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Chapter

Theoretical Approach of the Propagation of Electromagnetic Waves through Carbon Nanotubes and Behavior of Carbon Nanotubes as Capacitor using Electric Hertz Potential

Jay Shankar Kumar and Ashok Kumar

Abstract

The electromagnetic waves and its propagation through material medium described by maxwell's equations. We have identified that electromagnetic waves propagate through carbon nanotubes according to electric hertz potential with solution of Helmholtz equation and satisfied by using the concept of Gaussian beam or wave. When monochromatic electromagnetic wave propagates through a hollow single wall carbon nanotube, its energy absorbed by walls of nanotubes just like a capacitor because of carbon nanotubes have metallic as well as semiconductor characteristic which is shown by density of state and lattice vector. It is verified by Helmholtz equation and Schrödinger's wave equation. Thus, the electromagnetic waves can propagate through carbon nanotubes and carbon nanotubes absorb the energy as a capacitor.

Keywords: carbon nanotube, electromagnetic wave, electric hertz potential, Helmholtz equation, Schrödinger equation, Gaussian beam or wave, capacitor

1. Introduction

A new allotropes of carbon element is carbon nanotube which is in cylindrical form and made by folding of graphene sheet of graphite. By passing time, the various types of carbon nanotubes (carbon nano scrolls, carbon nano cones, carbon nano coils, carbon nanoribbon, carbon nanofibers, etc.) by variousare formed by various processes (Arc Discharge, Laser Ablation or Evaporation, Chemical Vapor Deposition (CVD), Plasma Enhanced Chemical Vapor Deposition (PECVD), etc.). The carbon nanotubes were discovered by S. Iijima in 1991 by fullerene synthesis [1, 2]. There are two forms of carbon nanotube. One is single walled carbon nanotubes that made up of rolling of graphene sheet and its dimeter vary from 0.7 to 3 nm and minimum dimeter

up to ~0.4 nm. The other nanotubes are multiwalled carbon nanotubes that are made up of multiple concentric cylinders and its dimeter range is of 10–20 nm and space is available between two layers (3.4 Å).

In atomic structure of carbon, six electrons are arranged according to electronic configuration $1s^2\ 2s^2\ 2p^2$ and designated as $1s^2$, 2 s, $2p_x$, $2p_y$, $2p_z$, if atoms bounded in molecules. In graphite sheet, carbon atoms bound together by sp^2 hybrid bonds and similarly, fullerenes, carbon nanotubes, and graphene are also formed by sp^2 hybrid bonds [3]. Graphene is a single layer carbon atoms of graphite and has 120^0 bond angle in hexagons with electronic structure characterized by π-bonds linear dispersion near Fermi surface (**Figures 1–3**). In a hexagonal lattice, the unit vectors $\vec{a}_1$ *and* $\vec{a}_2$ in the real space can be written as:

$$\vec{a}_1 = \frac{1}{2}a\left(\sqrt{3}, 1\right) \ , \ \vec{a}_2 = \frac{1}{2}a\left(\sqrt{3}, -1\right) \tag{1}$$

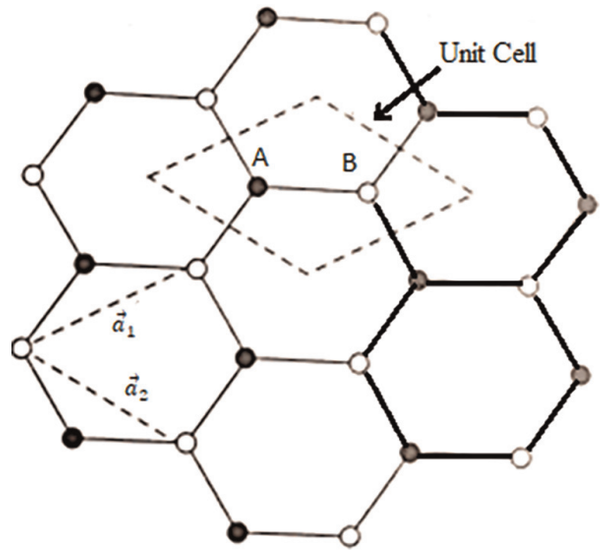

Figure 1.
Crystal structure of graphene with unit cell.

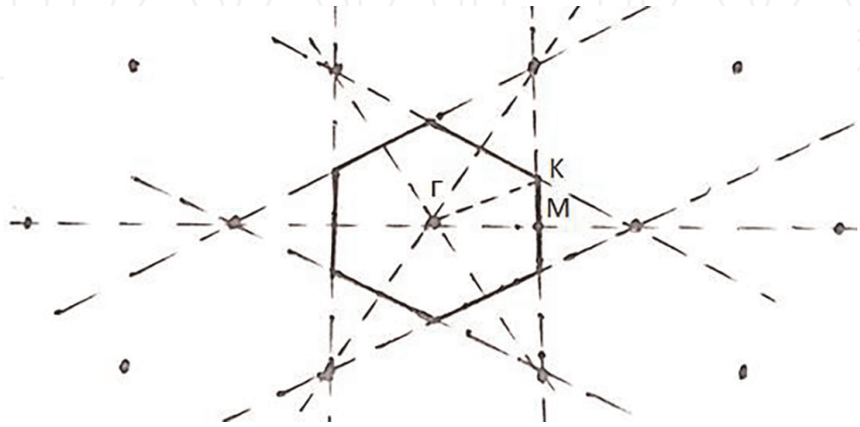

Figure 2.
Wigner-Seitz cell is a primitive cell which represents the Brillouin zone of the reciprocal lattice. To construct this cell, at first join the lattice point passing through central point and then join the other two lattice points each sides just like parallel the lines to both sides. The Brillouin zone of the graphene with location of the symmetrical points K, M and Γ.

