Physica B 498 (2016) 55–58

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Effect of magnetic field on quantum state energies of an electron confined in the core of a double walled carbon nanotube

Khurshed A. Shah*, Bashir Mohi Ud Din Bhat

Nanomaterials Research Laboratory, Department of Physics, Govt. Degree College for Women, K. P. Road, Anantnag 192101, India

ARTICLE INFO

Article history:
Received 7 September 2015
Received in revised form
21 June 2016
Accepted 22 June 2016
Available online 23 June 2016

Keywords:
Double walled carbon nanotube
Magnetic field
Quantum state energies
Core radius dependence
Electron confinement

ABSTRACT

In this paper we report the effect of external magnetic field and core radius on the excited quantum state energies of an electron confined in the core of a double walled carbon nanotube. The goal is accomplished by using Wentzel–Kramers–Brillioun (WKB) approximation method within the effective mass approximation and confinement potential. All numerical analysis were carried out in a strong confinement regime. The results show that the electron energy increases with the increase in external magnetic field at a given core radii. The electron energy is also found to increase as the core radius of the CNT decreases and for core radius $a > 5$ nm the energy becomes almost zero. The effect of magnetic field on the excited state energies of the confined electron is more evident for smaller core radius $a < 1$ nm. The observed results are important for calculations of spin polarized current in carbon nanotube quantum dot devices [1].

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1. Introduction

Carbon nanotubes (CNTs) are hollow cylinders made exclusively of carbon atoms and their aspect ratio is high due to the fact that the diameter of CNTs is of few nanometers and the length is in the range of micrometers. The CNTs have graphene layered like structure which differentiates them from other carbon materials such as activated carbon and carbon nanofibres. The CNTs can be of metallic or semiconducting in nature and have a tubular morphology [2]. Generally CNTs can be single walled nanotube (SWCNT), double walled nanotube (DWCNT) or multi-walled nanotube (MWCNT). A SWCNT with only one atomic thick cylindrical graphene layer attracts scientific community because of their extra-ordinary properties. Similar to MWCNTs, they are very robust due to the carbon-carbon bond formation, one of the strongest bonds in nature. Sawada et al. [3] predicted that the minimum diameter for an energetic stable SWCNTs is about 0.4 nm whereas Qin et al. [4] demonstrated narrowest attainable carbon nanotube with a diameter of 0.4 nm and at the same time Wang et al. [5] published a HRTEM micrograph of porous zeolite single crystals which contain a SWCNT of diameter 0.42 nm in their center.

The electronic and vibrational properties of the DWCNTs resembles with those of the SWCNTs, but when compared with SWCNTs, they are more resistant to thermal and mechanical stress [6]. This makes DWCNTs good for the fabrication of nano based electronic devices, such as field emitters [7]. In this context, we need better understanding of the energy transfer mechanisms between two concentric layers of DWCNT to unveil their potential for future applications. It is to mention that the DWCNTs provide more interest for studying the interaction between two concentric graphene layers. Generally the inner and the outer layers of double walled carbon nano tubes can be either metallic (M) or semi-conducting (S). The four possible configurations are: M@M, M@S, S@S and S@M, where S@M denotes an S inner tube and M outer tube. Each configuration is expected to possess distinct electronic properties [8]. The inner layer S can be approximated as an isolated SWNT exhibiting a rich variety of intriguing electronic properties and thus becomes promising material for nano based electronic devices.

Although in past hydrogen and its isotopes [9], KI and CsL nano crystals [10], molecules and peptides [11], metal nano particles [12] were confined inside CNTs, however to the best of our knowledge no effort has been made in confining the electron in the core of DWCNT and the dependence of its energy on external magnetic field and core radius. Therefore, the subject of this paper is to investigate and calculate the electron energy associated with the confined electron in the core of a S@M DWCNT that arises because of the quantum confinement effects and their dependence on applied external magnetic field and core radius. It is found that the change in energy of electron is more profound for higher excited states at a given core radius and applied magnetic field. Smaller magnetic fields less than 0.2 T does not affect too much on the electron energy and the electron energy becomes zero for CNTs of core radius greater than 8 nm. We believe that these

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* Corresponding author.
E-mail address: drkhursheda@gmail.com (K.A. Shah).

http://dx.doi.org/10.1016/j.physb.2016.06.024
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results will be very useful for the applications of CNTs in various sectors especially tunneling effect based nano devices.

The paper is organized as:

Section 2 describes the model and theoretical formulations and Section 3 presents the results and discussions. The conclusion remarks are presented in Section 4.

2. Model and theoretical formulations

Here in this study a theoretical model is developed to study quantum states energies of an electron confined in the core of a DWCNT under the application of external magnetic field. In our model, we choose the core of the tube being semiconducting (S) and outer wall metallic (M) in nature, as the configuration is expected to possess distinct electronic properties. The inner-outer tube distance is taken to be much less than the interlayer spacing in graphite. The magnetic field was assumed to be applied along *z*-direction such that a symmetric magnetic confinement occurs in the *x*–*y* plane. The geometrical two dimensional view of the S@M DWCNT under consideration is shown in Fig. 1. Here *a* is the radius of the core of the tube while *b* is the radius of the CNT as a whole.

For simplicity, we assume a parabolic confinement potential for electron, given by

$$V_e(r) = \frac{V_0}{a^2}\left(r^2 - a^2\right) \quad |r| \le a$$
$$\text{Otherwise} \quad 0 \qquad |r| > a \tag{1}$$

where $V_0 = 0.4$ eV is the potential barrier height for a semiconducting carbon nanotube of diameter 1 nm [13].

