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Transmission of charge ion in Single-walled Carbon Nanotube

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Transmission of charge ion in Single-walled Carbon Nanotube

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Abstract. In this paper, we investigate the effects of the chiral structure of single-wall carbon nanotube (SWCNT) on the probability that an electron is transmitted (or reflected) through SWCNT. We adopt the charge density calculated by using the density functional theory (DFT) method [New J. Phys. 18 (2016) 023029] to investigate the transmission of an electron through potential barriers from the charge density. We find that the alpha-electron density in SWCNT for the chiral structures (9,0), (9,2) and (9,3) causes resonant tunneling of electrons through potential barriers. For the chiral structures (9,1), (9,4) and (9,5), we obtain transmission and reflection as same as scattering at a finite potential barrier.

1. Introduction

Theoretical investigations were developed by several authors, focusing on the transport of fast charged particles through single-wall carbon nanotube (SWCNT). The hydrodynamic theory of a two-dimensional electron gas [1-2] has been used to derive energy loss of a probe electron when passing through or close by SWCNT. [3]. While the studies on results for stopping power in the linearized hydrodynamic model compared with the dielectric formalism in random-phase approximation had shown [4]. A close agreement between the two approaches is obtained for high speeds of a probe charged particle. The induced potential, the self-energy, and the stopping power for the examination charged particle moving parallel to the axis in CTNs had been derived. The numerical results show that the velocity dependents of these quantities are strongly affected by the damping factor, the nanotube radius, and the probe charged particle position. For fast molecular and cluster ion through solid and plasma targets had been studied [5]. For CNTs, problems in channeling H₂⁺ through SWCNTs were solved by the classical equation of motion, which involves both the repulsive continuum potential of SWCNT and the dynamical screened Coulomb repulsion between the two ions [6]. Strong vicinage effects are found in both the molecule self-energy and its stopping power when the speeds are high [7]. For other consideration, impact of the curvature on induced hybridization and modification of emission profiles for each chiral's index of SWCNT are showed that the maximum dipole vector circumference is obtained at the phase summation of π for the case of indirect transition [8] and electron transport in the chiral SWCNT and quantum dot coupling was showed in [9].



In the present paper, we adopt the charge density calculated by using the density functional theory (DFT) method [10] to investigate the transmission of an electron through potential barriers from the charge density.

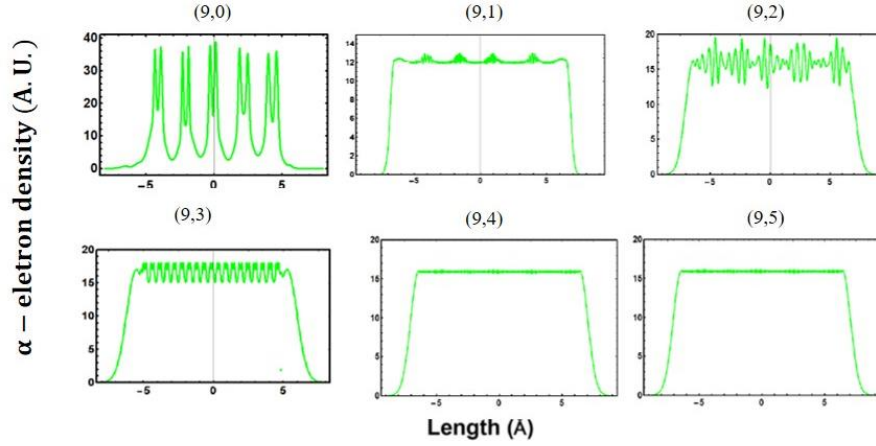


Figure 1. The α -electron density distribution along the tube axis of $(9, m)$ for $m = 0-5$, calculated by using the density functional theory (DFT) method [10].