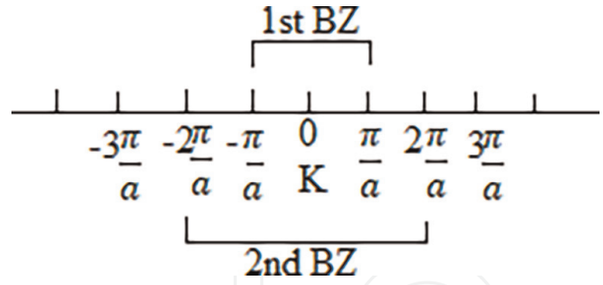

Figure 3.
The first two Brillouin zones of graphene for one dimensional.

Where, a represents the lattice constant and equal to $\sqrt{3}a_{c-c}$, here, a_{c-c} shows the bond length (0.144 mm) of carbon-carbon atom.

To describe quantum mechanical properties of the crystals in lattice the Brillouin zone were introduced and we can also describe the behavior of electrons in a perfect crystal on the concept of Brillouin zone. In reciprocal lattice space, a region where closest lattice point of primitive cell is the origin is known as the Brillouin zone (BZ). It is constructed by Wigner and Seitz and called Wigner-Seitz primitive cell i.e., Brillouin zone. In the Brillouin zone, the three symmetrical points is at the centre, corners, and centre edge. We have

$$K = \frac{n\pi}{a}, where, n = \pm 1, \pm 2, \pm 3, \ldots .etc. \tag{2}$$

The first and second Brillouin zone is defined between $K = -\frac{\pi}{a}$ *to* $K = +\frac{\pi}{a}$ in which electron has allowed energy value and $K = -\frac{2\pi}{a}$ *to* $K = +\frac{2\pi}{a}$ which is forbidden zone.

Carbon nanotube is formed by chiral and translation vector using chiral angle with indices (n, m) and (5, 5). Using Fourier series and transform and Schrödinger's equation, the Bloch theorem is determined with Brillouin zone. Bloch function helps to determine the determinant equation for Schrödinger's equation. The solution of this determinant equation gives energy dispersion over tight binding which shows the band structure of carbon nanotubes and taking wave vector components, metallic character found near Fermi point of graphene with Fermi energy of electrons. The density of state of carbon nanotubes is expressed by expanding the dispersion relation [4] around the Fermi surface. We have the condition for semiconducting and metallic carbon nanotubes near the K points that is proportional to the Fermi velocity $\left(v_f = 8 \times 10^5 \text{ m/s}\right)$ of the electrons in the graphene.

The Helmholtz equation [5] is obtained by curl of Maxwell's equations and its solution gives the plane monochromatic transverse wave [6, 7]. Helmholtz equation in cylindrical coordinate gives the Gaussian wave or beam and its spot size ensures that it can propagate through the cylindrical carbon nanotube. A monochromatic electromagnetic wave as radiation is called Gaussian beam that provided by a laser source [8]. The Gaussian wave represented by the amplitude function with very small spot size propagates through a carbon nanotube [9]. The parameters of Gaussian wave are the width, the divergence, the radius of curvature. The better beam quality and intensity is represented by the smaller angle of divergence. The propagation distance leads to intensity, spot size, radius of curvature and divergence [10].

When the wave travel through the carbon nanotube [11] then the inner surface of the carbon nanotube absorbs the energy of the wave as a capacitor and shown by the Schrödinger's and Helmholtz relation using the work-energy theorem.

2. Chiral and translation vector

Rolling up of graphene along the chiral vector as

$$\overrightarrow{C_h} = n\overrightarrow{a_1} + m\overrightarrow{a_2} \tag{3}$$

Where, n and m are integers and $\overrightarrow{a_1}$ *and* $\overrightarrow{a_2}$ are lattice vectors. The two corners K and K′ are the location of Dirac cones in the Brillouin zone. In reciprocal space, K and K′ are as

$$K = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right), \; K' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right) \tag{4}$$

Where, $a(\approx 1.42A°)$ is the distance of C-C.

In figure θ be the chiral angle between the chiral $\vec{C}_h$ *and* $\vec{a}_1$. The circumference of tube equal to $\vec{C}_h$ given by

$$\vec{C}_h = \frac{\sqrt{3}}{2}a(n+m)\hat{x} + \frac{1}{2}a(n+m)\hat{y} \tag{5}$$

In magnitude,

$$|\vec{C}_h| = a\sqrt{n^2 + m^2 + nm} \tag{6}$$

The dimeter d_T of the carbon nanotube obtained if $|\vec{a}_1| = |\vec{a}_2| = \sqrt{3}a_{c-c}$ (as)

$$d_T = \frac{\sqrt{3}a_{c-c}}{\pi}\sqrt{n^2 + m^2 + nm} \tag{7}$$

The chiral angle given as

$$cos\theta = \frac{m + 2n}{2\sqrt{n^2 + m^2 + nm}} \tag{8}$$

$$\text{And also } \; tan\theta = \frac{\sqrt{3}m}{m + 2n}, 0^\circ \le \theta \le 30^\circ \tag{9}$$

If the chiral angle is 30° then $n = m$ and the structure is armchair. $\vec{C}_h$ is obtained by the vector addition as $\vec{C}_h = 5\vec{a}_1 + 5\vec{a}_2$ (in **Figure 4**) and now the translation vector $\vec{T}$ is drawn perpendicular to the chiral vector $\overrightarrow{C_h}$ and expressed as (**Figures 5–9**)

$$\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2 \tag{10}$$

Where, t_1 and t_2 are components of vector $\vec{T}$ and they are written as

$$t_1 = \frac{2m + n}{d_T}, \; t_2 = -\frac{m + 2n}{d_T} \tag{11}$$

The Eq. (10) written as

$$\vec{T} = \frac{(m - n)}{d_T}\left(\frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}\right) \tag{12}$$

