

# Temperature Dependence Quantum State of Electron in One Dimensional Carbon Nano Tubes and The Expression for Temperature Co-efficient of Resistance in Terms of Quantum State

Ashrafuz Zaman Sk., Dr. Ranjit Chowdhury

**Abstract**— The Field of Carbon nano tube (CNT) is an promising area of research theoretically as well as experimentally [1],[2]. In fact the band structure of CNT determines its conductivity and in carbon nano tubes the structural pattern affects the conductivity type i.e the conductivity of CNT depends upon how graphene sheet is rolled up. So, CNT can be made to behave as conductor as well as semiconductor [2] It is well established that the samples of single wall carbon nano tubes with an arm chair wrapping have been produced and exhibit metallic behavior with an intrinsic resistivity which increases approximately linearly with temperature over a wide temperature range (see for instance ref.[4]. In this paper the quantized value of electric conductivity [1],[2] is used in an attempt to show theoretically that the quantum state of the electron of the carbon nano tube is directly related to temperature of the CNT as resistivity of CNT depends on quantum state and also found to depend on temperature. Finally, an effort has been made to find an approximate expression for the temperature co-efficient of resistance of the CNT.

**Index terms (keywords)** : Debye temperature, electrical conductivity, temperature co-efficient of resistance, quantum state

## I. INTRODUCTION

It has been already established {see for instance [1]} when CNT is extremely narrow (thin) for a very thin conductor

$\frac{1}{A^2} \ll L$  where A is the area of cross section and L is the length of the potential well, the total energy of a single electron in side a one dimensional well of infinite depth is

given by,  $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$  .....(i) 'm' is the mass of the

electron.

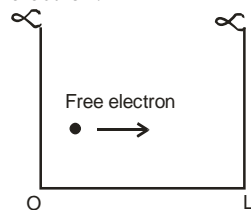


Figure-01

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For one electron system, electron spatial density

$$N_n = \frac{1}{AL} \dots\dots\dots(ii)$$

Many experiments show that CNT are ballistic conductor [2], [4]; therefore velocity of the electron in the  $n$ th quantum state

$$v_n = \frac{nh}{2mL} \dots\dots\dots(iii)$$

Introducing transit time of the electron in nano tube

$$\tau = \int_0^L \frac{dx}{v_n} = \frac{L}{v_n}$$

$$\tau_n = 2m \frac{L^2}{nh} \dots\dots\dots(iv)$$

With the help of (i), (ii), (iii) and (iv) we could readily establish the relation for conductivity for CNT.

$$\sigma_n = \frac{2Le^2}{Anh} \quad \text{or}$$

$$\rho_n = \frac{Anh}{2Le^2} \dots\dots\dots(v)$$

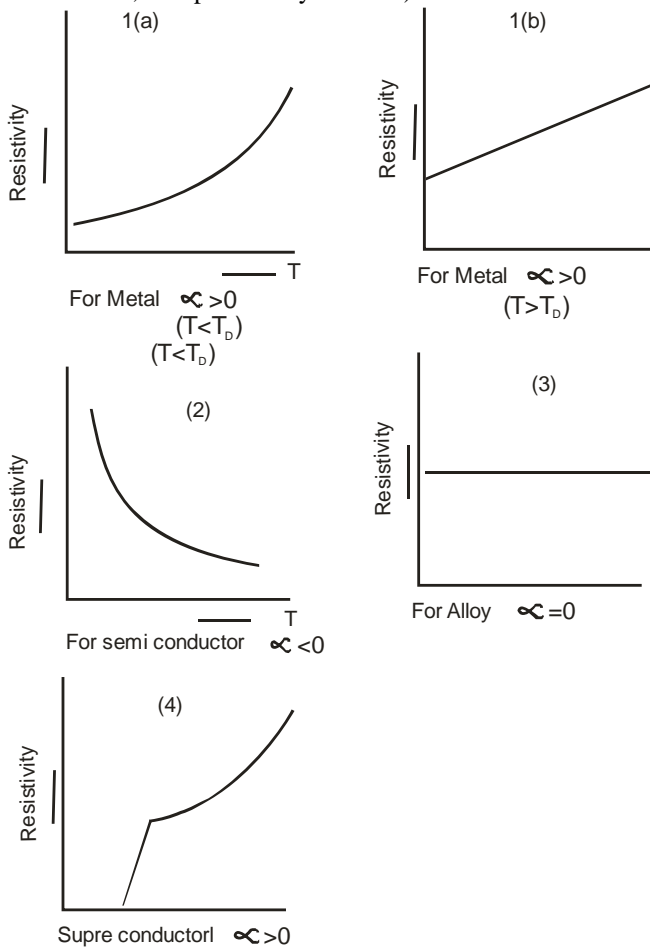
Since the resistivity is quantized so we must respect its quantum nature and hence resistivity has been denoted by  $\rho_n$  replacing ' $\rho$ '