2. Methods

In the present, the computer simulation technique has been used in solutions to the one-dimensional Schrodinger equation with an arbitrary potential. A numerical method for quantum tunneling is essential for understanding many quantum transport phenomena. Instead, we have used the Crank-Nicolson method [11], which is stable and conserves probability. In this method, we evaluate the right-hand side of the Schroedinger equation at both times k_1 and k and take the average. Our discretized Schrodinger equation is then

$$\left(2 + 2\alpha + \frac{i\Delta t}{\hbar} V_j\right) \varphi_{j,k} - \alpha \varphi_{j+1,k} - \alpha \varphi_{j-1,k} = \left(2 - 2\alpha - \frac{i\Delta t}{\hbar} V_j\right) \varphi_{j,k-1} - \alpha \varphi_{j+1,k-1} - \alpha \varphi_{j-1,k-1} \quad (1)$$

when. $\alpha = i\hbar\Delta t/2m\Delta x^2$. Eq. (1) can be rewritten in matrix form as

$$A\varphi_{j,k} = B\varphi_{j,k+1}, \quad (2)$$

and φ is the N-point array representing the wave function, k is the temporal index, and the matrices A and B are

$$A = \begin{pmatrix} 2 + 2\alpha + \frac{i\Delta t}{\hbar} V_1 & -\alpha & 0 & & 0 \\ -\alpha & 2 + 2\alpha + \frac{i\Delta t}{\hbar} V_2 & -\alpha & \dots & \vdots \\ 0 & -\alpha & 2 + 2\alpha + \frac{i\Delta t}{\hbar} V_3 & & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 2 + 2\alpha + \frac{i\Delta t}{\hbar} V_N \end{pmatrix}, \quad B = \begin{pmatrix} 2 - 2\alpha - \frac{i\Delta t}{\hbar} V_1 & -\alpha & 0 & & 0 \\ \alpha & 2 - 2\alpha - \frac{i\Delta t}{\hbar} V_2 & -\alpha & \dots & \vdots \\ 0 & -\alpha & 2 - 2\alpha - \frac{i\Delta t}{\hbar} V_3 & & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 2 - 2\alpha - \frac{i\Delta t}{\hbar} V_N \end{pmatrix}. \quad (3)$$

Finally, to evolve the wave function forward by one-time step we perform the matrix multiplication

$$\varphi_{j,k} = A^{-1}B\varphi_{j,k+1} = C\varphi_{j,k+1} \quad (4)$$

where C is known as the Crank-Nicolson matrix.

The shape of the transmitted wave packet can, in principle, be determined by looking at the transmission amplitude for each of its energy eigenstate components following ref. [6]. We assume that the potential wall of the free electron moving through the SWCNT is proportional to the charge density of the alpha-electron density in SWCNT. We adopt the charge density calculated by using the density

functional theory (DFT) method [10] to investigate the transmission of an electron through potential barriers from the charge density.

3. Result and discussion

The results of the calculated probability of an electron through SWCNT, we obtain two characteristics of tunneling shown in figure 2-7 as resonant tunneling and rectangular potential. The electron transmission coefficient through the chiral structure depends on the alpha-electron density in SWCNT for the chiral structures (9,0), (9,2) and (9,3) causes resonant tunneling of electrons through potential barriers. For the chiral structures (9,1), (9,4) and (9,5), we obtain transmission and reflection as same as scattering at a finite potential barrier.

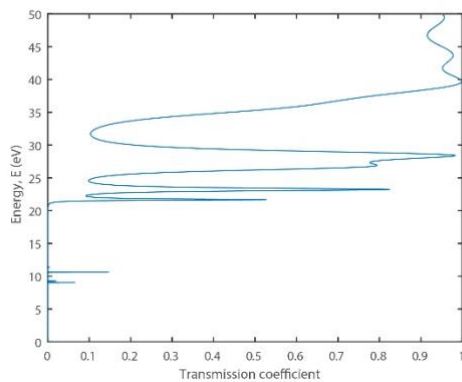


Figure 2. The electron transmission coefficient through the chiral structure (9,0) as a function of energy.