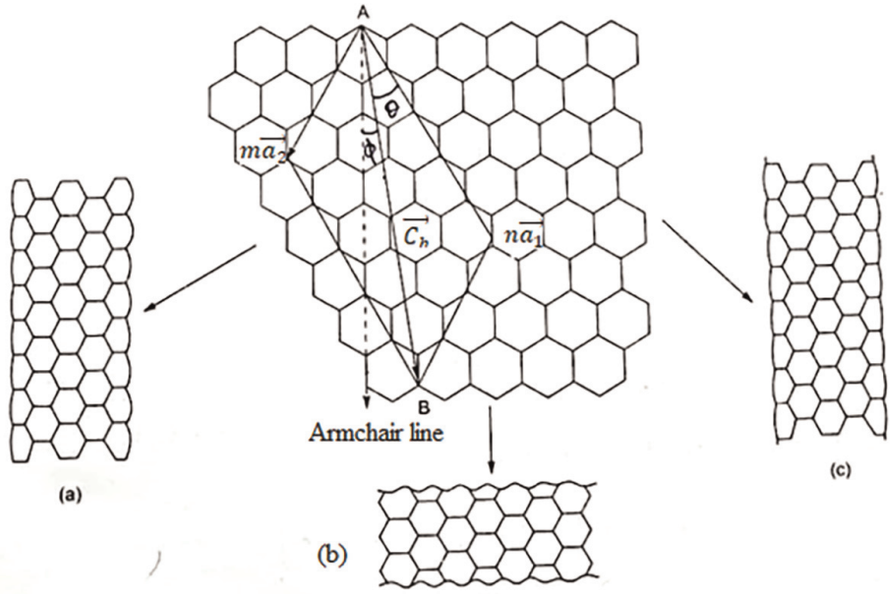

Figure 4.
Rolling graphene sheet along the chiral vectors (a), (b) and (c) show the armchair (m,m) zig-zag (n,0) and the chirl (n,m) nanotubes respectively.

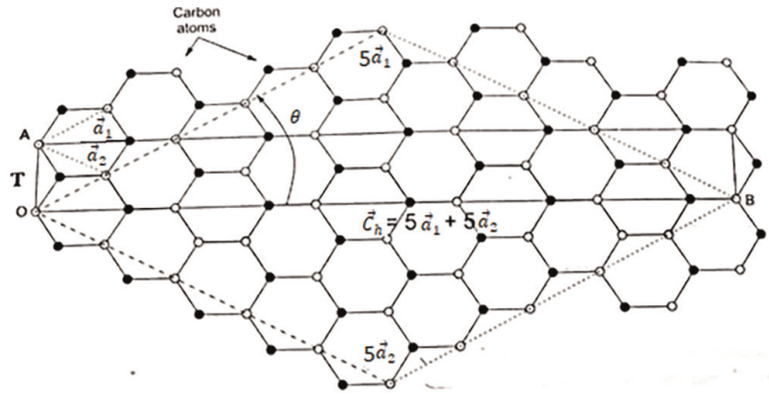

Figure 5.
The crystal structure of the carbon nanotube with the armchair (5,5) and rectangle shows the unit cell of the carbon nanotube and the angle between $\vec{C}_h$ *and* $\vec{a}_1$ *is* $0 < \theta < 30^\circ$ *called the chiral angle.*

In magnitude,

$$\text{In magnitude } |\vec{T}| = \frac{|\vec{C}_h|\sqrt{3}}{d_T} \tag{13}$$

In carbon nanotube the hexagons in unit cell of $a(n, m)$ is given by

$$N = \frac{2\,(n^2 + m^2 + nm)}{d_T} \tag{14}$$

3. Fourier series in carbon nanotubes

We have general Fourier series of sines and cosines for a periodic function $f(x)$ written as

$$f(x) = A_\circ + \sum_{f>0} A_f \cos\left(\frac{2\pi fx}{a}\right) + \sum_{f>0} B_f \sin\left(\frac{2\pi fx}{a}\right) \tag{15}$$

Where, the f is the positive integer and A_f and B_f are the real constants called Fourier coefficients. Consider the electron number density $n\left(\vec{r}\right)$ is a periodic function as $f(x)$ in the direction of crystal axes which invariant under translation $\vec{T}$. Thus

$$n\left(\vec{r}\right) = n\left(\vec{r} + \vec{T}\right) \tag{16}$$

The factor $\frac{2\pi}{a}$ ensures that $n(x)$ has a period $'a'$ (**Figure 6**);

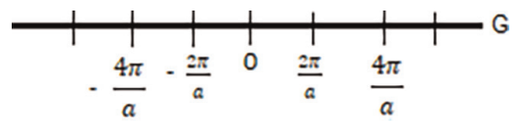

Figure 6.
The periodic function n(x) *of period* a *for the Fourier transform.*

$$n(x+a) = A_\circ + \sum A_f \cos\left(\frac{2\pi fx}{a}\right) + \sum B_f \sin\left(\frac{2\pi fx}{a}\right) = n(x) \tag{17}$$

For this condition, $\frac{2f}{a}$ is in Fourier space of the crystal and we can write the Fourier transform as

$$n(x) = \sum_f n_f e^{\frac{i2\pi fx}{a}} \tag{18}$$

Where, the sum is over all integers: positive, negative and zero. Similarly, the Fourier transform to periodic function $n\left(\vec{r}\right)$ in three dimensions with finding a vector set $\vec{G}$, such as

$$n\left(\vec{r}\right) = \sum_G n_G e^{i\vec{G}\bullet\vec{r}} \tag{19}$$

Where, $\vec{G}$ is a reciprocal lattice vector and expressed as

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3 \tag{20}$$

Where, v_1,v_2,*and* v_3 are integers and $\vec{b}_1$, $\vec{b}_2$, and $\vec{b}_3$ are the primitive vectors and also axis vectors of the reciprocal lattice and have the property $\vec{b}_i \bullet \vec{a}_j = 2\pi\delta_{ij}$, where, $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$.

