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The electronic spectra of double-wall zig-zag carbon nanotube affected by the magnetic field.

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Abstract. We study the electronic spectra of (9,0)-(18,0) double walled carbon nanotubes influenced by the external magnetic field. We choose the orientation of the magnetic field parallel to the axis of nanotube. We found the strong change of the electronic spectra due to external magnetic field. That means gap between valence and conductive bands in DWN will be changed.

1. Introduction

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. Of special interest is the prediction that the calculated electronic structure of a carbon nanotube can be either metallic or semiconducting, depending on its diameter and chirality. The energy gap for a semiconductor nanotube, which is inversely proportional to its diameters, can be directly observed by scanning tunneling microscopy measurements. We now consider the electronic structure of carbon nanotubes in a uniform external magnetic field. There are two high symmetry cases for the direction of the magnetic field: one with the magnetic field parallel to the nanotube axis (B $\parallel$ z) and the other with the magnetic field perpendicular to the nanotube axis, (B $\perp$ z). Hereafter the nanotube axis is taken along the z-axis. In this paper we consider the case of B $\parallel$ z. Especially we are interested in the zigzag $(9,0)-(18,0)$ double-wall nanotubes(DWNs) affected by the magnetic field. The synthesis of DWNs has been reported recently [1, 2]. Their electronic structure was investigated by the local density approximation [3, 4] and the tight-binding model [5, 6, 7, 8, 9]. When the magnetic field is parallel to the nanotube axis, electrons moving within the nanotube surface will feel a force perpendicular to the surface. As far as we consider only the transfer integral between two atoms within the nanotube surface, the electronic structure would appear to be unaffected by the magnetic field. This, however, is not correct. The wavefunction will change its phase factor and thus its momentum, k, will shift depending on the magnetic flux penetrating the cross section of the carbon nanotube. This phenomenon is generally known as the Aharonov-Bohm effect, discussed often in the case of cylindrical geometry. Since the carbon nanotube can be a metal or a semiconductor, depending on whether there is an allowed wavevector k in the circumferential direction that has the value of the K. point in the two-dimensional Brillouin

zone, this Aharonov-Bohm effect will modify the energy gap of a carbon nanotube as a function of magnetic field.

2. $(9,0)-(18,0)$ zigzag tubules

The π electronic structures are calculated from the tight-binding Hamiltonian

$$H=\sum_i \epsilon|\varphi_i^{out}\rangle\langle\varphi_i^{out}|+\sum_{i,j}\gamma_{ij}\left(|\varphi_i^{in}\rangle\langle\varphi_j^{in}|+h.c\right)+\sum_i \widetilde{\epsilon}|\varphi_i^{in}\rangle\langle\varphi_i^{in}|+\sum_{i,j}\widetilde{\gamma}_{ij}\left(|\varphi_i^{in}\rangle\langle\varphi_j^{in}|+h.c\right)$$
$$+\sum_{l,n}W_{ln}\left(|\varphi_l^{in}\rangle\langle\varphi_n^{out}|+h.c\right), \tag{1}$$

ϵ and $\widetilde{\epsilon}$ are Fermi energies of the outer and inner nanotubes; $|\varphi_i^{out}\rangle$, $|\varphi_i^{in}\rangle$ are π orbitals on site i at the outer and inner tubes; γ_{ij}, $\widetilde{\gamma}_{ij}$ are the intratube hopping integrals; W_{ij} are the intertube hoping integrals which depends on the distance d_{ij} and angle θ_{ij} between the π_i and π_j orbitals.

$$W_{ij}=\frac{\gamma_0}{8}\cos(\theta_{ij})e^{(\xi-d_{ij})/\delta}, \tag{2}$$

where θ_{ij} is an angle between the ith atom of the inner shell and the jth atom of the outer shell, d_{ij} is the interatom distance and ξ is a intertube distance. The characteristic length $\delta=0.45\mathring{A}$. We assume the symmetric geometry of zig-zag DWNT [7]. It was considered that hopping between shells takes place only between atoms which occupy position directly each above other. It means we take into account only the interactions

$$W_{ii}=\frac{\gamma_0}{8}. \tag{3}$$

We look for solution in the form

$$\Psi=\sum_{i=1}^{12}c_i\psi_i. \tag{4}$$

We have secular equations

$$\sum_{j=1}^{12}\langle\psi_i|H|\psi_j\rangle c_j=\tilde{E}c_i, \tag{5}$$

where

$$\langle\psi_i|H|\psi_j\rangle=\delta_{ij}E_i, \tag{6}$$

for $i,j=1,...8$ and $i,j=9,...12$, and the interaction between shells is described by the terms $\langle\psi_i|H|\psi_j\rangle$ for $i=1,...8$; $j=9,...12$, see [10]. The vector potential A for B$\|$ in this coordinate system is given by

$$A=\left(\frac{\Phi}{L},0\right), \tag{7}$$

where Φ is the magnetic flux penetrating the cross section of a carbon nanotube, and L is the diameter of tube. Thus the shift k is

$$k_x=k_x+\frac{\Phi}{L\Phi_0}, k_x=k_x+\frac{\Phi}{2L\Phi_0}, \tag{8}$$

for inner and outer tube, respectively. To construct the Hamiltonian, we use only the valence and conductive states of individual nanotubes in the absence of intertube interaction. The electronic structures can be calculated from the Hamiltonian

$$H=\begin{pmatrix}\Delta+b2 & 0 & H_{3,11} & H_{3,12}\\ 0 & \Delta-b2 & H_{4,11} & H_{4,12}\\ H_{11,3} & H_{11,4} & -\Delta+b6 & 0\\ H_{12,3} & H_{12,4} & 0 & -\Delta-b6\end{pmatrix} \tag{9}$$