But point to be noted regarding the behavior of the electrical conductivity of the metallic conductor. "The resistivity of metal at room temperature is of the order  $10^{-7}$  ohm meter and above ( $T_o$ ) Debye's temperature resistivity varies linearly with temperature i.e  $\rho \propto T$ .....(\*) but at very low temperature resistivity of pure conductor increases as higher power of temperature and for most of the metallic conductor at very low temperature  $\rho \propto T^5$ .....(\*\*), T is the absolute temperature. This variation of the resistivity with temperature can easily be represented by a specific dimensional physical quantity which needs to be introduce shortly. In fact, this quantity is very important dimensional quantity ' $\alpha$ ' called temperature co-efficient of resistance which is defined as change in resistance of the conductor per unit resistance per degree centigrade rise of temperature. For metallic conductor ' $\alpha$ ' is found to be positive and for insulator and for most of semi conductor ' $\alpha$ ' is negative. Thus, ' $\alpha$ ' (temperature co-efficient of resistance) is an indicator to mean and characterize the nature of electrical conductivity of a material.

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For most of the materials of one kind obeys their respective variation of  $\rho$  with temperature (T) which have been shown through the graphs.

(The following graphs are observed experimentally in most of the cases, exceptions may be there)



## II. THEORY

With the help of relation (v) we can find the quantum resistance of the carbon nano tube which is given by

$$R_n = \rho_n \frac{L}{A} = \frac{Anh}{2Le^2} \times \frac{L}{A}$$

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

$$R_n = \frac{nh}{2e^2} \dots\dots\dots(vi)$$

Let us now, bounce back to simply define  $\alpha$  (temperature co-efficient of resistance) Let,  $R_T, R_0$  be the resistance at  $T^\circ C$  and  $T_0^\circ C$  respectively then,

$$\alpha = \frac{R_T - R_0}{R_0 (T - T_0)} \dots\dots\dots(vii)$$

Since, we have experimental evidence for a range of temperature, that temperature variation results in change of the resistance, see for instance graphs 1(a),1(b), 2, 3, 4. The same happens to carbon nano tube and temperature dependence resistivity of CNT is now well established known property [4]. Relation (vi) makes it clear that  $R_n$  depends on the quantum state of the electron of CNT. But

we have just cited with proper evidences [4] and experimental graphs 1(a),1(b), 2, 3, 4 that the resistance and hence the resistivity of conductor including carbon nano tube depends on temperature. Therefore we can empirically and theoretically justify that variation of temperature has an impact on Resistance (R) but (iv) shows that  $R_n \propto n$ . But in carbon nano tubes as well as in other conductors the resistivity of the material depends on the number density of the electrons and average relaxation time which is given by the relation  $\rho_n = \frac{m}{N_n e^2} \tau$  but more

accurately for CNT  $\rho_n = \frac{m}{2N_n e^2} \tau_n$  [3]. It follows that the

