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Tight- binding study of electronic band structure of anisotropic honeycomb lattice

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Abstract: The two-dimensional structure of graphene, consisting of an isotropic hexagonal lattice of carbon atoms, shows fascinating electronic properties, such as a gapless energy band and Dirac fermion behavior of electrons at fermi surface. Anisotropy can be induced in this structure by electrochemical pressure. In this article, by using tight-binding method, we review anisotropy effects in the electronic nanostructure of graphene in one direction. For this purpose, we just consider π states, which express electronic characteristics, and compare electronic band of π states with that of isotropic honeycomb lattice in graphene. As a result, by applying pressure or stretching in one direction, the gap will be created in the electronic band at the fermion surface, which can be useful for semiconducting nano devices. The isotropic graphene has a band structure with no energy gap. By applying electrochemical pressure in one direction, the translational symmetry can be broken, therefore an energy gap appears between the two bands.

Keywords: graphene, electronic nanostructure, electrochemical pressure, tight-binding method, energy gap band.

Introduction

Graphene is a two-dimensional structure of the Carbon atoms, in which atoms form a honeycomb lattice, according to Fig 1 [1]. Wallas introduced graphene, for the first time in 1977, great efforts was afforded to build such a two-dimensional material [2, 3]. Finally Geim and Novoselov made graphene in 2004; they won the Nobel Prize in physics in 2010, for construction of the two-dimensional graphene [4]. There are six electrons of carbon atoms occupy 1S2,2S2,2P2 orbitals in graphene structure. Since the energy difference between

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levels 2S and 2P is smaller than the binding energy, the wave function, of the four electrons are easily hybridized. The orbitals form covalent bonds with neighboring atoms, which are called σ bonds. These bonds are responsible for the mechanical properties of graphene and they are usually be ignored in theories that explains electronic properties of graphene. Due to the electronic symmetry, 2Pz orbital doesn't overlap with 2S,2Px orbitals or 2py , 2pz orbitals that are perpendicular to the graphene page, link with neighboring atoms to form π-bond, and electrons in this case move between neighboring atoms. Therefore we use π states to study electronic properties of graphene. π orbitals in π-bonds and π*-anti bonds participation in the energy spectrum. π-bonds form valence band and π* -anti bonds form conduction band [3, 5].

Energy band structure is an important property of different materials. For electronic bands calculation of honeycomb lattice, we use tight-binding model, which is an suitable for calculating the band structure of both periodic and non-periodic systems by using superposition of wave functions for each isolated atoms placed in an atomic sites [6]. This method create a good description of occupied states in all kind of crystals, (metals, semiconductors, and nonconductor) [7]. Though the tight-binding approach is a one-electron model, it also provides a basis for more advanced calculations like the calculation of surface states and application to various kinds of many-body problem and quasiparticle calculations. [8, 9].

Graphene is a material with no gap between conduction and valence bands [3]. One could create anisotropy by applying stress to it's lattice. This anisotropy is generally created by application of single-axis pressure or stretch, in honeycomb lattice which increases or decreases the separation distance between neighboring atoms and changes the electronic wave function overlap [10]. In this research we use the same mechanism to create anisotropy in the system.

This article is arranged according to following order: In section 2 and 3, the tight binding Hamiltonian is introduced and the method is explained to obtain the energy bands. In section 4, spectral function is obtained by calculating the green's function. Finally, we give concluding points in section 5.

