QUANTUM TRANSPORT IN THE SINGLE WALL CARBON NANOTUBE QUANTUM DOTS

Abstract

The transport properties of carbon nanotubes can be dealt with using Tylor's series, Boltzmann transport equation and Boltzmann's H – theorem and other. The density of stateand energy dispersion relation represent the metallic and semiconducting characteristics of the carbon nanotubes explained by band gap.The quantum dot and electro-chemical potential deduce the electron transport related to single electron energy.The effect of scattering is on the transport characteristics in scattering potential can be calculated by Fermi's – Golden rule that gives scattering of phonon modes. The phonon modes are observed with ballistic transport related to single electron in single wall carbon nanotube quantum dots.

Keywords: Carbon Nanotubes, Boltzmann Transport, Band gap, Energy Dispersion, Quantum Dots.

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I. INTRODUCTION

Tylor's series[1-5] gives the transport properties that is used for Boltzmann transport equation. Density of state[7] explains the characteristics of the carbon nanotubes with the dispersion relation[6]. The molecules have wave nature shown by the Boltzmann transport equation with H – theorem. At discreet energy level, the transport characteristics is shown by the quantum dot that has zero – dimensional structure and it is related to single electron energy. Kumar and Kumar[6]has been given the theory for propagation of wave and absorption of energy that now shown the charging energy depends on or independent from the length of CNTs. Surface conductivity[7] of MWCNT is shown by the integral equation method. The conductivity of CNTs is compared with copper for the high frequency[8]. The electron transport is predicted by White and Todorov[9] through nanowires. The coulomb interactions[10]are explained for nanotubes.

An expression given by Amar and Kumar[11] for quantum conductance[12-13] of metallic CNTs is derived and dominated by transport using back scattering process that represents electron – electron interaction with phonon. The dispersion relation of phonon[14] for CNTs are calculated by many body that is used in this paper.Ab initio method[15] for lattice dynamics and Franck – Condon based model[16] for carbon nanotube with phonon mode are explained. Ando and et.al., give Berry's phase[17] in the single wall carbon nanotube with absence of back scattering.The transport characteristics are affected by scattering.

II. TYLOR'S SERIES:

If f(x) is a function up to $(n+1)^{st}q$ – derivatives in the interval [a, b] then expression near $x = x_0$in [a, b] written as

$$f(x) = f(x_0) + D_q f(x_0)(x - x_0) + D_q^2 f(x_0)\frac{(x-x_0)^2}{2!} + D_q^3 f(x_0)\frac{(x-x_0)^3}{3!} + \ldots\ldots\ldots\ldots\ldots\ldots + D_q^n f(x_0)\frac{(x-x_0)^n}{n!} + D_q^{n+1} f(x_0)\frac{(x-x_0)^{n+1}}{(n+1)!} \quad (1)$$

Where, exponent of $D_q$shows the first, second, third, …… $(n+1)^{st}$ derivatives of f(x) evaluated at x_0.

The term $D_q^{n+1} f(x_0)\frac{(x-x_0)^{n+1}}{(n+1)!}$ is term as remainder term. The expiration (5) is the Tylor's series. If the function $f(x) = \chi(y_0 + \lambda\cos\theta)$, Tylor's series written as

$$\chi(y_0 + \lambda\cos\theta) = (x_0 + \lambda\cos\theta)\left(\frac{d\chi}{dy}\right)_{y_0} \quad (2)$$

If the function $f(x) = \chi(y_0 - \lambda\cos\theta)$, the Tylor's series expressed as

$$\chi(y_0 - \lambda\cos\theta) = (x_0 - \lambda\cos\theta)\left(\frac{d\chi}{dy}\right)_{y_0} \quad (3)$$

1. **Boltzmann Transport Equation:** Consider the homogeneous electromagnetic fields in the caron nanotube in z – direction. The Boltzmann transport equation for electrons is written as

$$v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z} - \left(\frac{eE_x}{m} + \frac{e}{c}\frac{v_x}{m} H_z\right)\frac{\partial f}{\partial v_x} - \left(\frac{eE_y}{m} + \frac{e}{c}\frac{v_x}{m} H_z\right)\frac{\partial f}{\partial v_y} = \left(\frac{\partial f}{\partial t}\right)_{cool} \quad (4)$$

The Boltzmann transport equation is written in integral-differential form as

$$\frac{\partial f_1}{\partial t} + v\nabla_r f_1 + a\nabla_v f_1 = \iiint \left(f_1' f_2' - f_1 f_2\right) gb\, db\, d\varphi\, dv_2 \quad (5)$$

Where $f_1 \equiv f(r, v_1, t)$, $f_1' \equiv f\left(r, v_1', t\right)$, $f_2 \equiv f(r, v_2, t)$, $f_2' \equiv f\left(r, v_2', t\right)$

We have the Boltzmann - H function, $H = \int f \ln f \, dr dv$ and we obtain

$$\frac{dH}{dt} \leq 0 \quad (6)$$

Relation (6) is known as Boltzmann H −theorem.