The Fourier series for the electron density has the invariance under the crystal translation as $\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2 + t_3\vec{a}_3$. From (19),

$$n\left(\vec{r}+\vec{T}\right)=\sum_{G} n_G e^{i\vec{G}\bullet\vec{r}} e^{i\vec{G}\bullet\vec{T}} \tag{21}$$

4. The Schrödinger's equation and the bloch theorem

We have Schrödinger's wave equation in three dimensions as

$$-\frac{\hbar^2}{2m}\nabla^2\psi_k\left(\vec{r}\right)=\epsilon_k\psi_k\left(\vec{r}\right) \tag{22}$$

Where $\epsilon_k = E - U$, E is the kinetic energy and U is the potential energy. The potential function $U(r)$ has the period l of the lattice given as $U(r) = U(r+l)$. The wave function to be periodic in three dimensions with period l as

$$\psi(\rho, \theta, \varphi) = \psi(r+l, \theta, \varphi) \tag{23}$$

This is corresponding to $\psi(x, y, z) = \psi(r+l, y, z)$ because of angles are made with Cartesian axis. So, the form of a traveling plane wave given as

$$\psi_k\left(\vec{r}\right)=e^{i\vec{k}\bullet\vec{r}} \tag{24}$$

Where $\vec{k}$ is the wave vector and $= 0; \pm\frac{2\pi}{l}; \pm\frac{4\pi}{l}$. The solution of Schrödinger's wave equation for periodic potential given by Bloch as

$$\psi_k\left(\vec{r}\right)=u_k\left(\vec{r}\right)e^{i\vec{k}\bullet\vec{r}} \tag{25}$$

Where $u_k\left(\vec{r}\right)$ have the periods of the lattice with $u_k\left(\vec{r}\right)=u_k\left(\vec{r}+\vec{T}\right)=u_k\left(\vec{r}+l\right)$ and u_k is called the Bloch function. This expression (25) is the Bloch theorem (**Figure 7**).

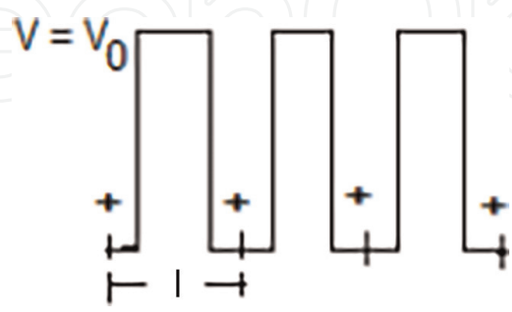

Figure 7.
The periodic potential distribution for the crystal.

When lattice translation carries $\vec{r}$ *to* $\vec{r}+\vec{T}$ then we have the form of Bloch theorem as

$$\psi_k\left(\vec{r}+\vec{T}\right)=e^{i\vec{k}\bullet\vec{T}}\psi_k\left(\vec{r}\right) \tag{26}$$

The Schrödinger's wave Eq. (22) also written as $\psi = \epsilon\psi$, where H,ψ, and ϵ are the Hamiltonian, the total wave function and the total energy of electron in π-orbital of graphene. The Bloch function u_k from $2p_z$ orbitals of atoms P and Q as

$$u_{P(Q)} = \frac{1}{\sqrt{N}} \sum_{P(Q)} e^{i\vec{k}\cdot\vec{r}_{P(Q)}} X\left(\vec{r} - \vec{r}_{P(Q)}\right) \tag{27}$$

Where $X\left(\vec{r}\right)$ is the orbital $2p_z$ wave function for the isolated carbon atom.

5. Energy dispersion for carbon nanotubes

We have determinant equation for Schrödinger's wave equation as

$$\begin{vmatrix} H_{PP}-\epsilon & H_{PQ} \\ H_{QP} & H_{QQ}-\epsilon \end{vmatrix} = 0 \tag{28}$$

$$\text{Here } H_{PP} = \int X^*\left(\vec{r} - \vec{r}_P\right) H X\left(\vec{r} - \vec{r}_P\right) d\tau = \epsilon_0 \tag{29}$$

$$\text{and } H_{PQ} = \left(e^{i\vec{k}\cdot\rho_1} + e^{i\vec{k}\cdot\rho_2} + e^{i\vec{k}\cdot\rho_3}\right) \int X^*\left(\vec{r}\right) H X(r - \rho_1) d\tau$$

$$= \gamma_0 \left(e^{-\frac{ik_x a}{\sqrt{3}}} + e^{\frac{ik_x a}{2\sqrt{3}}} \cos\left(\frac{k_y a}{2}\right)\right) \tag{30}$$

By the symmetry of graphene lattice, $H_{PP} = H_{QQ}$ *and* $H_{PQ} = H_{QP}$, now, we have the solution of the Eq. (28) given as

$$\epsilon = H_{PP} \mp |H_{PQ}| \tag{31}$$

From the Eqs. (29)–(31), the obtained energy dispersion relation as follows

$$\epsilon = \epsilon_0 \mp \gamma_0 \sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)} \tag{32}$$

Where γ_0 is the tight-binding or transfer integral. The negative sign represents the valence band of the graphene which is formed by π-orbitals bonding but the positive sign indicates the conduction band that is formed by π^*-orbitals antibonding. The energy dispersion of graphene is shown in **Figure 8**.

