Edge states of graphene bilayer strip

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(Dated: May 5, 2014)

Abstract

The electronic structure of the zig-zag bilayer strip is analyzed. The electronic spectra of the bilayer strip is computed. The dependence of the edge state band flatness on the bilayer width is found. The density of states at the Fermi level is analytically computed. It is shown that it has the singularity which depends on the width of the bilayer strip. There is also asymmetry in the density of states below and above the Fermi energy.

PACS numbers: 73.63.-b, 73.63.Fg, 73.22.-f

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I. INTRODUCTION

Carbon atoms can create a variety of forms such as graphite, diamond, carbon fibers, fullerences and carbon nanotubes. A carbon nanotube can be described as a graphene sheet rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry and in general exhibiting a spiral conformation called chirality. They are interesting because of their unique mechanical and electronic properties. From the pioneering works, the electronic properties of graphite have attracted interest because of unconventional physical properties of a graphite layer. The development in the fabrication of the single layers of graphite (graphene) caused a striking level of interest in the investigation of the carbon compositions. In addition to the closed carbon molecules, systems with boundaries also show interesting features. The nanographite zig-zag ribbon possesses localized edge states near the Fermi level. States like that are absent for ribbons with armchair edges. The graphite sheet is a zero-gap semiconductor with the density of states (DOS) vanishing at the Fermi level, the edge states of the zig-zag ribbons produce a peak in the DOS at the Fermi level. Both the carbon nanotubes and graphite layers have the edge states because of their boundary. The presence of the edge state results in the relatively important contribution to the density of states (DOS) near the Fermi energy. It was found that the HOMO-LUMO (highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively) gap is inversely proportional to the length of the zig-zag carbon nanotube segment. The zig-zag ribbons have partly flat bands at the Fermi level. In the presented paper, we focus on the computation of the electronic spectra of the zig-zag bilayer strip and also on the computation of the DOS of the edge states near the Fermi level.

II. THEORY

Firstly, we describe the model for the zig-zag bilayer strip. We will study the edge and size effects using the tight-binding model for this strip shown in Fig.

The \( \pi \) electronic structures are calculated from the tight-binding Hamiltonian

\[
H = \sum_i \epsilon_i |\varphi_i^u\rangle\langle \varphi_i^u| + \sum_{i,j} \gamma_{ij} (|\varphi_i^u\rangle\langle \varphi_j^x| + h.c) + \sum_i \epsilon_i |\varphi_i^d\rangle\langle \varphi_i^d| + \sum_{i,j} \tilde{\gamma}_{ij} (|\varphi_i^d\rangle\langle \varphi_j^u| + h.c) \\
+ \sum_{l,n} W_{ln} (|\varphi_l^u\rangle\langle \varphi_n^u| + h.c),
\]

(1)
$\epsilon_i$ and $\tilde{\epsilon}_i$ are the site energies of the upside and down layer; $|\varphi_i^u\rangle$, $|\varphi_i^d\rangle$ are $\pi$ the orbitals on site $i$ at the upside and down layer; $\gamma_{ij}$, $\tilde{\gamma}_{ij}$ are the intralayer hopping integrals; $W_{ij}$ are the interlayer hoping integrals which depend on the distance $d_{ij}$ and angle $\theta_{ij}$ between the $\pi_i$ and $\pi_j$ orbitals.