Let the transport property be χ associated with molecule then at $y_0 \pm \lambda \cos\theta$ where $y_0$is the plane of particle, the transport property of a particle be $\chi_0$can be expressed by the Taylor series expansion (2) and (3) and we get net transport χ per unit area per second is

$$J_\chi = \int \chi\, v.\, \hat{n}\, f(v)\, dv \quad (7)$$

The net flux of χ, J_χ crossing $y = y_0$ surface is given by

$$J_\chi = -\frac{1}{3}\rho\langle v\rangle\lambda\left(\frac{d\chi}{dy}\right)_{y_0} \quad (8)$$

2. **Density of State:** The single layer of graphite in a flat honeycomb hexagonal structure determined by C – C bond is graphene. The energy dispersion relation for graphene sheet calculated by Wallace [13] by using the scheme of tight binding (see in figure 1) given as

$$E = \gamma_0 \left\{1 + 4\cos^2\left(\frac{k_y a}{2}\right) + 4\cos\left(\frac{\sqrt{3}\,k_x a}{2}\right)\right\}^{1/2} \quad (9)$$

For carbon nanotubes density of states described as

$$D(E) = \frac{\sqrt{3}a^2}{2\pi R}\sum_k \int \left|\frac{\partial E}{\partial K}\right|^{-1} (K - K_i)\, dK \quad (10)$$

On expanding the relation (9) around Fermi surface and obtained [15] as

$$D(E) = \frac{a\sqrt{3}}{\pi^2 \gamma R} \sum_{m=1}^{N} \frac{|E|}{\left(E^2 - \epsilon_m^2\right)^{1/2}} \quad (12)$$

Where $\epsilon_m = |3m + 1|\left(\frac{a\gamma}{2R}\right)$ shows the semiconducting properties of carbon nanotubes and $\epsilon_m = |3m|\left(\frac{a\gamma}{2R}\right)$ shows the metallic properties of carbon nanotubes. With the crossing plane passing through K point and then the carbon nanotube will have finite density of state at Fermi energy $(E_f = 0)$ is explained by Fermi – Dirac statistics given by

$$f(E) = 1/[1 + e^{(E - E_f)/K_B T}] \quad (13)$$

The band gap of semiconducting carbon nanotube depends on dimeter given by

$$E_g = \frac{\sqrt{a}}{R} \quad (14)$$

In graphene, the dispersion is directly proportional to the Fermi velocity of electrons near

K points $v_f = 8 \times 10^5$ m/s[15] given as

$$\frac{dE}{dK}|_k = \hbar v_f \quad (15)$$

3. **Quantum Transport in the Carbon Nanotubes:** The transport properties of carbon nanotubes as the quantum systems having zero - dimensional structure called quantum dots at the discreate energy levels arise because of quantum confinement. The quantum dot and electro-chemical potential deduce the electron transport related to single electron energy U_c or $\Delta E \gg K_B T$. The energy within metallic carbon nanotube of length l can be estimated as

$$\Delta E = \frac{\partial E}{\partial K_{||}} \frac{\Delta K_{||}}{2} = \hbar v_f \frac{\pi}{2l} = \frac{h v_f}{4l} = \frac{0.8\, MeV}{l\ (\mu m)} \quad (16)$$

Where at Fermi level of carbon nanotube, the factor 2 has come from the two degenerate one dimensional sub bands. The Boltzmann equation can be written for quantum transport as

$$\frac{\partial f_1}{\partial t} + v \cdot (\nabla)_r f_1 + a(\nabla)_v f_1$$

$$= \iiint \left[f_1' f_2' (1 + \theta f_1)(1 + \theta f_2) - f_1 f_2 \left(1 + \theta f_1'\right)\left(1 + \theta f_2'\right)\right] \alpha(g, \chi) \sin\chi \, d\chi \, d\varphi \, dv_2 \quad (17)$$

Where $\alpha(g, \chi)$ is called the scattering probability. This equation (17) shows the wave nature of carbon molecules. So, surface wave propagates on a bundle of CNTs. The effect of scattering is on the transport characteristics in scattering potential can be calculated by Fermi's – Golden rule written as

$$W_{fi} = \frac{2\pi}{\hbar}|V_{fi}|^2 \cdot \delta(E_f - E_i) \quad (18)$$

Where V_{fi} is the scattering potential final state to initial state.

III. RESULTS AND DISCUSSION

Equation (9) of dispersion relation along high symmetrical point of reciprocal space if E_0 = 0 shown by figure 1. At K points, the two bands meet and known as valence and conduction band. So, K point behaves as Brillouin zone.

The calculation of energy dispersion and density of state of graphene have been performed with the calculation of ab initio and tight binding. We obtained the results with dispersion near at K points for the electron transport through the carbon nanotubes is proportional to the electrons Fermi velocity. At Fermi level the band structure makes metallic single walled carbon nanotube quantum dots depending on temperature and length and transport occurs in T – L liquid regime or coulomb blocked regime.The scattering potential can be a screened or non-screened Coulomb potential due to charged impurities. Metallic single wall carbon nanotubes have long mean free path at room temperature and it is suppressed back – scattering due to armchair as the results. On transport properties of single walled carbon nanotubes, the impurities, and pair of penta-hepta-gone are affected the electrical transport characteristics of metallic single wall carbon nanotubes away from the Fermi level shown in figure 2(a).