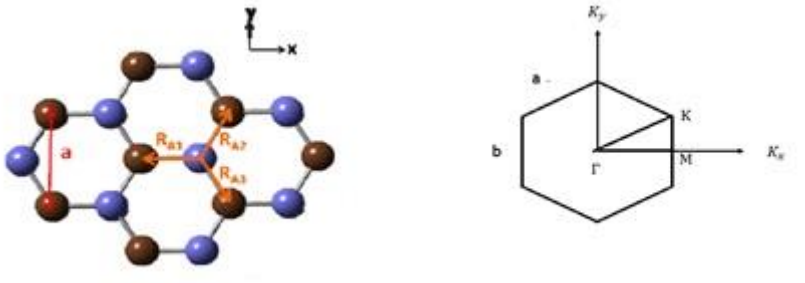

Fig. 1 Graphene honeycomb lattice (left), first Brillouin zone (right)

1. TIGHT-BINDING CALCULATION

The tight-binding Hamiltonian for graphene honeycomb lattice, reads as:

$$H = H_0 + \sum_{t_m} t e^{i\boldsymbol{k}.\boldsymbol{t_m}} \tag{1}$$

In the above equation, H_0 is the non-interaction Hamiltonian, t is the hopping amplitude between two adjacent lattice sites, k is the wave vector and t_m points to the nearest neighbor site. The second term in Eq (1) the sum is taken over the nearest neighboring sites. In the momentum space, the solution of the tight-binding method is:

$$F(k) = \sum_{t_m} t e^{i\boldsymbol{k}.\boldsymbol{t_m}} = t\left(e^{-ik_x.a} + 2cos\left(\frac{\sqrt{3}}{2}k_y a\right)e^{i\frac{1}{2}k_x a}\right) \tag{2}$$

To calculate the band structure, we have to solve the following eigenvalues

problem:

$$|[H] - E(k)[S]| = 0 \tag{3}$$

In which Hamiltonian matrix is:

$$H = \begin{bmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{bmatrix} \tag{4}$$

Each matrix element is determined using the relations below:

$$H_{AA} = \langle \phi_{A2p_z} | H | \phi_{A2p_z} \rangle = \varepsilon_{2p} \tag{5.1}$$

$$H_{AB} = \langle \phi_{A2p_z} | H | \phi_{B2p_z} \rangle = \sum_{i=1}^{3} H_{pp\pi} e^{i\boldsymbol{k}.\boldsymbol{R_{Ai}}} \tag{5.2}$$

In this approximation *S* matrix is equal to the unit matrix. In particular eigenvalues are calculated by the following determinate equation:

$$\begin{vmatrix} \varepsilon_{2p} - E(k) & H_{pp\pi}F(k) \\ H_{pp\pi}F^{\dagger}(k) & \varepsilon_{2p} - E(k) \end{vmatrix} = 0 \qquad (6)$$

where we put for $H_{pp\pi}$ =-3.1 and ε_k=0 [11]. The band structure *E (k)* may be described by a simple one-orbital tight-binding model as:

$$E(k) = \pm t\sqrt{H_{pp\pi}^2\left(1 + 4cos\left(\frac{\sqrt{3}}{2}k_y a\right)cos\left(\frac{3}{2}k_x a\right) + 4cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)\right)} \qquad (7)$$

Solving this eigenvalue problem yields the electronic band structure of graphene. Since all possible eigenstates are specified by the wave vector *k* within any one primitive cell of the periodic lattice in reciprocal space, the first Brillouin zone is the uniquely defined cell that is the most compact possible cell. We can obtain π and π^* electronic bands for the graphene honeycomb lattice by plotting eigenvalues of energy in the first Brillouin zone, [12, 13].

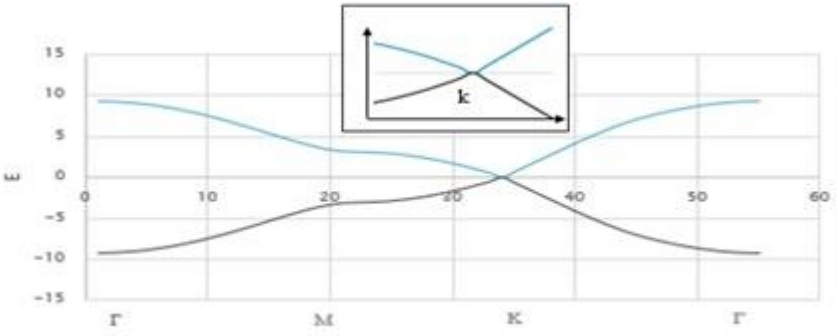

Fig. 2 Electronic bands graphene honeycomb lattice without pressure in one direction with a=b.