resistivity of carbon nano tubes is inversely proportional to the average relaxation time of the free electron, since it is not a constant parameter and changes with change in temperature of the CNT. In fact, if the temperature of the CNT increases the amplitudes of the vibration of the lattice ions increase in addition to the increase of the speeds of free electrons. Consequently, free electrons collide more rapidly with vibrating lattice ions results in decrease of the relaxation time. Therefore, resistance of the tube increases as the temperature increases. Empirically as well as experimentally it can be perceived that temperature has an impact on the quantum relaxation time  $\tau_n$ , quantum resistivity  $\rho_n$  whereas  $\tau_n$  and  $\rho_n$  are all found to depend on the quantum state  $n$ . Thus, it is reasonable to think that once temperature is change this physical quantities  $\rho_n, \tau_n$  and  $R_n$  are to be changed. But since we respect quantum nature of  $\rho_n, \tau_n$  and  $R_n$  (see result iv, v and vi) with special reference to CNT hence,  $\rho, \tau, R$  to be replaced by  $\rho_n, \tau_n$  and  $R_n$  so, change of temperature can be attributed to change of quantum state. In other words, 'n' quantum state ( $n = 1, 2, 3, \dots$ ) is a function of temperature. If ' $R_T$ ' is resistance at temperature  $T^\circ C$  corresponding to the quantum state  $n$ , Similarly  $R_0$  is the resistance at temperature  $T_0^\circ C$  corresponding to quantum state  $n_0$ . So,

$$R_T = \frac{nh}{2e^2} \quad \text{and} \quad R_0 = \frac{n_0 h}{2e^2} \quad . \text{ So, relation (vii) can be put in}$$

$$\text{terms of the quantum state. } \alpha = \frac{\left( \frac{nh}{2e^2} - \frac{n_0 h}{2e^2} \right)}{\frac{n_0 h}{2e^2} \times (T - T_0)}$$

$$\text{Or, } \alpha = \frac{(n - n_0)}{n_0 (T - T_0)} \dots\dots\dots(viii)$$

$$\alpha = \left( \frac{n}{n_0} - 1 \right) (T - T_0)^{-1}$$

$$\Rightarrow (T - T_0) \alpha = \frac{n}{n_0} - 1$$

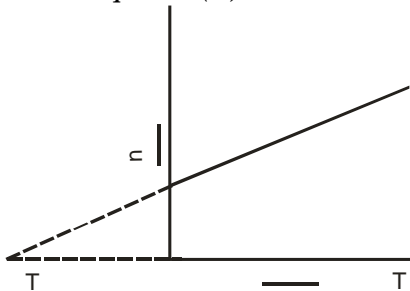
$$\Rightarrow \frac{n}{n_0} = (T - T_0) \alpha + 1$$

$$\Rightarrow n = \frac{1}{n_0} (T - T_0) \alpha + \frac{1}{n_0} \dots\dots\dots(ix)$$

For a given initial quantum state  $n_0$ , temperature  $T_0$  is

constant thus if we plot a graph between  $n$  and  $T$  or  $(T - T_0)$ , then the graph is a straight line intercepting 'n'(quantum axis) axis at a distance  $\frac{1}{n_0}$  from the origin with slope  $\frac{\alpha}{n_0}$ .

Therefore **Quantum state 'n' varies linearly in accordance with the equation (ix)**



Graph-5

Here, point to be noted that temperature co-efficient of resistance has been assumed constant for a wide range of temperature and it is logical to assume which is evident from experimental result and table no. 1

