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Effect of the magnetic field on the edge states of zig-zag single wall carbon nanotubes

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ABSTRACT

The influence of the static magnetic field on the edge states of finite zig-zag nanotubes has been explored theoretically by the tight-binding approximation. It was found that the magnetic field removes the degeneracy of the energy levels of the edge states. Investigation of the formation of new edge states by the magnetic field indicated the dependence of the number of these states on the length of a nanotube.

1. Introduction

Carbon nanotubes are extensively studied experimentally and theoretically because of their unusual electronic properties. A carbon nanotube can be viewed as a graphene sheet rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry and in general exhibits a spiral conformation called chirality. Nanotubes show unique mechanical and electronic properties [1]. Properties of the finite-length nanotubes are strongly influenced by the types of edges. From the category of edges the most intensively studied are the zig-zag and armchair types. For the nanographite ribbons with the zig-zag edge the presence of localized states near the Fermi level was already shown. However, similar states were absent in ribbons with armchair edges [2].

The graphite sheet is considered as a zero-gap semiconductor with the density of states (DOS) vanishing at the Fermi level. In contrast, the edge states of the zig-zag ribbons produce a peak in the DOS at the Fermi level. The finite nanotubes with the edges bring about the change of the dimensionality of the system from one to zero dimensional system, as it is in the case of fullerenes [3]. The existence of edge states for arbitrarily oriented graphene ribbons with a large class of edge shapes was already investigated [4]. From these studies new geometrical understanding of the edge state has emerged. The relation of the edge states to the topological nature of nanotubes was also found [5]. In addition, the presence of the edge state results in the relatively important contribution to the density of states (DOS) near the Fermi energy [6]. Apparently, the length of single-wall carbon nanotubes [7] affects the edge states. In short nanotubes the edge states could play an important role by contribution to conductivity. Specifically, it was found [8] 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. Another factor showing the potentiality of controlling the electronic properties of a carbon nanotube is an external magnetic field [9]. To explore this possibility, we have also conducted in this Letter a theoretically study of the electronic properties of finite-length carbon nanotubes under the influence of the magnetic field.

2. Theory

We investigate the zigzag nanotubes in the static magnetic field $\vec{B}$ parallel to the nanotube axis. We assume Hamiltonian for an electron in a potential $V(r)$ and in the magnetic field in the form

$$H = \frac{1}{2m}(\vec{p} - e\vec{A})^2 + V. \tag{1}$$

The potential $V(r)$ reflects the structure of the crystal lattice such as the symmetry and periodicity properties. Here this potential describes the structure of the zig-zag single wall carbon nanotube. The vector potential $\vec{A}$ in the Landau gauge can be expressed in the form [1]

$$\vec{A} = \left(\frac{\Phi}{L}, 0\right), \tag{2}$$

where $\Phi = B\pi r^2$ is the magnetic flux penetrating the cross section of the carbon nanotube, and $L = 2\pi r$ is a circumference of the nanotube (r-nanotube radius). Here the coordinate x is in the circumferential direction, and the coordinate y denotes the direction parallel to the nanotube axis. To describe the parameters which characterize the zig-zag tubules, we start from the graphene

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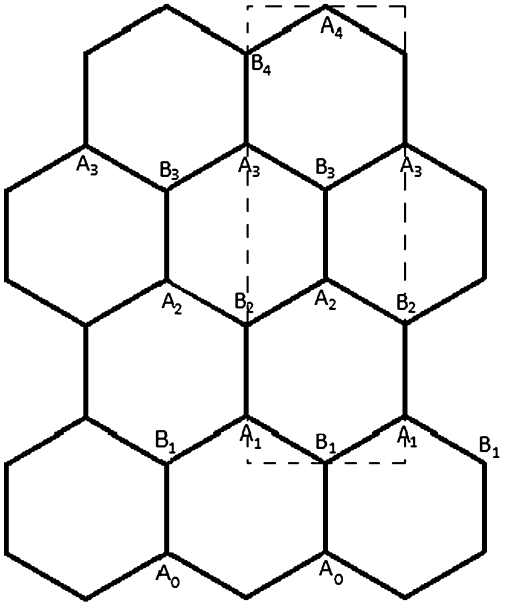

Fig. 1. Structure of the finite-length open ended single wall carbon nanotube with the zig-zag edges. A unit cell for the width $M = 4$ which creates a nanotube is depicted.

layer [10] where we can define the vectors connecting the nearest neighbor carbon atoms for the zig-zag nanotubes in the form:

$$\vec{\tau_1} = a\left(0; \frac{1}{\sqrt{3}}\right),$$
$$\vec{\tau_2} = a\left(\frac{1}{2}; -\frac{1}{2\sqrt{3}}\right),$$
$$\vec{\tau_3} = a\left(-\frac{1}{2}; -\frac{1}{2\sqrt{3}}\right), \tag{3}$$

where $a = 0.246$ nm is the lattice constant. The finite length open ended zig-zag carbon nanotubes can be assumed to be rolled from the finite length zig-zag graphene nanoribbons [2]. In confining the structure along the length, the edge states are induced by terminating the length dimension with the zig-zag shaped edges. We will study the edge and size effects using the tight-binding model for the carbon nanotube shown in Fig. 1. We want to find the solution to the above problem in the form of the Bloch function

$$\psi(\vec{r}) = \sum_{i=0}^{M} (C_{A_i}\psi_{A_i} + C_{B_{i+1}}\psi_{B_{i+1}}) \tag{4}$$