By expressing K_x and K_y in terms of components for band structure of carbon nanotubes of wave vector perpendicular and parallel to the tube axis and substituting in (32). We have

$$\epsilon(K) = \pm \sqrt{1 + 4\cos\left(\frac{3C_x Ka}{2C} - \frac{3\pi faC_y}{C^2}\right)\cos\left(\frac{\sqrt{3}C_y fa}{2C} + \frac{\sqrt{3}faC_x}{C^2}\right) + 4\cos^2\left(\frac{\sqrt{3}C_y Ka}{2C} + \frac{\sqrt{3}faC_x}{C^2}\right)} \tag{33}$$

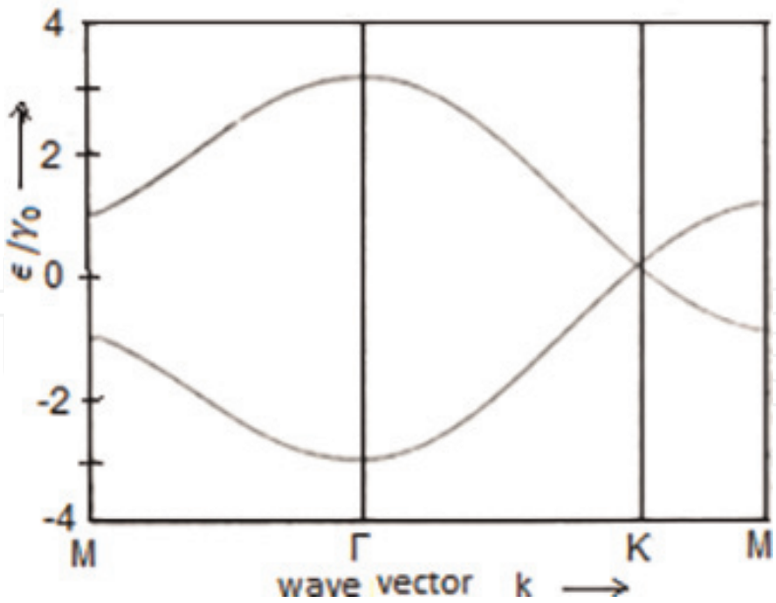

Figure 8.
Energy dispersion of the graphene in the reciprocal space along the symmetrical points.

Where K represents the wave vector along the axial direction and $C_x = \sqrt{3}a\left(n + \frac{m}{2}\right)$ *and* $C_y = \frac{3}{2}am$. For carbon nanotubes, the condition to be metallic of the allowed lines $\left(\frac{2\pi f}{C_y} - \frac{C_x}{C_y}K_x\right)$ cross one of the Fermi points of the graphene.

The band gap of the semiconducting carbon nanotubes depends on the diameter as shown in **Figure 9** and they are inversely proportional to each other. The relationship between the band gap and the radius or as diameter can be obtained in **Figure 10** by closing the two lines to the Fermi point of the graphene and given as (**Figures 11–20**)

$$\epsilon_g \simeq \frac{\sqrt{a}}{R_{CNT}} \tag{34}$$

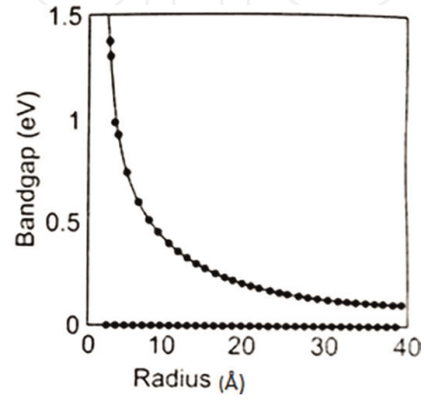

Figure 9.
The bandgap and radius for the zig-zag carbonnanotubes. The bandgap decreases with increasing the diameter for semiconducting carbon nanotubes.

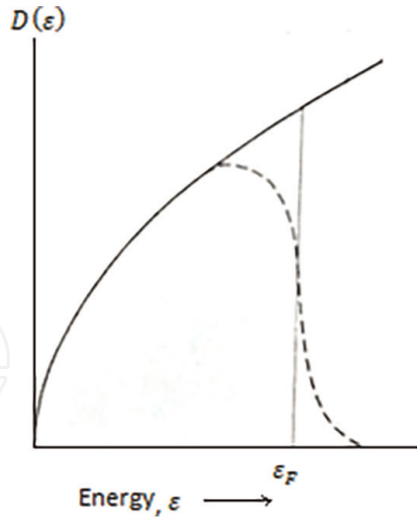

Figure 10.
Density of state as function of energy. The dashed curve shows the density at the finite temperature comparing with the Fermi energy ε_F at the absolute temperature.

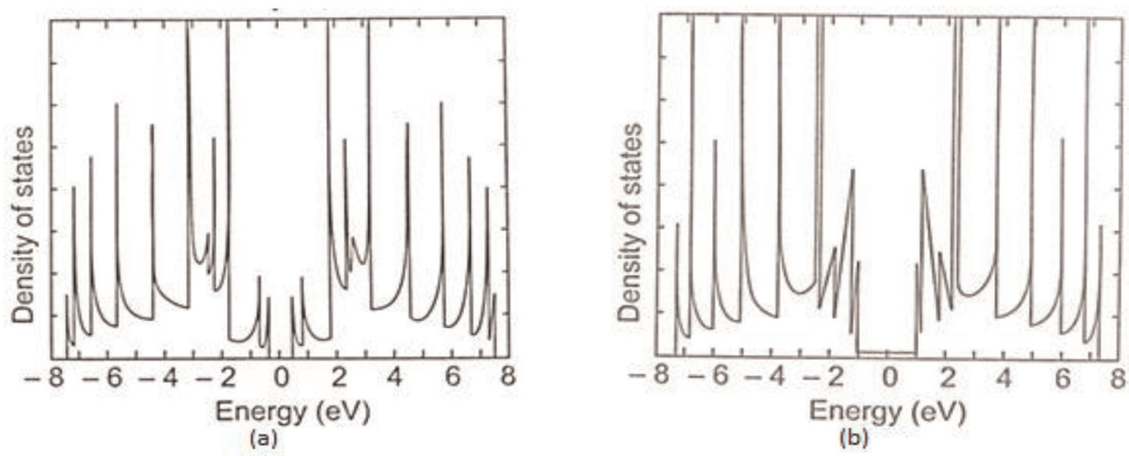

Figure 11.
Density of state for carbon nanotubes calculated from Eqs. (36) and (37) for the armchairs (11, 0) and (12, 0) of the carbon nanotubes and computed from the tight binding.

