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Short Communication

Berry curvature and energy bands of graphene

ABSTRACT

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In this paper energy bands and Berry curvature of graphene was studied. Desired Hamiltonian regarding the next-nearest neighbors obtained by tight binding model. By using the second quantization approach, the transformation matrix is calculated and the Hamiltonian of system is diagonalized. With this Hamiltonian, the band structure and wave function can be calculated. By using calculated wave function the Berry connection and Berry curvature of our system are calculated. Our results are exactly consistent with previous methods and the Berry curvature throughout the Brillouin zone get zero.

Keywords: *Graphene; Tight binding model; Band structure; Berry curvature; Brillouin zone.*

INTRODUCTION

Graphene produces a lot of excitement in the scientific world and has generated intense interest since it was firstly discovered in 2004.[1] Carbon atoms are strongly bonded by sp^2 hybridization and form one-atom thick hexagonal network, which is called graphene and can be seen with an ordinary optical microscope[1-3]. It is well known that graphene is a zero-gap semiconductor and conducts electricity better than silicon.[4] Tight-binding (TB) approach is widely used to investigate physical properties of graphene and carbon nanotubes [5-10]. The first TB description of graphene was given by Wallace, who only took the nearest and second-nearest neighbor atoms into account. [10] After that, Saito et al.[11] considered the nonfinite overlap between the basic function, but included only the nearest neighbors within the graphene sheet.

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EXPERIMENTAL

Graphene energy band structure by next nearest neighbors

Graphene is made out of carbon atoms arranged in hexagonal structure, as shown in Figure 1.

The structure can be seen as a triangular lattice with a basis of two atoms per unit cell. The lattice vectors can be written as $a_1 = \frac{a}{2}(3, \sqrt{3})$, $a_2 = \frac{a}{2}(3, -\sqrt{3})$ where $a = 1.42 \text{ \AA}$ is the carbon-carbon distance. The reciprocal-lattice vectors are given by

$$b_1 = \frac{2\pi}{3a}(1, \sqrt{3}), b_2 = \frac{2\pi}{3a}(1, -\sqrt{3}).$$

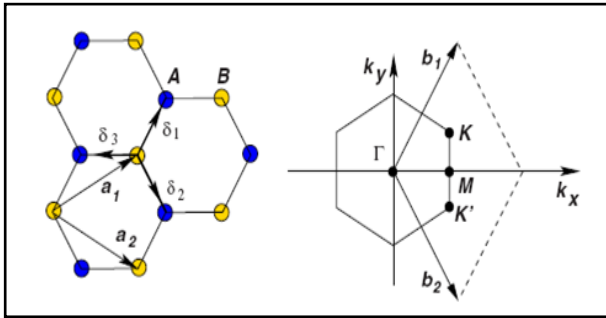


Fig. 1. Honeycomb lattice and its Brillouin zone

Of particular importance for the physics of graphene is the two points K and K' at the corners of the graphene Brillouin zone (BZ). These are named Dirac point. Their positions in momentum space are given by $K = (\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a})$, $K' = (\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a})$. Three nearest-neighbor vectors in real space are given by $\delta_1 = \frac{a}{2}(1, \sqrt{3})$, $\delta_2 = \frac{a}{2}(1, -\sqrt{3})$, $\delta_3 = -a(1, 0)$. While the six second-nearest neighbors are located at $\delta'_1 = \pm a_1$, $\delta'_2 = \pm a_2$, $\delta'_3 = \pm(a_2 - a_1)$.

The tight-binding Hamiltonian for electrons in graphene considering that electrons can hop to both nearest- and next-nearest-neighbor atoms has the form (we use units such that $\hbar = 1$)

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger b_j + \text{H. c.}) - t' \sum_{\langle\langle i,j \rangle\rangle} (a_i^\dagger a_j + b_i^\dagger b_j + \text{H. c.}) \quad (1)$$

Where $a_{i,\sigma}$ ($a_{i,\sigma}^\dagger$) annihilates (creates) an electron with spin σ ($\sigma = \uparrow, \downarrow$) on site R_i on sublattice A (an equivalent definition is used for sublattice B), t ($\approx 2.8 \text{ eV}$) [12] is the nearest-neighbor hopping

energy (hopping between different sublattices), and t' is the next nearest-neighbor hopping energy (hopping in the same sublattice). [12] The value of t' is not well known but *ab initio* calculations [6] find $0.02t \lesssim t' \lesssim 0.2t$ depending on the tight-binding parameterization. By means of Fourier transformation on operator and our Hamiltonian is $H =$

$$-t \sum_i (a(k)^\dagger b(k) \exp(ik \cdot \delta_i) + b(k)^\dagger a(k) \exp(-ik \cdot \delta_i)) + t' \sum_i (a(k)^\dagger a(k) (\exp(ik \cdot \delta_i) + \exp(-ik \cdot \delta_i)) + b(k)^\dagger b(k) (\exp(ik \cdot \delta_i) + \exp(-ik \cdot \delta_i))).$$

By definition of $f(k) = -t(\exp(ik \cdot a_1) + \exp(ik \cdot a_2) + \exp(ik \cdot (a_2 - a_1)))$ and $s(k) = \cos(k \cdot a_1) + \cos(k \cdot a_2) + \cos(k \cdot (a_2 - a_1))$ and relation between a and δ the Hamiltonian have the form

$$H = \begin{pmatrix} a(k)^\dagger & b(k)^\dagger \end{pmatrix} \begin{pmatrix} t^\dagger s(k) & t f(k) \\ t f(-k) & t^\dagger s(k) \end{pmatrix} \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} \quad (2)$$