where

$$\psi_\alpha(\vec{k}, \vec{r}) = \frac{1}{\sqrt{M}} \sum_n \exp\left(i\vec{k}(\vec{r_n} + \vec{d}_\alpha) + i\frac{e}{\hbar} G(\vec{r_n} + \vec{d}_\alpha)\right) \times |\varphi(\vec{r} - \vec{r}_n - \vec{d}_\alpha)\rangle, \tag{5}$$

where α denotes A or B atoms. Here $\vec{d}_\alpha$ are the coordinates of the α atom in the unit cell and $\vec{r_n}$ is a position of a unit cell, M is the number of the unit cell; $|\varphi(\vec{r})\rangle$ is a π orbital which is generally different for the outer and inner shell; $G(\vec{R})$ is the phase factor associated with the magnetic field and is expressed by [11]

$$G(\vec{R}) = \int_{\vec{R}}^{\vec{r}} \vec{A}(\vec{x}).d\vec{x} = \int_0^1 (\vec{r} - \vec{R}).\vec{A}\big(\vec{R} + \lambda(\vec{r} - \vec{R})\big)\, d\lambda. \tag{6}$$

Employing Eq. (2) we get

$$G(\vec{R}) = \int_0^1 (\vec{r} - \vec{R}).\left(\frac{\Phi}{L}, 0\right) d\lambda = (x - X)\frac{\Phi}{L}. \tag{7}$$

We denote

$$\epsilon = \langle\varphi(\vec{r} - \vec{A}_i)|H|\varphi(\vec{r} - \vec{A}_i)\rangle = \langle\varphi(\vec{r} - \vec{B}_i)|H|\varphi(\vec{r} - \vec{B}_i)\rangle. \tag{8}$$

Now we define the hopping integrals

$$\langle\varphi(\vec{r} - \vec{A}_i)|H|\varphi(\vec{r} - \vec{B}_i)\rangle = \gamma_0\beta,$$
$$\langle\varphi(\vec{r} - \vec{A}_i)|H|\varphi(\vec{r} - \vec{B_{i+1}})\rangle = \gamma_0. \tag{9}$$

The electronic spectrum of finite zig-zag single wall carbon nanotubes can be described by the following system of equations:

$$\epsilon C_{A_m} + H_{A_mB_{m+1}} C_{B_{m+1}} + H_{A_mB_m} C_{B_m} = E C_{A_m}, \tag{10}$$
$$\epsilon C_{B_m} + H_{B_mA_{m-1}} C_{A_{m-1}} + H_{B_mA_m} C_{A_m} = E C_{B_m}, \tag{11}$$

where

$$H_{A_mB_{m+1}} = \gamma_0, \tag{12}$$
$$H_{A_mB_m} = 2\gamma_0\beta\cos\left(\frac{n\pi}{N} + \frac{\Phi}{2N\Phi_0}\right) \tag{13}$$

here $\Phi_0 = \hbar/e$, $n = 0, \ldots, N-1$, $\beta = 1 - \frac{1}{2}(\frac{\pi}{N})^2$ for the $(N, 0)$ zig-zag nanotube [12] and γ_0 (≈ 3 eV) is the nearest neighbor hopping integral in the flat graphene. The site index $m = 1, \ldots, M$, where M describes the length of the nanotube. So we have

$$\tilde{E} C_{A_m} + \gamma_0 C_{B_{m+1}} + \gamma_0 g_n C_{B_m} = 0, \tag{14}$$
$$\tilde{E} C_{B_m} + \gamma_0 C_{A_{m-1}} + \gamma_0 g_n C_{A_m} = 0, \tag{15}$$

where $\tilde{E} = \epsilon - E$ and

$$g_n = 2\beta\cos\left(\frac{n\pi}{N} + \frac{\Phi}{2N\Phi_0}\right) = 2\beta\cos\left(\frac{n\pi}{N} + \frac{NB}{B_1}\right) \tag{16}$$

where $B_1 = 4h/ea^2$. We assume that the A_0 and B_{M+1} sites are missing. So we have the boundary condition $C_{A_0} = C_{B_{M+1}} = 0$ [13]. The solutions of Eqs. (14) and (15) in two cases (cases I and II) are found. The solution is assumed to be (case I)

$$C_{A_m} = Ae^{ipm} + Be^{-ipm}, \tag{17}$$
$$C_{B_m} = Ce^{ipm} + De^{-ipm}. \tag{18}$$

Here A, B, C and D are the coefficients which have to be determined and p is the wave number in the direction of the nanotube axis. From the boundary condition we have

$$C_{A_0} = A + B = 0, \tag{19}$$
$$C_{B_{M+1}} = Ce^{ip(M+1)} + De^{-ip(M+1)} = 0. \tag{20}$$

And so

$$C_{A_m} = A\left(e^{ipm} - e^{-ipm}\right), \tag{21}$$
$$C_{B_m} = C\left(e^{ipm} - z^2e^{-ipm}\right) \tag{22}$$

where $z = e^{ip(M+1)}$. Substituting Eqs. (21) and (22) into Eqs. (14) and (15) we obtain

$$\tilde{E}\left(e^{ipm} - z^2e^{-ipm}\right)C + \gamma_0\left[\left(e^{ip(m-1)} - e^{-ip(m-1)}\right) + g_n\left(e^{ipm} - e^{-ipm}\right)\right]A = 0, \tag{23}$$
$$\gamma_0\left[\left(e^{ip(m+1)} - z^2e^{-ip(m+1)}\right) + g_n\left(e^{ipm} - z^2e^{-ipm}\right)\right]C + \tilde{E}\left(e^{ipm} - e^{-ipm}\right)A = 0. \tag{24}$$