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Quantum drift velocity and current density in one dimensional carbon nano tubes

***Ashrafuz-Zaman SK, PK Saikia**
Department of Physics, Dibrugarh University, Dibrugarh, Assam, India

Abstract
The Material Science in modern times seem to be incomplete without nano-materials[9]. The distinction of nano materials with other bulk materials lies in dimensionality of the systems. For instance, we cite the field of carbon nano tubes and other nano materials have in recent days been a promising and emerging area of research due to its dimensionality. In fact, when the particular dimension of a three dimensional system becomes comparable to the de-Broglie wave length, the energy level associated with the dimension become quantized. This quantized energy is found to be fruitful stating point to account for other quantized electrical quantities in composite nano structures and other similar systems. With the help of the quantized energy, a semi classical approach has been adopted to investigate the quantized nature of the drift velocity of electrons and finally an expression of current density in ideal one dimensional carbon nano tubes has been proposed.

Keywords: conductivity, drift velocity, potential well, quantized state, current density

1. Introduction

It has been so far found See, for instance ref. [1, 8], electrical and mechanical properties of carbon nano tubes depend on the structure of carbon nano tubes. when CNT is extremely narrow (Thin) *i.e* for a very thin carbon nano conductor for which $A^{1/2} << L$ where the diameter of the tube is a few nano meter, then we may approximate that the de-Broglie wave length of the electrons may be assumed to be comparable with the diameter, hence energy associated with transverse dimension is quantized [10] due to the quantum confinement of the electrons. Well, we start with an ideal one dimensional potential well of infinite depth and of length 'L' in which eletron moves almost freely *i.e* assuming infinite depth of the well, then the well known wave function

$$\psi_n(x) = A\text{Sin}\frac{n\pi x}{L}, \quad n = 1, 2, 3............$$

In deriving the result total quantized energy we could normalise the wave function of the electron by solving the schroodinger wave equation, which for an electron turns out to be11

$$\psi_n(x) = \sqrt{\frac{2}{L}}\,\text{Sin}(\frac{n\pi x}{L}), \quad n = 1, 2, 3........$$

Hence, the total quantized energy is given by

$$E_n = \frac{n^2 h^2}{8mL^2} \text{-----------------} \qquad (1)$$

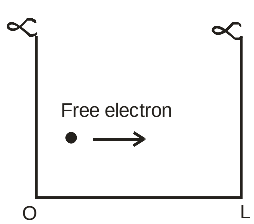

Figure-01

Now, since the electron spatial density in the nano tube varies directly with the probability density of the electron, that is we can write $N_\rho(x) = C\sum_{1}^{N_0}\left|\psi_{n_i}\right|^2$, where C is a positive constant.

Note the carbon nano tubes with armchair wrapping have been produced so far which exhibit metallic or conducting nature with helicity indices *(m,n) with m=n* or m-n/3 is an integer. Further more, many experiments show that CNT are ballistic conductors provided that the mean free path of the electron is greater than the length of the tube [1, 4] However, the velocity v_n of the electron

$$v_n = \frac{nh}{2ml} \text{---------------------} \qquad \text{(iii)}$$

Introducing transit time of the electron in nano tube

$$\tau_n = \int_0^L \frac{dX}{V_n} = \frac{L}{v_n}$$

$$\tau_n = 2m\frac{L^2}{nh} - - - - \qquad \text{(iv)}$$

With the aid of equation (ii), (iii) & (iv) it has been so far established theoretically

$$\sigma_n = \frac{2Le^2}{Anh} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad \text{(v)}$$

See for instance ref [1, 3, 5, 7, 8].

Equations (i), (ii), (iii), (iv) & (v) have been referred in ref. [1] and (v) is referred in ref. [1, 2, 4, 8]. However, the same can be attained through various approach, see for instance [1, 4] and valid for many electron system as well.