To describe the parameter which characterizes the zig-zag bilayer strip, we start from the graphene layer where we can define the vectors connecting the nearest neighbor carbon atoms in the form:

$$
\vec{\tau}_1 = a(0; \frac{1}{\sqrt{3}}),
\vec{\tau}_2 = a\left(\frac{1}{2}; -\frac{1}{2\sqrt{3}}\right),
\vec{\tau}_3 = a\left(-\frac{1}{2}; -\frac{1}{2\sqrt{3}}\right).
$$

(2)

The distance between atoms in the unit cell is $d = |\hat{\tau}_i| = \frac{a}{\sqrt{3}}$. We want to find a solution to the double-layer graphene strip in the form:

$$
\psi(\vec{r}) = \psi^u(\vec{r}) + \psi^d(\vec{r})
$$

(3)

where

$$
\psi^u(\vec{r}) = \sum_{i=0}^{M+1} (C_{Ai}\psi_{Ai} + C_{Bi}\psi_{Bi}),
$$

(4)
\[
\psi^d(\vec{r}) = \sum_{i=0}^{M+1} \left( C_{A_i} \psi_{A_i} + C_{B_i} \psi_{B_i} \right). \tag{5}
\]

We want to find a solution to the above equation in the form of the Bloch function
\[
\psi_\alpha(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_n e^{i\vec{k} \cdot \vec{r}_n} |\varphi(\vec{r} - \vec{r}_n)\rangle, \tag{6}
\]
where \(\alpha\) denotes A or B atoms. Here \(\vec{k} = (k_x, 0)\), \(\vec{r}_n\) is the position of a unit cell and \(N\) is the number of a unit cell; \(|\varphi(\vec{r})\rangle\) is a \(\pi\) orbital. We denote
\[
\epsilon_i = \tilde{\epsilon}_i = \Delta = \langle \varphi^{\text{out}}(r - A_i)|H|\varphi^{\text{out}}(r - A_i)\rangle = \langle \varphi^{\text{out}}(r - B_i)|H|\varphi^{\text{out}}(r - B_i)\rangle, \tag{7}
\]
\[
\epsilon_i = \tilde{\epsilon}_i = -\Delta = \langle \varphi^{\text{out}}(r - B_i)|H|\varphi^{\text{out}}(r - B_i)\rangle = \langle \varphi^{\text{out}}(r - A_i')|H|\varphi^{\text{out}}(r - A_i')\rangle. \tag{8}
\]

Now we define the intratube hopping integrals as \(\gamma_{ij} = \bar{\gamma}_{ij} = \gamma_0\). We take into account only the interaction between nearest-neighbors also in the case of interlayer interaction and denote
\[
\langle \varphi(r - A_i)|H|\varphi(r - B_i')\rangle = \gamma_1. \tag{9}
\]

In confining the structure along the width, the edge states are induced by terminating the width dimension with zig-zag shaped edges. The presence of edges in the bilayer strip changes the dimensionality of the system from a two-dimensional to a one-dimensional system. The electronic spectrum of the zig-zag bilayer strip can be described by the following system of equations:
\[
(E - \Delta)C_{A_m} = -\gamma_0 C_{B_{m-1}} - g_k C_{B_m} - \gamma_1 C_{B_{m+1}}, \tag{10}
\]
\[
(E + \Delta)C_{B_m} = -\gamma_0 C_{A_{m+1}} - g_k C_{A_m}, \tag{11}
\]
\[
(E + \Delta)C_{A_m} = -\gamma_0 C_{B'_{m-1}} - g_k C_{B'_m}, \tag{12}
\]
\[
(E - \Delta)C_{B'_m} = -\gamma_0 C_{A'_{m+1}} - g_k C_{A'_m} - \gamma_1 C_{A_m}, \tag{13}
\]
where
\[
g_k = 2\gamma_0 \cos(k_x a/2). \tag{14}
\]

Here \(m = 1, \ldots, M\), are site indices, where \(M\) describes the width of the graphene bilayer.