We consider particle like an electrons experience strong confinement potential within the core of the tube due to the presence of outer layer of the tube, in other words the particle experiences a strong confinement regime. The single particle wave functions under such situation can be described by the Wentzel Kramers Brillouin (WKB) wave functions [14], given by

$$\psi(a,b) = \begin{cases} \dfrac{A_s}{\sqrt{k_j}}\exp\left[-\displaystyle\int_a^b K_j dr\right] & \text{For } -b < r < -a \\ \dfrac{A_c}{\sqrt{k_j}}\mathrm{Sin}\left[\displaystyle\int_{-a}^{a} K_j dr + \frac{\pi}{4}\right] & \text{For } -a < r < a \\ \dfrac{A_s}{\sqrt{k_j}}\exp\left[-\displaystyle\int_a^b K_j dr\right] & \text{For } a < r < b \end{cases} \tag{2}$$

Here *j* can be an electron (*e*) or a hole (*h*), A_c and A_s are the normalization constants of the inner core and outer shell of the DWCNT and the wave vector K_j associated with the electron is given by [13]

$$k_j = \frac{2n\pi}{8\sqrt{3}\,a_{c-c}} \tag{3}$$

where $a_{c-c} = 1.44A^0$ the distance between the carbon atoms and *n* is an integer.

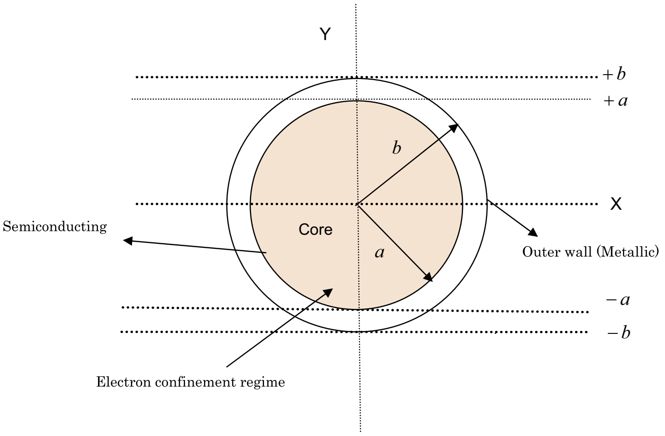

Fig. 1. Geometrical two dimensional view of S@M DWCNT.

2.1. Theoretical formulations

The electron Hamiltonian of confined electron in the presence of magnetic field B_Z (applied along the *z*-direction) is given by

$$H_e = -\frac{\hbar^2}{2m_e^*}\nabla^2 + V_e(r) + \frac{1}{2}g_e{}^*\mu_B B_Z \tag{4}$$

where m_e^* is the effective mass of the electron, $g_e{}^*$ and μ_B are the effective *g*-factor for the electron and Bohr magnetron respectively. The first term of Eq. (4) is the kinetic energy operator term, the second term $V_e(r)$ represents the geometrical confinement potential, while the last term represents Zeeman energy.

The application of an external magnetic field restricts the motion of electron within the cyclotron radius $r_c = \sqrt{\hbar/em_e}$, accordingly, the in plane confinement of electron will be due to magnetic effect as well as the geometry chosen. In the presence of magnetic field, the energy levels in the plane perpendicular to the magnetic field get quantized resulting into the formation of degenerate energy levels. Furthermore, the applied magnetic field modifies the electron momentum giving rise to Zeeman splitting, thus the splitting of energy levels depends significantly on the applied magnetic field, effective g-factor.

The energy Eigen value of the confined electron can be obtained by diagonalising H_e using wave function given by Eq. (2)

$$E_e = \left\langle \psi \middle| -\frac{\hbar^2}{2m_e^*}\nabla^2 + V_e(r) \middle| \psi \right\rangle + \frac{1}{2}g_e{}^*\mu_B B_z \tag{5}$$

where ∇^2 operator in spherical polar coordinates is given by

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\varphi}\left(\sin\theta\frac{\partial}{\partial\varphi}\right)$$

After rigorous mathematical calculations, we obtained the final expression for the electron energy as,

$$E_e = \frac{4}{3}\frac{\pi^2 A_c^2\hbar^2 n^2}{m_e^* a^2} + \frac{4}{a}A_c^2 V_o a_{c-c} + \frac{1}{2}g_e{}^*\mu_B B_z \tag{6}$$

3. Results and discussions

We calculated the electron energies of an electron confined in the core of S@M DWCNT as a function of external magnetic field strength and the core radius using mathematical software Mathcad 8 professional [15]. The parameters used in the calculations are $m_e^* = 0.13m_o$, where m_o is the mass of free electron, lande g factor for electron $g_e = 1.2$ and *c*–*c* distance $a_{c-c} = 1.44A^0$ and $\mu_B = 9.27 \times 10^{-24}$ J/T. Using values for all variables in the Eq. (6) and varying the applied magnetic field in the range 0–1 T at constant value of core radius, the splitting energies of the excited states of confined electron are shown in Fig. 2.

From the Fig. 2 it is clear that the splitting of energy states of an electron in a S@M DWCNT depends both on applied magnetic field strength B_z and the radius of the core. For a given core radius, the energies of the electron increases as magnetic field B_z increases. The electron energy decreases sharply with increasing core radii and the change in electron energy is more evident for smaller core

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