2. Materials and Methods

For dealing with our problem we consider previous model of CNT with the one dimensional approach of carbon nano tubes in which electron is confined within the well of infinite depth, so that electron is completely free to to move within the well. That means electron is confined from transverse directions in the tube that results in the quantized nature of the total energy of the electron[1].Hence one dimensional box model with single electron constitute the starting point for fruitful approach to find the quantized resistance. Apart from this, we use well established Ohm's law in order to find the quantized current through the circuit and hence the current density.

Theory

Respecting the quantum behavior of the conductivity, we denote 'σ' as

$$\sigma_n = \frac{2Le^2}{Anh}$$

Note, 'σ_n' depends on the length & area of the cross section of the tube. Thus, for a conducting CNT 'σ_n' and hence 'ρ_n' resistivity depends on its dimension, whereas for an ordinary conductor 'σ_n' & 'ρ_n' are independent of the dimension of the given conductor.

Equation (v) shows conductivity is quantized, so does the resistance also

$$R_n = \rho\frac{L}{A} = \frac{Anh}{2Le^2}\cdot\frac{L}{A} = \frac{nh}{2e^2} \Rightarrow R_n = \frac{nh}{2e^2} - - - - - - - - - - (vi)$$

This value agrees with first two values for n=1 and n=2 observed in ref [4]

So, the resistance no longer depends upon the dimensional aspect such as on length and its area of cross section but for an ordinary conductor

$R_n \alpha L$

$\alpha \frac{1}{A}$

It is here the beautiful nature manifested by the quantum nano wire unlike bulk ordinary conductor, draws attention of the Researchers for further fruitful investigations in quantum nano technological field. Furthermore, under the effect of electric field E, the free electron in the wire get accelerated and acquire velocity component in a direction opposite to the direction of electric field in addition to their thermal random velocity. However, the gain in velocity of an electron (e) due to electric field takes place only for a short duration of time as the electron accelerates, it gets scattered or deflected on suffering collision with the positive ions in the conductors.

The short time for which an electron get accelerated before it under goes a collision is called relaxation time. If an electron having initial random thermal velocity $\boldsymbol{u_1}$ (Bold letters indicate vectors) get accelerated for a time τ_1, then it will attain a velocity $\boldsymbol{v_1}$,

$$\boldsymbol{v_1} = \boldsymbol{u_1} + \boldsymbol{a}\,\tau_1$$
$$\boldsymbol{v_2} = \boldsymbol{u_2} + \boldsymbol{a}\,\tau_2$$

For many electron system, we can extend the idea up to n^{th} electron

$$v_n = u_n + a\tau_n$$

Now, by definition of drift velocity, drift velocity is the average velocity with which free electrons get drifted under the influence of an external electric field.

$$\vec{v}_d = \frac{\vec{v}_1 + \vec{v}_2 + \ldots\ldots}{n}$$

$$\vec{v}_d = \frac{(\vec{u}_1 + \vec{u}_2 + \ldots + \vec{u}_n) + \vec{a}(\tau_1 + \tau_2 + \tau_3 + \ldots\ldots\ldots)}{n}$$

$$\because \frac{(\vec{u}_1 + \vec{u}_2 + \ldots\ldots + \vec{u}_n)}{n} = 0$$

$$\boldsymbol{v_d} = \boldsymbol{0} + \boldsymbol{a}\tau$$

τ average relaxation time and in an conductor random thermal velocities of electrons get cancelled due to random direction of thermal velocities

$$\frac{\vec{U}_1 + \vec{u}_2 + \ldots\ldots\ldots\ldots\ldots \vec{U}_n}{n} = 0$$

$$v_d = -\frac{eE\,\tau}{m} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad \text{(vii)}$$

It is to be noted the result given by equation (vii) does not strictly hold for single electron system, which involves a factor $\frac{1}{2}$, that comes out as a result of the average of final and initial velocity of the electron between two successive collisions, which has been derived by simple mathematical calculation as follows first by considering the fresh journey of the electrons after each collision (starts with zero velocity).Secondly assigning random thermal velocities to all the electrons. Nevertheless the identical result is achieved.