We assume that the \(A_0\) and \(B_{M+1}\) sites are missing. So we have the boundary condition \(C_{A_0} = C_{B_{M+1}} = C_{A'_0} = C_{B'_{M+1}} = 0\). The solution is assumed to be \[11\]
\[
C_{A_m} = Ae^{ipm} + Be^{-ipm}, \tag{15}
\]

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Here $A$, $B$, $C$ and $D$ are the coefficients which have to be determined, and $p$ is the transverse wave number. From the boundary condition we have

$$C_{A_0} = A + B = 0,$$  \hspace{1cm} (17)

$$C_{B_{M+1}} = Ce^{ip(M+1)} + De^{-ip(M+1)} = 0.$$  \hspace{1cm} (18)

And so

$$C_{A_m} = A(e^{ipm} - e^{-ipm}),$$  \hspace{1cm} (19)

$$C_{B_m} = C(e^{ipm} - z^2 e^{-ipm}),$$  \hspace{1cm} (20)

where $z = e^{ip(M+1)}$. And similarly,

$$C'_{A_m} = A'(e^{ipm} - e^{-ipm}),$$  \hspace{1cm} (21)

$$C'_{B_m} = C'(e^{ipm} - z^2 e^{-ipm}).$$  \hspace{1cm} (22)

Substituting Eqs. (19-22) into Eqs. (10-13) we obtain

$$(E - \Delta) (e^{ipm} - z^2 e^{-ipm}) A + [\gamma_0 (e^{ipm-1} - e^{-ipm-1}) + g_k (e^{ipm} - e^{-ipm})] C +$$  \hspace{1cm} (23)

$$+ \gamma_1 (e^{ipm} - e^{-ipm}) C' = 0,$$

$$[\gamma_0 (e^{ip(m+1)} - z^{2} e^{-ip(m+1)}) + g_k (e^{ipm} - z^2 e^{-ipm})] A + (E + \Delta) (e^{ipm} - e^{-ipm}) C = 0,$$  \hspace{1cm} (24)

$$(E - \Delta) (e^{ipm} - e^{-ipm}) C' + [\gamma_0 (e^{ip(m-1)} - z^{2} e^{-ip(m-1)}) + g_k (e^{ipm} - z^2 e^{-ipm})] A' +$$  \hspace{1cm} (25)

$$+ \gamma_1 (e^{ipm} - z^2 e^{-ipm}) A = 0,$$

$$[\gamma_0 (e^{ip(m+1)} - e^{-ip(m+1)}) + g_k (e^{ipm} - e^{-ipm})] C' + (E + \Delta) (e^{ipm} - z^2 e^{-ipm}) A' = 0.$$  \hspace{1cm} (26)

This homogenous system of equations has a solution only if the following conditions are fulfilled:

$$E^2 - \gamma_1 (E + \Delta) - (\gamma_0 e^{-ip} + g_k) (\gamma_0 e^{ip} + g_k) e^{2ipm} +$$

$$z^2 [E^2 - \gamma_1 (E + \Delta) - (\gamma_0 e^{-ip} + g_k) (\gamma_0 e^{ip} + g_k)] e^{-2ipm} -$$

$$-(E^2 - \Delta^2 - \gamma_1 (E + \Delta) (z^2 + 1) + (g_n + \gamma_0 e^{ip})^2 + z^2 (g_n + \gamma_0 e^{-ip})^2 = 0,$$  \hspace{1cm} (27)

or

$$E^2 - \Delta^2 + \gamma_1 (E + \Delta) - (\gamma_0 e^{-ip} + g_k) (\gamma_0 e^{ip} + g_k)] e^{2ipm} +$$
\[ z^2 \left[ E^2 - \Delta^2 + \gamma_1 (E + \Delta) - (\gamma_0 e^{-ip} + g_k) (\gamma_0 e^{ip} + g_k) \right] e^{-2ipm} - \\
- (E^2 - \Delta^2 + \gamma_1 (E + \Delta)) (z^2 + 1) + (g_k + \gamma_0 e^{ip})^2 + z^2 (g_k + \gamma_0 e^{-ip})^2 = 0. \] (28)

