The electronic properties of double wall carbon nanotubes

2012 J. Phys.: Conf. Ser. 393 012028

(http://iopscience.iop.org/1742-6596/393/1/012028)

The electronic properties of double wall carbon nanotubes

R. Pincak[1,2] and M. Pudlak[1]

[1] Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47,043 53 Kosice, Slovak Republic

[2] Joint Institute for Nuclear Research, BLTP, 141980 Dubna, Moscow region, Russia

E-mail: pincak@saske.sk, pudlak@saske.sk

Abstract. The electronic spectra double wall carbon nanotubes using tight binding approximation are investigated. We focus on the double wall armchair nanotubes. The influence of nanotube curvature on the electronic spectra is also treated. The impact of the external magnetic field on the spectral characteristic of double wall nanotubes is computed. We found the big change of the electronic spectra for the double walled carbon nanotubes due to the external magnetic field.

1. Introduction

Carbon based materials has attracted scientific interest in recent years from both an experimental and a theoretical viewpoint. Among them carbon nanotubes are very interesting because of their unique mechanical and electronic properties [1]. A single-wall 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. The electronic states of carbon nanotubes are classified by the chiral vector that assigns the diameter and chirality of the nanotubes [2]. The primary symmetry classification of carbon nanotubes is either achiral or chiral. Achiral carbon nanotubes are defined by a carbon nanotube whose mirror images have an identical structure to the original one. There are only two cases of achiral nanotubes, armchair and zig-zag nanotubes. The names of armchair and zig-zag nanotubes arise from the shape of the cross-section ring at the edge of the nanotubes. Chiral nanotubes exhibit spiral symmetry whose mirror image cannot be superposed onto the original one. There is a variety of geometries in carbon nanotubes where the diameter, chirality and cap structures are different [3]. The electronic structure of carbon nanotubes is derived by a simple tight-binding calculation for the π-electrons of carbon atoms.

2. $(5,5)-(10,10)$ armchair tubules in a static magnetic field

We investigate the armchair nanotubes in a 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

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

Potential $V(r)$ reflects the structure of the crystal lattice such as the symmetry and periodicity properties. Here this potential describes the structure of armchair. Vector potential $\vec{A}$ in the Landau gauge can be expressed in the form $\vec{A} = (\frac{\Phi}{L}, 0)$, where $\Phi = B\pi r^2$ is the magnetic flux penetrating the cross section of carbon nanotube and $L = 2\pi r$ is a circumference of the nanotube (r-nanotube radius). Here coordinate x is in the circumferential direction and coordinate y denotes the direction parallel to nanotube axis.

$$\psi_\alpha(\overrightarrow{k}, \overrightarrow{r}) = \frac{1}{\sqrt{M}} \sum_n \exp\left(i\overrightarrow{k}(\overrightarrow{r_n} + \overrightarrow{d}_\alpha) + i\frac{e}{c\hbar} G(\overrightarrow{r_n} + \overrightarrow{d}_\alpha) \right) |\varphi(\overrightarrow{r} - \overrightarrow{r}_n - \overrightarrow{d}_\alpha)\rangle, \qquad (2)$$

where α denotes A or B atoms. Here $\overrightarrow{d}_\alpha$ are the coordinate of the α atom in the unit cell and $\overrightarrow{r_n}$ 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

$$G(\vec{R}) = \int_{\vec{R}}^{\vec{r}} \vec{A}(\vec{x}).d\vec{x} = \int_0^1 (\vec{r} - \vec{R}).\vec{A}(\vec{R} + \lambda(\vec{r} - \vec{R}))d\lambda \qquad (3)$$

Employing Eq.(2), we get $G(\vec{R}) = \int_0^1 (\vec{r} - \vec{R}).(\frac{\Phi}{L}, 0)d\lambda = (x - X)\frac{\Phi}{L}$. We denote $\epsilon = \langle\varphi^{out}(\vec{r} - \vec{A}_i)|H|\varphi^{out}(\vec{r} - \vec{A}_i)\rangle = \langle\varphi^{out}(\vec{r} - \vec{B}_i)|H|\varphi^{out}(\vec{r} - \vec{B}_i)\rangle$,$\widetilde{\epsilon} = \langle\varphi^{in}(\vec{r} - \vec{A}_i)|H|\varphi^{in}(\vec{r} - \vec{A}_i)\rangle = \langle\varphi^{in}(\vec{r} - \vec{B}_i)|H|\varphi^{in}(\vec{r} - \vec{B}_i)\rangle$ and the intertube hopping integrals $\langle\varphi^{out}(\vec{r} - \vec{R}_i)|H|\varphi^{in}(\vec{r} - \vec{R}_j)\rangle = W_{ij}$, ϵ and $\widetilde{\epsilon}$ are Fermi energies of the outer and inner nanotubes; $|\varphi^{out}(\vec{r} - \vec{R}_i)\rangle$, $|\varphi^{in}(\vec{r} - \vec{R}_j)\rangle$ are π orbitals on site i at the outer and on site j at the inner tubes; $W_{ij} = \frac{\gamma_0}{8}\cos(\theta_{ij})e^{(\xi - d_{ij})/\delta}$, where γ_0 is the hopping integral in the graphene,θ_{ij} is an angle between the i-th atom of the inner shell and the j-th atom of the outer shell, d_{ij} is the interatom distance and ξ is the intertube distance. The characteristic length $\delta = 0.45\mathring{A}$. We can define the vectors connecting the nearest neighbor carbon atoms for armchair nanotubes in the form:$\overrightarrow{\tau_1} = a(\frac{1}{\sqrt{3}}; 0)$, $\overrightarrow{\tau_2} = a(-\frac{1}{2\sqrt{3}}; -\frac{1}{2})$,$\overrightarrow{\tau_3} = a(-\frac{1}{2\sqrt{3}}; \frac{1}{2})$. The distance between atoms in the unit cell is also $|\overrightarrow{\tau_i}| = \frac{a}{\sqrt{3}}$. Now we define the