where

$$b2 = \gamma_0(1 - 2\xi\cos\frac{\sqrt{3}ka}{2} + \xi^2)^{\frac{1}{2}}, \tag{10}$$

$$b6 = \gamma_0(1 - 2\widetilde{\xi}\cos\frac{\sqrt{3}ka}{2} + \widetilde{\xi}^2)^{\frac{1}{2}}, \tag{11}$$

$$H_{3,11} = H_{4,12} = \frac{1}{4\sqrt{2}}\frac{\gamma_0}{8}\left(1 + e^{-i(\varphi_6-\varphi_2)}\right), \tag{12}$$

$$H_{4,11} = H_{3,12} = \frac{1}{4\sqrt{2}}\frac{\gamma_0}{8}\left(1 - e^{-i(\varphi_6-\varphi_2)}\right), \tag{13}$$

$$e^{i(\varphi_6-\varphi_2)} = \gamma_0^2\frac{1 - \xi e^{i\frac{\sqrt{3}ka}{2}} - \widetilde{\xi}e^{-i\frac{\sqrt{3}ka}{2}} + \xi\widetilde{\xi}}{b2\ b6}. \tag{14}$$

$2\Delta(\approx\ 0.21eV)$ is a Fermi energy difference of the outer and inner nanotubes, $\Psi(k) = (d_3, d_4, d_{11}, d_{12})$ and d_i is an amplitude to find electron in state ψ_i. The wave functions ψ_3, ψ_4 are conductance and valence states of outer nanotube and ψ_{11}, ψ_{12} are conductance and valence states of inner nanotube in the absence of the intertube interaction [10]. The parameter $\gamma_0(\simeq 3eV)$ is the hoping integral in the graphene.

The parameters ξ, $\widetilde{\xi}$ can be expressed in the form

$$\widetilde{\xi} = 2\tilde{\beta}\cos(\frac{m\pi}{9} + \frac{\Phi}{9\Phi_0}), \tag{15}$$

and

$$\xi = 2\beta\cos(\frac{m\pi}{9} + \frac{\Phi}{18\Phi_0}), \tag{16}$$

where the parameters $\tilde{\beta}$ and β are the same as in [10, 12]

The eigenvalues of Hamiltonian (1) for some values of $\sqrt{3}ka/2$ near the point $k = 0$ are depicted on Fig.1. and was computed in [12]. The Fig.2. shows broadening of the gap between valence and conductive bends due to the influence of the magnetic field parallel to the z axes.

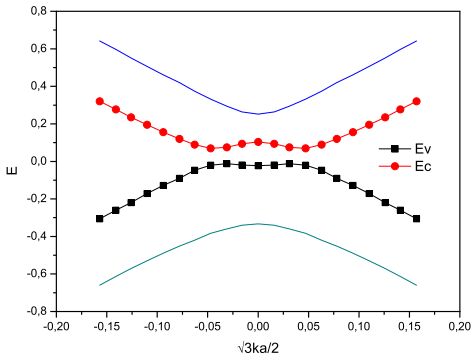

Figure 1. Spectra of zigzag DWN where E_c and E_v are conductive and valence band.

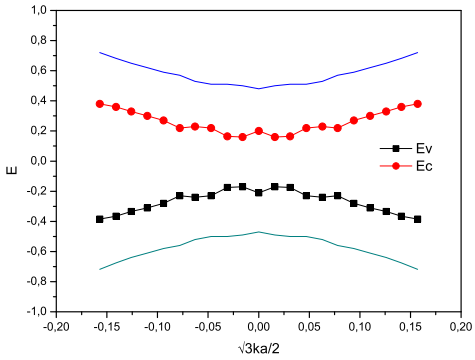

Figure 2. Spectra of zigzag DWN affected by the magnetic field with value $\Phi/\Phi_0 = 0.5$.

3. Conclusion

As was described in [10, 12] the Fermi level of the outer shell is about 0.21 eV higher than the Fermi level of the inner shell in the case of zig-zag SWNs. In the case of zig-zag DWNs the curvature do not shift the k_F of the individual nanotubes. The result is that these DWNs are semiconductors. Generally we can say that the conductivity depends on the relative position of the Fermi points k_F of individual nanotubes. If there is no shift the DWN is a semiconductor. If there is a shift in the dependence on Fermi levels and the energy gaps of individual nanotubes the DWN can be semimetal or semiconductor. Since the presence of an energy gap in a carbon nanotube is determined by whether or not the one-dimensional energy bands cross or do not cross at the K or K' points at the corners of the 2D Brillouin zone, a semiconducting carbon nanotube can become metallic in a parallel magnetic field at certain values of the phase shift, and conversely a metallic nanotube can become semiconducting in a parallel magnetic field, the energy gap thus oscillates. The significance in a carbon nanotube is that the semiconducting or metallic nature of the nanotube can be altered only by applying a magnetic field parallel to the nanotube axis. This is because the distinction between a semiconducting and a metallic carbon nanotube arises from a quantum effect in which discrete wave numbers in the circumferential direction distinguish between metallic and semiconducting properties. It is noted that the one-dimensional energy dispersion relations for carbon nanotubes at the top of the valence band and the bottom of the conduction band follow a linear t relation only when the carbon nanotube is metallic. When the carbon nanotube has a semiconducting energy gap, the energy dispersion is quadratic at the top of the valence band and at the bottom of the conduction band. Thus the effective mass of an electron contributing to the transport properties of a carbon nanotube is a function of magnetic field.

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