According to free electron model, the electron in a solid move freely. If free time *i.e* time taken between two successive collision be $'\tau'$, *mean free path* $'\lambda$ 'then, $\tau = \frac{\lambda}{v}$, If the applied field on electron of charge $-e$ is $'\vec{E}'$, *then the equation of motion of the* electron

$$-e\,\vec{E} = m\frac{d^2x}{dt^2} \text{---------------------------------} \quad \text{(viii)}$$

Integrating the above equation, taking magnitude only

$$v = \dot{x} = e\frac{E}{m}\tau + C$$

C is the constant of integration

When $t' = \tau$ then $v = v_{max}$

At t=0, $C=0$ as $\dot{x}_0 = 0$, Maximum velocity of electron corresponds to a time duration 'τ' as the electron start with a fresh velocity after a collision. since the electron moves with uniform acceleration

$$v_{\max} = \dot{x}_{\max} = e\frac{E}{m}\tau$$

During the time interval 'τ', average velocity between successive collision

$$v_d = \frac{v_{max}+0}{2} = e\frac{E}{m}\tau\frac{1}{2} \text{ --------------------}(ix)$$

So, this idea of drift velocity can be extended to many electron system as well, instead of taking single electron system as so far, we have considered only single electron in one dimensional well of CNT.

For a system of 'n' electrons with assignment of random thermal velocities (before the field works on the chare carriers), we can arrive at the same result as before

We could see a factor '$\frac{1}{2}$' in the expression, since the drift velocity has to be an average velocity of the journey not the terminal velocity between successive collision.

$$\mathbf{v}_d = (u_1+v_1) + (\mathbf{u}_2 + \mathbf{v}_2) + \text{-----------------} + (\mathbf{u}_n + \mathbf{v}_n)/2n$$

Note bold letters have been used to denote vectors

$$\mathbf{v}_d = (\mathbf{u}_1 + \mathbf{u}_2 + \mathbf{u}_3 + \text{---------}\mathbf{u}_n)/2n +$$

$$(\mathbf{v}_1 + \mathbf{v}_2 \text{-+-----+} \mathbf{v}_n)/2n$$

$$= 0 + \vec{a}\,(\tau_1 + \tau_2 + \tau_3 + \cdots \dots \dots \dots \tau_n)/2n$$

'τ' is here referred to average relaxation time

$$\tau = \frac{\tau_1+\tau_2+\tau_3+\cdots\cdots+\tau_n}{n}$$

$$\overrightarrow{v_d} = \vec{a}\frac{\tau}{2} = -e\frac{E}{m}\frac{\tau}{2} = \text{..................} \qquad (x)$$

So, the correct value of drift velocity is expected to be given by equation(x)

Now, equation (ix) and(x) gives same drift velocity. But many authors use drift velocity as

$$\overrightarrow{v_d} = -e\frac{E}{m}\tau$$ Ref [5, 6]

Since, current through the nano tube can be given [7]

$$\bar{i} = N_n A\, v_d e \text{.............................} \qquad (xi)$$

'N_n' *is the electron density*

Current density 'J' can now be given as

$$J = \bar{N}_n e v_d \text{ ....} \quad \text{(xii)}$$

After substituting the value of 'v_d 'in the above equation, we have

$$J= \frac{N_n e^2 E\tau}{2m} \text{ ....} \quad \text{(xiii)}$$

$$J = \sigma E \text{ ....} \quad \text{(xiv)}$$

From equation, (xiii) & (xiv), we can write as follows

$$\rho = \frac{1}{\sigma} = \frac{2m}{N_n e^2 \tau} \text{ ....} \quad \text{(xv)}$$

From relations-(xii) & (xiv), we can write

$$E= \frac{V_{p.d}}{L}$$

$V_{P.d}$ is the potential difference across the carbon nano tube

$$v_d = \frac{E}{\bar{N}\rho e} \Rightarrow v_d = \frac{V_{p.d}}{L\bar{N}\rho e} \text{.........................}(xvi)$$