The coefficient of \( e^{\pm2pm} \) terms and the constant term have to be equal to zero. Thus, we obtain the energy spectrum

\[ E_{1,2} = \frac{\gamma_1}{2} \pm \sqrt{\frac{\gamma_0^2}{4} + 2\gamma_0 g_k \cos(p) + \left( \frac{\gamma_1}{2} + \Delta \right)^2}, \] (29)

\[ E_{3,4} = -\frac{\gamma_1}{2} \pm \sqrt{\frac{\gamma_0^2}{4} + 2\gamma_0 g_k \cos(p) + \left( \frac{\gamma_1}{2} - \Delta \right)^2}. \] (30)

and the equation which gives the longitudinal wave number \( p \) is

\[ \sin [pM] + \frac{g_k}{\gamma_0} \sin [p(M + 1)] = 0. \] (31)

For \( M \gg 1 \) Eq.\( (31) \) can be written as

\[ \sin [pM] = 0. \] (32)

The solution is given by

\[ p = \frac{2\pi}{M} l. \] (33)

Substituting this solution into Eq.\( (29,30) \) we get the energy spectrum for the graphene bilayer with the periodic boundary condition along the \( y \)-axis.

### III. EDGE STATES OF GRAPHENE BILAYER

Now we are interested in the edge state of the graphene bilayer. This solution can be obtained in the form \( p = \pi + i\eta \) \[12\]. We get the following equation for \( \eta \):

\[ \sinh [\eta M] - \frac{g_k}{\gamma_0} \sinh [\eta(M + 1)] = 0. \] (34)

The edge state can exist when the condition

\[ |2 \cos (k_x a/2)| < \frac{1}{1 + 1/M}, \] (35)

is fulfilled. The energy spectrum of a state like that is given as

\[ E_{1,2} = \frac{\gamma_1}{2} \pm \sqrt{\frac{\gamma_0^2}{4} - 2\gamma_0 g_k \cosh(\eta) + g_k^2 + \left( \frac{\gamma_1}{2} + \Delta \right)^2}, \] (36)
\[E_{3,4} = -\frac{\gamma_1}{2} \pm \sqrt{\frac{\gamma_0^2}{2} - 2\gamma_0 g_k \cosh(\eta) + g_k^2 + \left(\frac{\gamma_1}{2} - \Delta\right)^2}. \]  

(37)

For big enough \(M\) the solution of Eq. (34) can be expressed in the form \[\eta = \ln\left[\frac{c_k + 1 - c_k^2}{c_k + 1 + c_k^2 + 1}\right], \]  

(38)

where \(1/c_k = |2 \cos \left(\frac{ka}{2}\right)|\). We denote \(k_x = k\). From Eq. (38) we have

\[
\cosh \eta \approx \frac{1 + c_k^2}{2 c_k} - \frac{(c_k^2 - 1)^2}{2 c_k^{2M+3}},
\]

(39)

and so

\[
E_{1,2} = \frac{\gamma_1}{2} \pm \sqrt{\gamma_0^2 \frac{(c_k^2 - 1)^2}{c_k^{2M+4}} + \left(\frac{\gamma_1}{2} + \Delta\right)^2},
\]

(40)

\[
E_{3,4} = -\frac{\gamma_1}{2} \pm \sqrt{\gamma_0^2 \frac{(c_k^2 - 1)^2}{c_k^{2M+4}} + \left(\frac{\gamma_1}{2} - \Delta\right)^2}.
\]

(41)

Now we assume, similarly as in \[13\], that \(\gamma_1 > 2\Delta\) and also it is assumed that the width of the graphene bilayer is big enough and the following condition is fulfilled:

\[
\gamma_1 \gg \frac{\gamma_0^2 (c_k^2 - 1)^2}{c_k^{2M+4}}.
\]

(42)

The bands are given by

\[
E_1(k) = \gamma_1 + \Delta - \frac{\gamma_0^2}{\gamma_1 + 2\Delta} \frac{(c_k^2 - 1)^2}{c_k^{2M+4}},
\]