**Table for Resistivity and Temperature Co-efficient of Resistance at 0° and 20°c 0**

**Table No-1**

Material	Resistivity $\rho$	Resistivity $\rho$	$\alpha$ at 0°c	$\alpha$ at 20°c
Metal	$\times 10^{-8} \Omega m$	$\times 10^{-8} \Omega m$	$\times 10^{-3} / ^\circ C$	$\times 10^{-3} / ^\circ C$
Silver	1.6	~1.6	~3.8	~3.8
Copper	1.7	~1.7	~3.9	~3.9
Aluminum	2.7	~2.8	~3.9	~3.9
Gold	2.42	~2.4	~3.4	~3.4
Iron	10	~11	~5	~5
Platinum	11	~11	~3.92	~3.92
Tungsten	56	~5.6	~4.5	~4.5
Material semiconductor	Resistivity $\rho$	Resistivity $\rho$	$\alpha$ at 0°c	$\alpha$ at 20°c
Carbon	$3.5 \times 10^{-5}$	$\sim 3.5 \times 10^{-5}$	$-0.5 \times 10^{-3}$	$-0.5 \times 10^{-3}$
Germanium	0.46	~0.5	$-48 \times 10^{-3}$	$-48 \times 10^{-3}$
Silicon	2300	~1000	$-75 \times 10^{-3}$	$-75 \times 10^{-3}$
Material Insulators	Resistivity $\rho$	Resistivity $\rho$	$\alpha$ at 0°c	$\alpha$ at 20°c
Wood	$10^8 - 10^{11}$	$\sim 10^8 - 10^{11}$	-	-
Glass	$10^{10} - 10^{14}$	$\sim 10^{10} - 10^{14}$	-	-
Mica	$10^{11} - 10^{15}$	$\sim 10^{11} - 10^{15}$	-	-
	$\Omega m$ =ohmmeter	$\Omega m$ =ohmmeter	$^\circ C =$ per degree celcius	(-) means data is not available

**Remarks :**

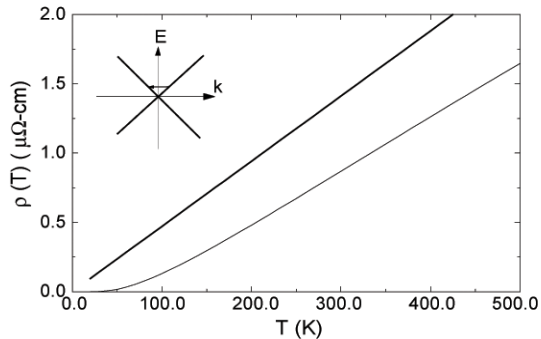
1. If the initial quantum state is known somehow corresponding to given initial  $T_0$  and then knowing the value of temperature co-efficient from the experimental data or table, we can find the higher order of quantum state of CNT provided the corresponding temperature is known and vice versa.
2. If we suppose  $n=0$  for the sake of argument, it would lead us to have value of quantum resistance  $R_n=0$  i.e.

$\rho_n = 0$ , i.e CNT behaves as super conductor, perhaps this super conducting state is not achieved, in CNT. Hence,  $n=0$  is restricted. On the other hand classically speaking at  $T=0^\circ K$ , the resistance approaches 0, thus we may expect at this point  $n=0$  and the ground state of the electron in CNT is more likely to be  $n=1$ . On the other hand classically speaking at  $T=0$  K, The resistance of the CNT approaches zero, then we may expect at this point  $n=0$  but  $n=0$  is restricted in CNT as at the beginning of our theoretical work we considered one dimensional potential of infinite depth. Therefore two consequences might come out from the theoretical approach;( i)one is that even if  $T=0$  K(Absolute temperature) is achieved, yet resistance of CNT does not vanish. Unless and other wise  $n=0$  That is even we have  $T=0K$  still we are not having super conducting state.(ii)Secondly, if the surrounding of the electrons within CNT is at 0 yet the electron in the lattice may not be cooled down to zero degree Kelvin, there by preserving its inherent quantum nature  $n \neq 0$ , therefore resistivity is retained even although the surrounding of the tube is at absolute zero Kelvin temperature. But, these two striking facts deserve special attention from the researcher to ascertain whether my points are trustworthy or not.