2. CALCULATION IN THE FIRST BRILLUIN ZONE

By plotting eigenvalues of energy *E* in the first Brillouin zone, we can obtain electronic band structure of honeycomb lattice for the isotropic and anisotropic graphene. We can obtain gap between the two bands in every two states. In Fig. 2 we shows π and π^* electronic bands when the honeycomb lattice is not affected by pressure, or in other words, the lattice is isotropic with the condition *a=b*. In this figure the electronic bands are connected without any gap in point K.

The following M, Γ and K points

$$\Gamma = \frac{2\pi}{a_0}(0,0) \qquad M = \frac{2\pi}{a_0}\left(\frac{1}{3}, 0\right) \qquad K = \frac{2\pi}{a_0}\left(\frac{1}{3}, \frac{1}{3\sqrt{3}}\right)$$

Are high symmetry points in the first Brillouin zone, shown in Fig. 1 (right), and a_0 constant lattice. We obtained eigenvalues of energy by replacing the coordinates of high symmetry points in equation (7). Applying electrochemical pressure in one direction of the honeycomb lattice creates anisotropy in the lattice. For an anisotropic lattice, with the condition $b = 1.05a$ and c changed constant lattice, the high-symmetry points are converted to the following coordinates:

A) $\Gamma = \frac{2\pi}{c}(0,0) \qquad M = \frac{2\pi}{c}\left(\frac{1}{3}, 0\right) \qquad K = \frac{2\pi}{c}\left(\frac{1}{3}, \frac{1}{3\sqrt{3}}\right)$

Moreover energy gap between the π and π^* electronic bands appears because of anisotropy, in point K (Fig. 3). In this calculations energy gap is obtained approximately 0.8ev.

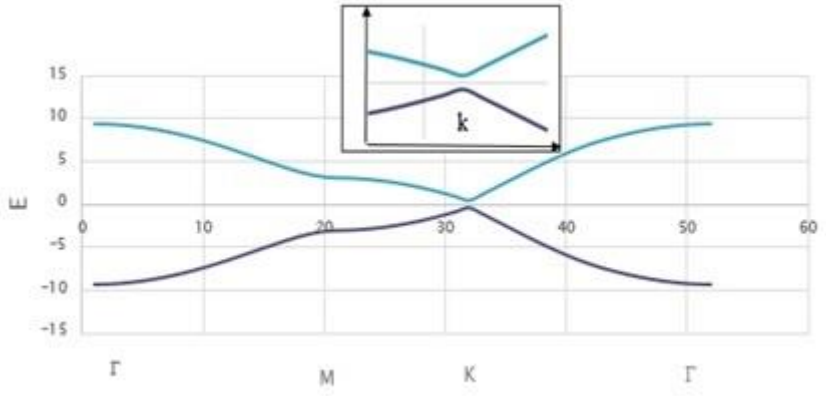

Fig. 3 Electronic bands graphene honeycomb lattice by the electrochemical pressure in one direction lattice with b=1.05a

3. Spectral Function

The spectral function provides information about the nature of the allowed electronic states, that can be considered as a generalized density of states regardless whether they are occupied or not. Spectral function gives the number of state (or density of state if you divide volume...etc.), peak in spectral function means there's a state or there're several degenerate states there. In single particle

system without interaction, the spectral function consists of only delta function sets at places where eigenstates exist.