Now, using the quantized value of $'\rho'$ in the above equation, we have

$$v_d = \frac{V_{p.d}}{L N_n e} X \frac{2Le^2}{Anh}$$

$$v_d = \frac{2V_{p.d}e}{Anh\bar{N}_n} \text{.............................}(xvii)$$

Since, in a given ordinary conductor, resistivity is independent of the size and dimension therefore in ordinary conductor drift velocity depends on length and varies inversely as the distance. Whereas for a given CNT, drift velocity is independent of the length of the tube or wire but varies inversely as the area of its cross section; on the other hand for a give an ordinary conductor drift velocity is independent of area of cross section of the bulk material. However, the quantum conditions rest on our assumption of for which $A^{1/2}$<<L where the diameter of the tube is a few nano meter, so that we may approximate that the de-Broglie wave length of electron is much smaller than its length.
It is now convenient to express current density 'J' in terms of the electric t field 'E'
Since***;***

$$I= N_n A v_d e \text{ or } J = \bar{N}_n e v_d$$

Now, substituting the quantized value of ' v_d' in the above expression' we have

$$J = N_n\left(\frac{2V_{p.d}e}{Anh N_n}\right)e$$

$$J = \frac{2V_{p.d}e^2}{Anh} \text{ ....} \quad \text{(xviii)}$$

Note one would get the expression of the current density as given below due to the factor $\frac{1}{2}$ if he considers the drift velocity as given by relation (vii)

$$J = \frac{V_{P.d}e^2}{Anh} \text{ ....} \quad \text{(xix)}$$

If one wishes to apply an potential drop of 6 Volt across a carbon nano tube of typical radius of 15 nm as the most general nano scale measurements involve 1-100nm as the size limit, then the current density is so larger than ordinary conductor which in our theoretical consideration comes out to be 10^8amp/$cm^{2.}$

3. Results & Discussion

Thus, the ordinary conductor and CNT differ in many respects such as in the conductivity, resistivity, resistance and the drift velocity of the electron etc. ρ_n or σ_n depends on the dimension for a CNT whereas for ordinary conductor ρ_n or σ_n does not depend on the dimension of the conductor. Thus, ρ_n or σ_n in carbon nano tube are no longer constants for a given nano-tube unlike as that of the case in ordinary conductors. Also, v_d (drift velocity) of the electron in carbon nano- tube is independent of the length of the CNT whereas in ordinary conductor drift velocity depends on its length.

In addition to this, the drift velocity of electron in CNT depends on its area of cross section and its quantum state but ordinary conductor classically does not contain its area of cross section and quantum state in the expression of drift velocity. Since, the expression of current density varies inversely as the area of cross section, diameter of the tube is dominant factor which is expected to play a role on the electrical properties subject to quantum condition or confinement of the electrons. Thus the quantum nature of the conductivity and hence same for the drift velocity and current density may be marked theoretically all of which varies inversely as the quantum state. Note that we have not taken the interactions among electrons which perhaps could give a perturbed potential instead of perfect square well potential, which is in fact would be more realistic model for multiple electron system in CNT. In such a case, the derived electrical quantities including the eigen energy the of the electron would have been different but our approach is in fact semi classical and semi quantum in nature with ideal case of perfect transitivity T=100% of the electron. In fact our findings is more accurate fore n=1, 2 lower states as quantized conductance of CNT for these states are found to be consistent [1, 4]

It remains incomplete without citing that our expression of drift velocity is believed to be consistent and hence the current density for n=1(ground state) gives current density 10^8a/cm^2>10^7 A/cm^2 for a radius of tube of 15 nm, with applied voltage of 6 volt which is claimed verified by group of researcher S.Frank [5, 2] discovered to be 10^7 A/cm^2 and as per citation made by author of ref [5]. Never the less the exact current density in metallic behavior of carbon nano tubes has to be reconfirmed experimentally for solidification of the accurate result.

4. Conclusions

Thus the one dimensional box model seems to be fruitful starting point for theoretical simulation of the electrical properties such as drift velocity, current and current density of the electrons in one dimensional CNTs. Never the less, the exact result need to be confirmed experimentally.

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