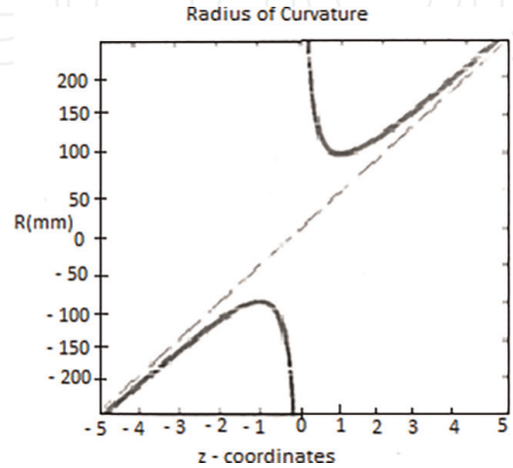

Figure 12.
Radius of curvature around beam waist position of Gaussian wave at a distance of $+z_R$ and $-z_R$ from beam waist. The point source is at beam waist along propagation, the radius of curvature is larger [9].

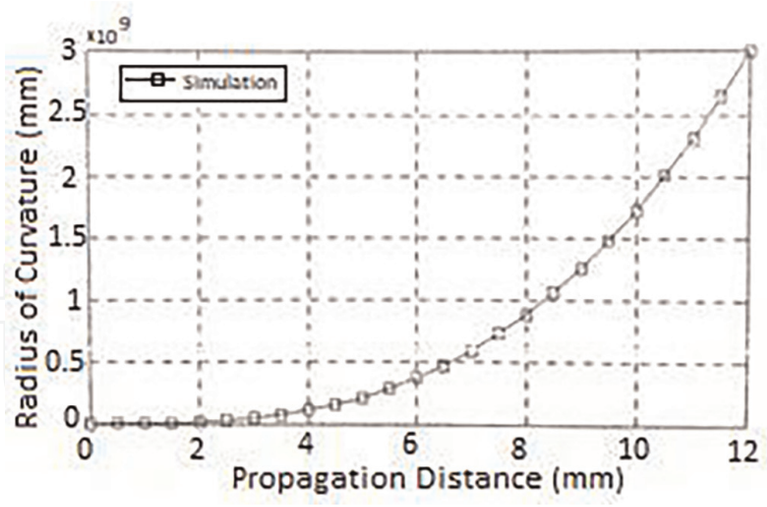

Figure 13.
Radius of curvature of Gaussian beam as a function of the propagation distance. The radius of curvature of the Gaussian beam is increased from 0mm to 2.99×10^9mm *for the propagation distance 0 mm to 12 mm. Therefore, the radius of curvature represents the linear variation with distance [10].*

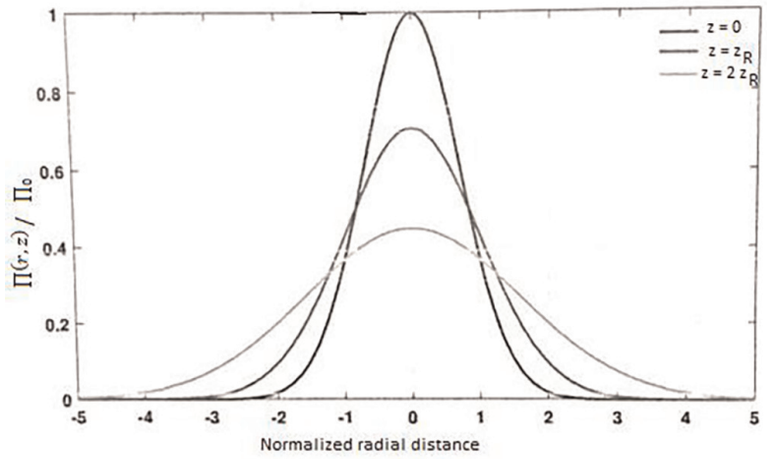

Figure 14.
The Gaussian wave along the radial direction for various "z".

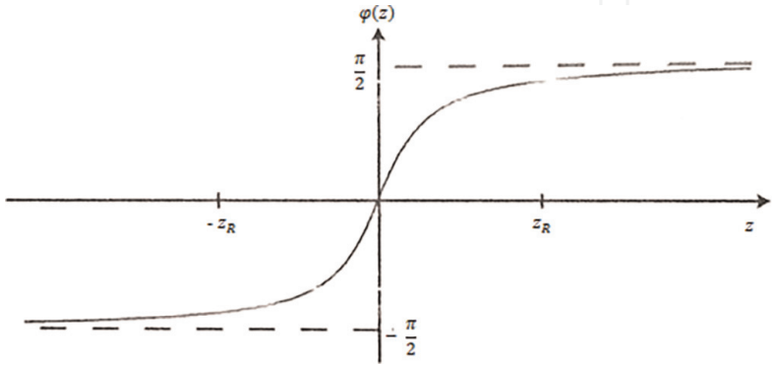

Figure 15.
Guoy phase shift around the Rayleigh length on both sides of the waist if the beam is at origin. There is the π phase shift in the Gaussian wave propagating from $z = -\infty$ to $z = +\infty$ *relative to the plane wave called the Guoy effect.*

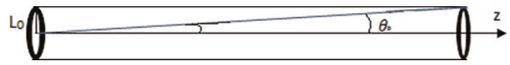

Figure 16.
Angle of divergence with z – axis.