The short-range potential for vacancies affects the transport nearer to the Fermi level represented in figure 2(b). The vacancy defects with ion irradiation influences on resistance of the nanotube. Phonons are the main source of the scattering by equation (18) or Fermi's golden rule in defects of single walled carbon nanotubes at high temperatures. The modes of phonon have been studied by theoretically and experimentally with Raman spectroscopy.

Equation (16) shows the charging energy is approximately six times larger than the energy level in the quantum dots of single walled carbon nanotubes which is independent of length and the number of electrons in metallic single walled carbon nanotubes. If the charging energy depends on the length, it is inversely proportional to the length which is expressed in figure 3 shows that for larger length of nanotubes the charging energy will be small.

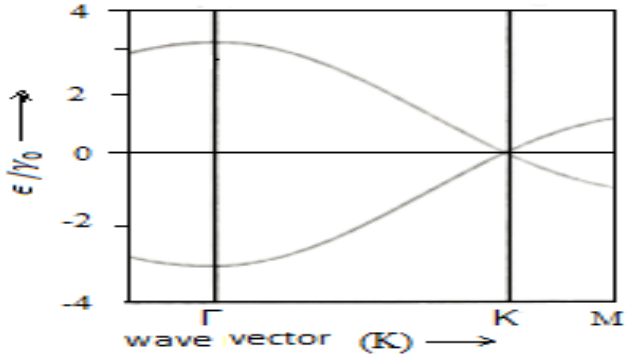

Figure 1: Energy dispersion of the graphene and gives Density of state for metalic and semiconducting propreties of carbon nanotube.

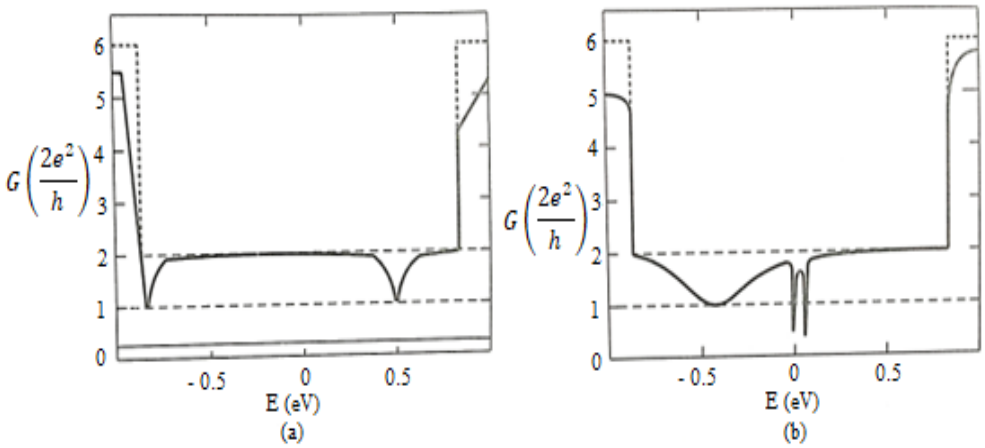

Figure 2: Conductance of the armchair single – walled carbon nanotube [12-13].

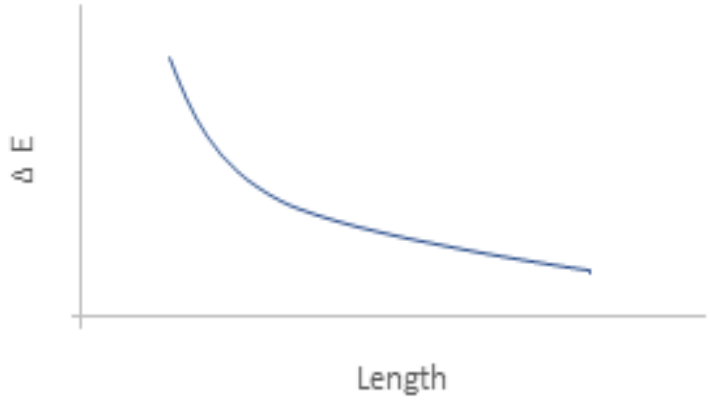

Figure 3: Plot of variation the charging energy with length of nanotubes.

IV. CONCLUSIONS

Density of state gives the metallic and semiconducting properties. Transport properties for carbon nanotubes using Boltzmann equation gives the wave nature of molecules and we have scattering potential by Fermi's – Golden rule.When the length of nanotube will be finite, $K_{\|}$ is quantized and leading the discrete energy levels in quantum dot. The coupling of the suspended single wall carbon nanotube quantum dot with phonon modes have observed. The single electron charging becomes negligible, the recovery of single wall carbon nanotube will be as one-dimensional quantum wire of electron wave guide and electron waves demonstrates the ballistic transport in the single wall carbon nanotubes. The transport properties related to single electron are observed when the energy ΔE is larger than the thermal energy K_BT.

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