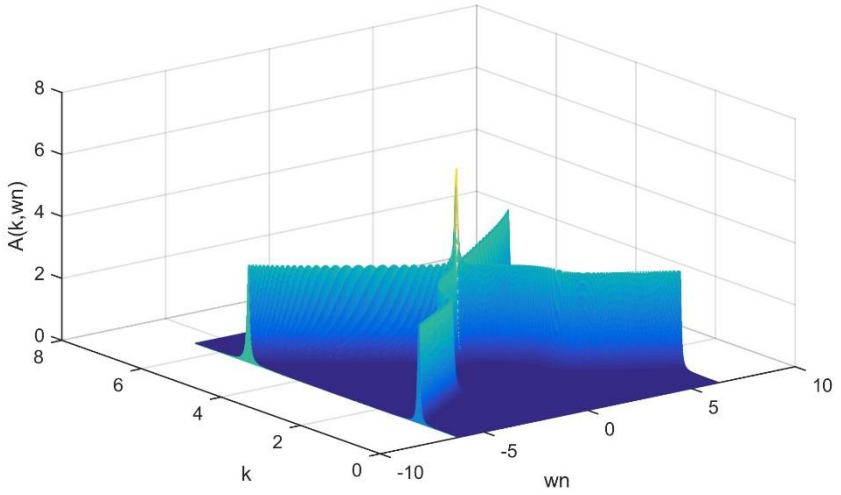

Fig. 4 Spectral function graphene honeycomb lattice without pressure in one direction with a=b and t=2.7 eV.

To calculate spectral function, the first step is introducing the green's function in lattice:

$$G(k,\omega) = (z - H)^{-1} \tag{8}$$

Where $z = \omega - i\eta$ and $\omega = \frac{(2n+1)\pi}{\beta}$ is the Matsubara frequencies for fermions. Therefore Spectral function can be written as:

$$A(k,\omega) = \frac{-1}{\pi}\Im TrG(k,\omega) \tag{9}$$

Trace of the spectral function represents the density of states [14, 15]:

$$\rho(\omega) = Tr[A(k,\omega)] = \int dk A(k,\omega) \tag{10}$$

Fig. 4 shows spectral function for the graphene honeycomb lattice, which is not affected by pressure, or *a=b*; by applying electrochemical pressure in one direction, a band gap is created shown in Fig. 5.

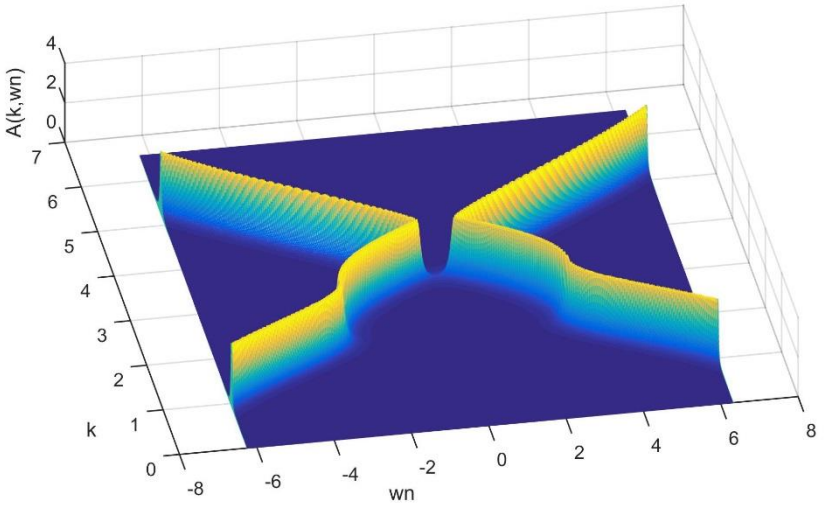

Fig. 5 Spectra function graphene honeycomb lattice by the electrochemical pressure in one direction lattice with $b = 1.05\ a$.

4. CONCLUSION

The isotropic graphene has a band structure with no energy gap. By applying electrochemical pressure in one direction, the translational symmetry can be broken, therefore an energy gap appears between the two bands. The created gap is due to the energy difference between the π and π^* bands. By coherent stretching lattice in the *x* axis direction by size of 1.005, the band gap opens up. If pressure on the lattice is more than of 1.3 in direction *x* axis, the reciprocal lattice would not remain honeycomb shape and the electronic properties would be changed.

5. References

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