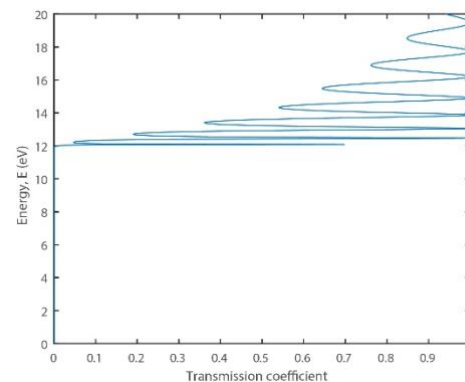


Figure 3. The electron transmission coefficient through the chiral structure (9,1) as a function of energy.

From Figure 2-4, the result of our simulation had predicted that the electron transmission coefficient through the chiral structure threshold is a complex phenomenon that compiles two quantum phenomena as quantum tunneling and quantum interference that show in low energy region. It refers to resonant tunneling in which the electron transmission coefficient through a structure is sharply peaked about certain energies in Figure 2. The total amplitude to transfer the electron through the chiral structure can be viewed as a sum of partial waves, executed several reflections in the central area.

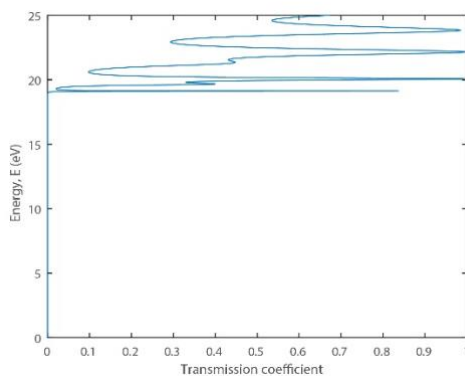


Figure 4. The electron transmission coefficient through the chiral structure (9,3) as a function of energy.

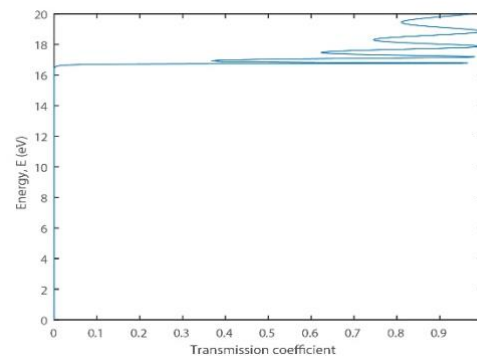


Figure 5. The electron transmission coefficient through the chiral structure (9,4) as a function of energy.

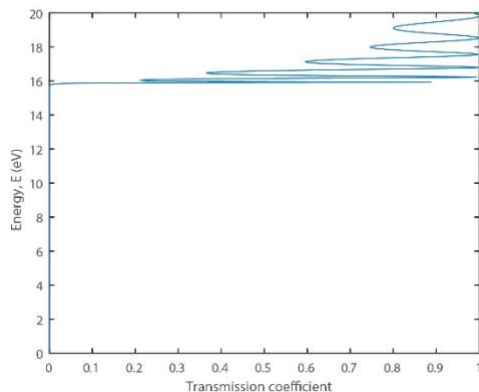


Figure 6. The electron transmission coefficient through the chiral structure (9,4) as a function of energy.

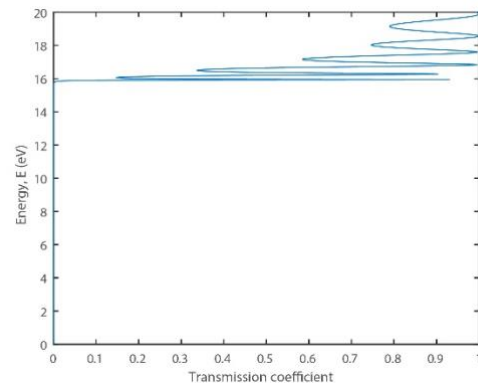


Figure 7. The electron transmission coefficient through the chiral structure (9,5) as a function of energy.

4. Conclusions

In this study, we investigate the dependence of the transmission coefficient of the electron through along the tube axis of the chiral structure (9, m) from 0 – 5. Our simulation had predicted the transmission coefficient threshold and show that the low energy electron is possible through the chiral SWCNT is decreasing while the chiral angle is increased.

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