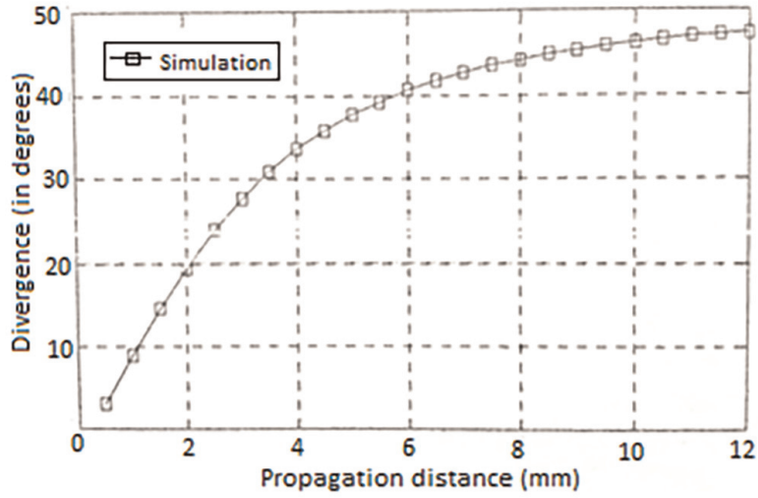

Figure 17.
Divergence of Gaussian beam as the function of the propagation distance. The Eqs. (58) and (59) repersents divergence angle range $(27.67^\circ \leq \theta \leq 35.85^\circ)$ *at the distance 3 mm to 4.5 mm. The divergence and the propagation distance are proportional to each other [10].*

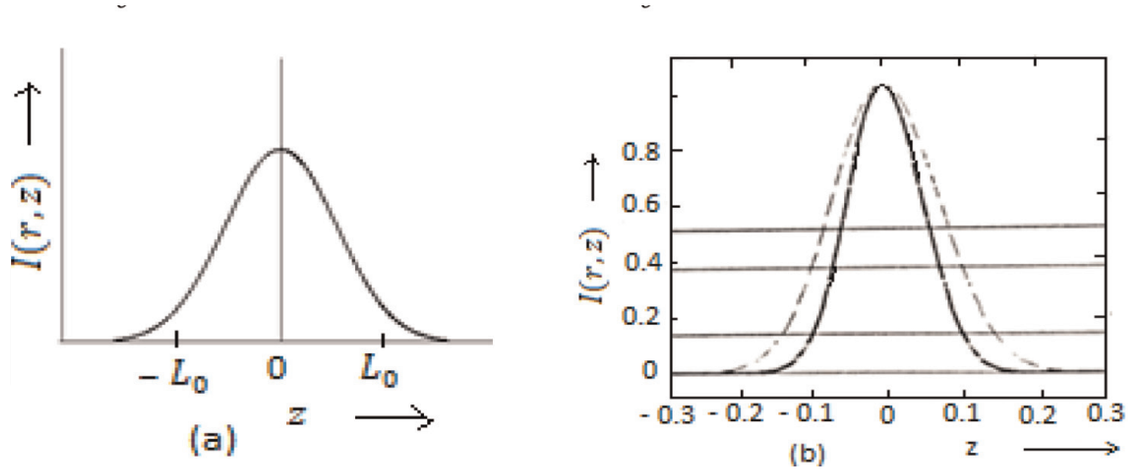

Figure 18.
Figure (a) represents the intensity distribution as function of z with the spot size. Figure (b) represents the amplitude and the intensity of Gaussian wave at beam waist with the dashed line and solid line respectively. They have been normalized to the maximum value. Here, the value of the spot size $L_0 = 0.1$ *mm. the horizontal line shows the maximum amplitude by factor 1/e and the maximum intensity by factor* $1/e^2$ *[7, 9].*

6. Fermi energy and density of state

In graphene, the energy of carbon nanotubes in the ground state of N electrons described as the Fermi energy given as

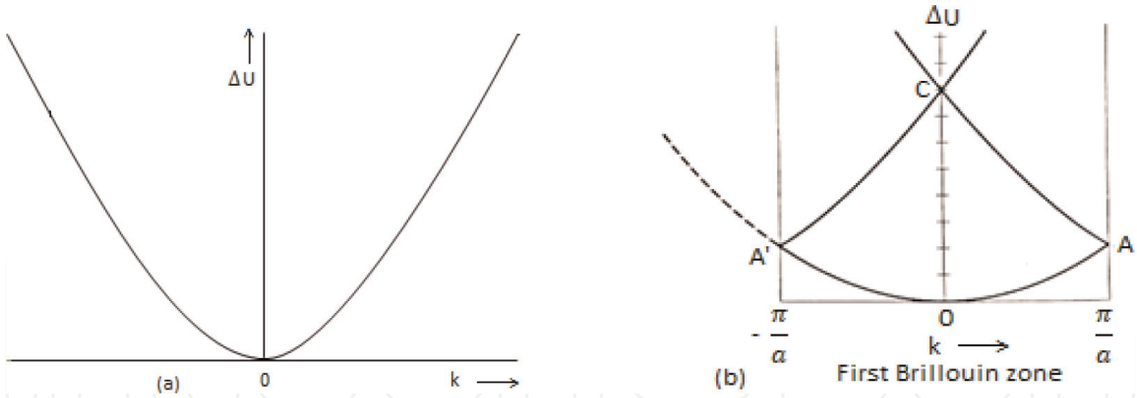

Figure 19.
Plot energy ΔU *verses wave vector* k *i.e.,* $\Delta U \alpha k^2$. *The construction in figure (b) represents the band structure of crystal of carbon nanotube. The crystal potential as well as Hertzian potential* $\prod_e$ *gives the band gap at A and A' and at C.*

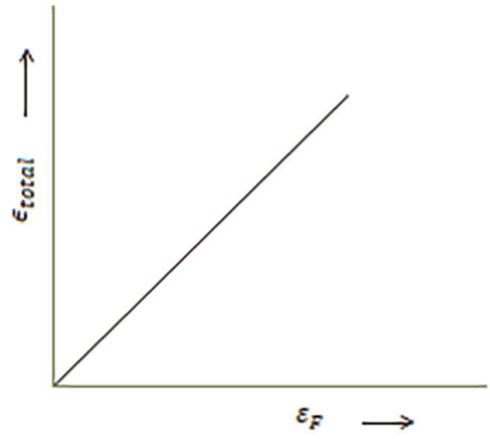

Figure 20.
Plot total stored energy ϵ_{total} *and Fermi energy* ε_F.

$$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2l}\right)^2 \tag{35}$$

The Fermi function described by the probability $f(\varepsilon)$ for the particular energy level ε by electron expressed as

$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\mu}{K_B T}} + 1} \tag{36}$$

Where μ is a function of temperature called the chemical potential. At absolute zero, we have $\mu = \varepsilon_f$ if $\varepsilon = \mu$ then $f(\varepsilon) = \frac{1}{2}$ at all temperatures.