The energy bands derived from this Hamiltonian obtained by diagonalization of Hamiltonian by transformation matrix S . So

$$H = (a(k)^\dagger b(k)^\dagger) S S^{-1} H S S^{-1} \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} \quad (3)$$

S and S^{-1} can be found by some calculation

$$S = \begin{pmatrix} \sqrt{\frac{f(k)}{f(-k)}} & -\sqrt{\frac{f(k)}{f(-k)}} \\ 1 & 1 \end{pmatrix}$$

$$S^{-1} = \frac{1}{2} \begin{pmatrix} \sqrt{\frac{f(-k)}{f(k)}} & 1 \\ -\sqrt{\frac{f(-k)}{f(k)}} & 1 \end{pmatrix} \quad (4)$$

Diagonalized Hamiltonian has the form

$$H_d = \begin{pmatrix} t s(k) + t \sqrt{f(k)f(-k)} & 0 \\ 0 & t s(k) - t \sqrt{f(k)f(-k)} \end{pmatrix} \quad (5)$$

And energy dispersion relations are

$$E_1 = t's(k) + t\sqrt{f(k)f(-k)} \quad (6)$$

$$E_2 = t's(k) - t\sqrt{f(k)f(-k)} \quad (7)$$

And in this stage by choosing (6), (7) for upper and lower energy band, we show the full band structure of graphene with both t' and t .

Berry curvature throughout Brillouin zone

In the next step we focused on calculation of Berry curvature. Now, let us define the Berry connection in the following way

$$A_{\vec{k}} = \sum_{\text{occupied state}} \langle \psi | i \partial_{\vec{k}} | \psi \rangle \quad (8)$$

Berry connection implies Berry curvature as follows [13].

$$\Omega_{k_x, k_y} = \partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x} \quad (9)$$

So finding the eigenstate of Hamiltonian in new state is necessary. The total functions for $c_1(k)^\dagger$ is linear combination of $|\varphi_A\rangle$ that located in position A and $|\varphi_B\rangle$ that located in position B . Also for

$c_2(k)^\dagger \cdot |\varphi_A\rangle = \frac{1}{\sqrt{N}} \sum_R e^{ik \cdot R} |p_z, R\rangle, |\varphi_B\rangle = \frac{1}{\sqrt{N}} \sum_R e^{ik \cdot R} |p_z, R-d\rangle$, the p_z atomic-orbitals are oriented perpendicular to the plane and are rotational symmetric around the z -axis. By

$$c_1(k)^\dagger = \sqrt{\frac{f(k)}{f(-k)}} a(k)^\dagger + b(k)^\dagger \quad (10)$$

$$c_2(k)^\dagger = -\sqrt{\frac{f(k)}{f(-k)}} a(k)^\dagger + b(k)^\dagger \quad (11)$$

We find $|\psi\rangle$ as

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_R e^{ik \cdot R} \left(\sqrt{\frac{f(k)}{f(-k)}} |p_z, R\rangle + |p_z, R-d\rangle \right) \quad (12)$$

By finding eigenstate and replace on Berry curvature equation we have $\Omega_{k_x, k_y} = 0$.

RESULTS AND DISCUSSION

Energy band structure that obtained by Wallace [10] was $E_{\mp}(k) = \mp t\sqrt{3 + g(k)} - t'g(k)$ with specific $g(k)$. But in our calculation we diagonalized Hamiltonian and plot it on Figure 2. And in resumption Berry curvature of these states has been calculated and get zero. Our assumption was that we don't know two symmetry of graphene, and calculated from eigenstates.

We know if the system has time reversal symmetry, the symmetry condition requires that $\Omega(-k) = -\Omega(k)$. And if the system has spatial inversion symmetry, then $\Omega(-k) = \Omega(k)$. Therefore, for crystals with simultaneous time-reversal and spatial inversion symmetry the Berry curvature vanish identically throughout the Brillouin zone [13].

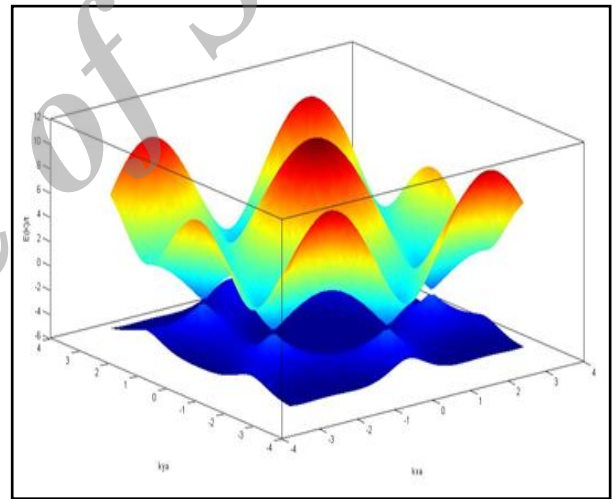


Fig. 2. Electronic dispersion in the honeycomb lattice.

CONCLUSION

There are many important physical systems where both symmetries are not simultaneously present. For example single-layer graphene sheet with staggered sublattice potential, which breaks inversion symmetry, so in this situation Berry curvature is not zero [14]. In our calculation all the symmetries was established. Results show that the next nearest neighborhood hopping did not break the symmetry of system.

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