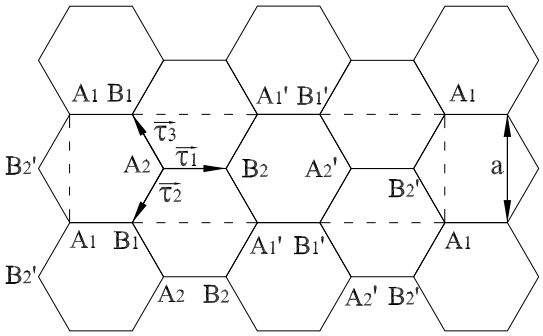

Figure 1. The outer shell part of the unit cell in the case of armchair nanotubes.

intratube hopping integrals $\langle\varphi^{out}(r - A_1)|H|\varphi^{out}(r - B_1)\rangle = \gamma_0\alpha$, $\langle\varphi^{out}(r - A_1)|H|\varphi^{out}(r - B_2^{'})\rangle = \gamma_0\beta$, and $\langle\varphi^{in}(r - A)|H|\varphi^{in}(r - B)\rangle = \gamma_0\widetilde{\alpha}$, $\langle\varphi^{in}(r - A)|H|\varphi^{in}(r - B^{'})\rangle = \gamma_0\widetilde{\beta}$, where $\alpha(\widetilde{\alpha})$, $\beta(\widetilde{\beta})$ are parameters which describe the dependence of hopping integrals on the surface curvature [4]. From Figures 1 and 2 we get the system of equations which describe the electronic properties of the armchair DWCNT [5]. The spectra for some values of $ka/2$ near the Fermi points of double wall armchair nanotubes without and with static magnetic field are depicted in Figure 3,4.

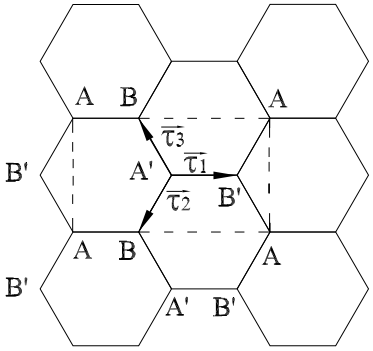

Figure 2. The inner shell part of the unit cell in the case of armchair nanotubes.

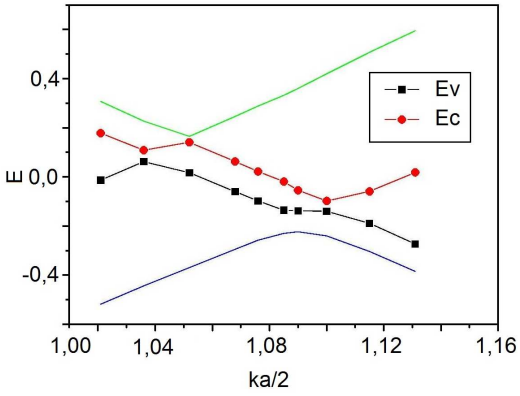

Figure 3. Spectra of armchair DWCNT with the intertube interactions without static magnetic field.

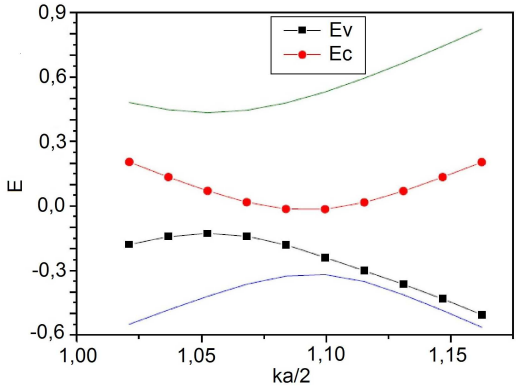

Figure 4. Spectra of armchair DWCNT with the intertube interactions when the static magnetic field $\Phi = 0.5\Phi_0$ is imposed.

3. Conclusion

When the static magnetic field is applied the character of conductivity is changing. For instance we get for armchair carbon nanotube that the conductivity is changed from semimetal to semiconductor.

ACKNOWLEDGEMENTS — 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.

References

[1] Meijer F E, Morpurgo A F and Klapwijk T M 2002 *Phys.Rev.* B **66** 033107
[2] Saito R, Dresselhaus G and Dresselhaus M S 1998 *Physical Properties of Carbon Nanotubes* (London:Imperial Colledge Press)
[3] Molnar B ,Peeters F M and Vasilopoulos P 2004 *Phys.Rev.* B **69** 155335
[4] Pudlak M and Pincak R 2009 *Eur.Phys.J.* B **67** 565-76
[5] Pincak R, Pudlak M and Smotlacha J 2012 *Carbon Nanotubes: Synthesis,Properties and Applications* (New York: Nova Science Publisher)