3. Apart from this, in one dimensional theory of scattering of electrons by twistons which predicts then intrinsic resistivity varies directly with temperature[4], more over, calculated temperature dependence resistivity due to twistons scattering including both one dimensional and three dimensional case, we have been able to observe  $\rho \propto T$ . In research paper [4], it has been shown for three dimensional model of the nano tubes  $\rho \propto T$  for  $T > 100K$ , which is well below the Debye temperature  $T_D$ . To test the validity of the theory of their works, the researcher compared their results with experimental results which were almost in harmony except a few exceptions which are perhaps due to the structural composition and dimensional aspects. As an evidence we forward here with my paper the observed variation of the resistivity with temperature and the theoretical plotting of the graphs as follows from ref.[4].If we ignore the factors affecting linear behavior of the resistivity and considering merely ideal one dimensional potential well subject to the condition  $\sqrt{A} < L$  and  $\alpha$  is a constant over a wide range of temperature, then in contrast to the observed and theoretical works[4] experimental results then we could assure you the linear temperature dependence of the quantum state.. in CNT.  $\alpha$
4. At  $T=0K$ , equation reduces to  $n = \alpha T / n_0 + 1/n_0$
5. The assumption made at the beginning  $A^2 \ll L$  and presumption that  $\alpha$  is a constant for wide range of temperature in CNT may not be achieved because of its structural defects as it has been observed that rolling of graphene sheet on nano meter scale has dramatic consequences on the electrical property of the carbon nano tube as well as on the mechanical property.[6] Apart from this in one dimensional theory of scattering of electrons by twistons which predicts the intrinsic resistivity varies directly with temperature [4], Moreover, calculated temperature dependence

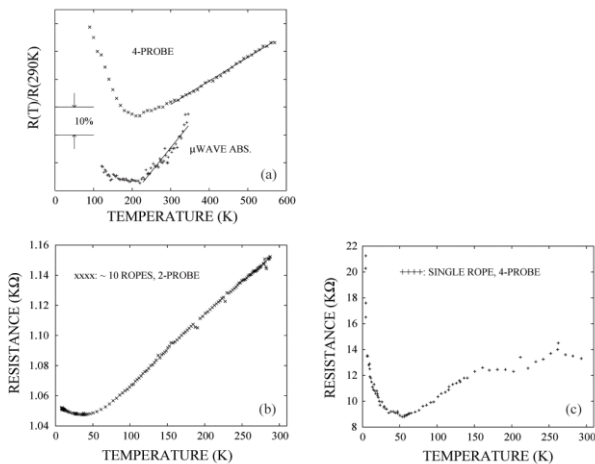
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resistivity due to twiston scattering including both one and three dimensional cases, we have been able to observe that  $\rho \propto T$ . In paper [4] 3D model assured that  $\rho \propto T$  for  $T > 100$  K, which is below the Debye temperature.[4] To test the validity of the temperature dependence of resistivity experiment were carried on which were in harmony with the theory.



Graph-5

Calculated temperature dependent resistivity due to twiston scattering. The upper Bold curve is calculated for one dimensional model for which  $\rho \propto T$ . Including 3D (three dimensional) inter tubes effects in both the electrons and twiston degrees of freedom we obtained the lower curve which shows  $\rho \propto T$  in 3D sample relatively above low crossover temperature.[4]



Graphs-6

Measured resistivity of samples of CNT (a) Bulk material. The top curve is a 4probe measurement. The lower curve is measured by microwave absorption. (b) 2 probe measurement on several ropes of CNT in parallel (c) 4Terminal measurement of a single rope. N.B.- graphs (5) and (6) have been extracted from the research paper [2]

## CONCLUSION

With our semi classical approach, despite of its adequate simplicity, we have tried to simulate the observed temperature dependence resistivity which in turn establishes the linear dependence of the quantum state of the electron in CNT under a few restrictions such as  $\sqrt{A} < L$  and  $\alpha$  is a constant over a wide range of temperatures and conditions. Perturbation to the small extent of the presumptions and conditions of the physical aspects in internal structures in CNT may slightly change the

conclusive result and hence may perturb the quantum behaviour of the CNT. Finally in short, the exceptions to our result if any, can be attributed to the structural defects and internal interactions arising out of electro electron interactions, electron ions interactions and interactions of the composite layers or ropes of the tubes et[2]and[4]c. It is .how ever logical to argue that linear electrical behavior of single wall one dimensional carbon nano tubes still holds good in ideal situation which can be a fruitful starting point of further researches.

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