(43)

\[
E_2(k) = -\Delta - \frac{\gamma_0^2}{\gamma_1 + 2\Delta} \frac{(c_k^2 - 1)^2}{c_k^{2M+4}},
\]

(44)

\[
E_3(k) = -\Delta + \frac{\gamma_0^2}{\gamma_1 - 2\Delta} \frac{(c_k^2 - 1)^2}{c_k^{2M+4}},
\]

(45)

\[
E_4(k) = -\gamma_1 + \Delta - \frac{\gamma_0^2}{\gamma_1 - 2\Delta} \frac{(c_k^2 - 1)^2}{c_k^{2M+4}}.
\]

(46)

We are interested in the \(E_2(E_3)\) band which is the valence(conductance) band of the edge states. The minimum of the \(E_2\) band is

\[
E_{2,\text{min}} = -\Delta - \frac{2}{e^2 M} \frac{\gamma_0^2}{\gamma_1 + 2\Delta}.
\]

(47)
where it was used that \( e^x = (1 + x/M)^M \) for \( M \to \infty \) and also Eq.(35). We found \( E_{2,max} = -\Delta \). Similarly for the \( E_3 \) band

\[
E_{3,max} = -\Delta + \frac{2}{e^2 M} \frac{\gamma_0^2}{\gamma_1 - 2\Delta},
\]

(48)

and \( E_{3,min} = -\Delta \). We can see that the width of the band is inversely proportional to the width of the bilayer.

The density of states can be expressed in the form

\[
N(E) = \frac{L}{2\pi} \frac{1}{\frac{dE}{dk}},
\]

(49)

where \( L \) is the length of the bilayer in the \( x \) direction. We get the density of the state in the region \( E_{3,min} - E_{3,max} \) in the vicinity of the energy \( E = -\Delta \) in the form

\[
N(E) = \frac{L}{2\pi a M (E + \Delta)^{2M+1} \left( \gamma_0^2 / (\gamma_1 - 2\Delta) \right)^{1/2(M+1)}}.
\]

(50)

The density of the state in the region \( E_{2,min} - E_{2,max} \) in the vicinity of the energy \( E = -\Delta \) has the form

\[
N(E) = \frac{L}{2\pi a M (E + \Delta)^{2M+1} \left( \gamma_0^2 / (\gamma_1 + 2\Delta) \right)^{1/2(M+1)}}.
\]

(51)

Both these densities of the states have a singularity at the energy \( E = -\Delta \). The strength of the singularity depends also on the width of the bilayer. The width of the bilayer is characterized by the parameter \( M \). The density of the state of the \( E_4(k)(E_1(k)) \) band is the same as the \( E_3(k)(E_2(k)) \) band.

IV. CONCLUSION

In the presented paper the electronic spectra of the zig-zag bilayer strip was studied analytically. We get for big enough \( M \) that the electronic spectra of the graphene bilayer strip are similar to the spectra of the graphene bilayer with the periodic boundary condition. Because of the boundary we also get edge states. It was shown that the width of the edge state band is inversely proportional to the width of the bilayer strip which is characterized by the parameter \( M \). So for big enough \( M \) we get partly flat bands of the edge states. The density of states at the Fermi level has a singularity which also depends on the width of the bilayer strip. There is asymmetry in the DOS at the Fermi energy, similarly to the electron-hole asymmetry in the bilayer graphene [14]. This asymmetry is caused by the parameter
\[ \Delta \] which describes the difference in the site energy of the atoms at the sites \( A_i, B'_i \) and the atoms at the sites \( B_i, A'_i \).

**Acknowledgment**

The work was supported by the Slovak Academy of Sciences in the framework of CEX NANOFLUID, and by the Science and Technology Assistance Agency under Contract No. APVV 0509-07 , 0171 10, VEGA Grant No. 2/0069/10 and Ministry of Education Agency for Structural Funds of EU in frame of project 26220120021.

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