The density of states of carbon nanotubes expressed as

$$D(\varepsilon) = \frac{\sqrt{3}a^2}{2\pi R}\sum_K \int dK(K - K_i)\left|\frac{\partial \varepsilon}{\partial K}\right|^{-1} \tag{37}$$

On expending the dispersion relation (33) around the Fermi surface, we have

$$D(\varepsilon) = \frac{a\sqrt{3}}{\pi^2 R\gamma} \sum_{m=1}^{N} \frac{|\varepsilon|}{\sqrt{\varepsilon^2 - \varepsilon_m^2}} \tag{38}$$

Where $\varepsilon_m = |3m+1|\left(\frac{a\gamma}{2R}\right)$ for semiconducting carbon nanotubes and $\varepsilon_m = |3m|\left(\frac{a\gamma}{2R}\right)$ for metallic carbon nanotubes. The dispersion near K points is proportional to the Fermi velocity of electrons in graphene, $v_f = 8 \times 10^5\ m/s$ as –

$$\frac{d\varepsilon}{dK}\Big|_K = \frac{\sqrt{3}}{2} a\gamma_0 = \hbar v_f \tag{39}$$

7. Maxwell's equation and Helmholtz equation

The carbon nanotube is like hollow cylinder and the spaces are available as free space in the carbon nanotube. So, the Maxwell's free space equations are as

$$\vec{\nabla} \bullet \vec{D} = 0 \tag{40}$$

$$\vec{\nabla} \bullet \vec{B} = 0 \tag{41}$$

$$\vec{\nabla} \bullet \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{42}$$

$$\vec{\nabla} \bullet \vec{H} = \frac{\partial \vec{D}}{\partial t} \tag{43}$$

Where $\vec{D} = \varepsilon_0 \vec{E}$ *and* $\vec{B} = \mu_0 \vec{H}$. Taking the curl of Eqs. (42) and (43) and using (40) and (41), we have

$$\nabla^2 \vec{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} \tag{44}$$

$$\text{And } \nabla^2 \vec{H} = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{H}}{\partial t^2} \tag{45}$$

These wave equations with components satisfy the eigen function wave Eq. (12);

$$\nabla^2 \prod = \mu_0 \varepsilon_0 \frac{\partial^2 \prod}{\partial t^2} \tag{46}$$

The plane wave along z-direction, thus, $\prod$ will be the function of z and t i.e.,

$$\prod = \prod(z, t) = \prod_0 \cos\omega\left(t - \frac{z}{C}\right) \tag{47}$$

On deriving (47) and (49), we obtain

$$\left(\nabla^2 + k^2\right) \prod = 0 \tag{48}$$

Where $k = \omega\sqrt{\varepsilon_0\mu_0}$ and $\prod = \prod(r)$ is the electric Hertz vector. The Eq. (49) is known as Helmholtz equation and the solution is given by

$$\prod(r) = \hat{e}_z e^{i\vec{k}\bullet\vec{r}} \tag{49}$$

Where $\hat{e}_z$ is a unit vector along z-direction. Eq. (49) represents the plane wave in transverse nature traveling through carbon nanotubes.

8. Gaussian wave

The Helmholtz Eq. (48) can also be written as

$$\frac{\partial^2 \prod}{\partial x^2} + \frac{\partial^2 \prod}{\partial z^2} - 2ik\frac{\partial \pi}{\partial z} = 0 \tag{50}$$

Or

$$\left(\nabla_T^2 - 2ik\frac{\partial}{\partial z}\right)\prod(x, y, z) = 0 \tag{51}$$

Where ∇_T^2 is the transverse gradient operator. The above Eq. (51) is termed as the paraxial wave equation and expressed in cylindrical coordinate system as

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \prod}{\partial r}\right) - 2ik\frac{\partial \prod}{\partial z} = 0 \tag{52}$$

Where $\prod = \prod(r, z)$ and $r = \sqrt{x^2 + y^2}$ is the transverse radial distance. The solution of Eq. (52) gives

$$\prod = e^{\frac{-ikr^2}{2q(z)}}e^{-iP(z)} \tag{53}$$

Where $q(z)\ \{= q_0 + z\}$ is a complex variable within the reciprocal of Gaussian width; q_0 is the value of q at z = 0 and the imaginary number equal to iz_R, where z_R is a constant and a real part. So, $q(z)$ is known as the complex radius of curvature and it expressed as $q(z) = iz_R + z$ and $\frac{1}{q(z)} = \frac{z}{z^2+z_R^2} - i\frac{z_R}{z^2+z_R^2}$ These are in order for the electromagnetic wave intensity, $I \sim |\prod|^2$ to show r-dependence in the transversal direction, if $|\prod(r,\ z = 0)|^2 = e^{\frac{-kr^2}{z_R}}$, where, the imaginary value of z_R has no radial dependence. z_R is also called Rayleigh distance of Rayleigh range and related to minimum spot size or minimum wave or beam waist, L_0, of Gaussian wave. P(z) gives the information to the phases of the waves. If q_0 is real then we have (**Figures 12–18**) [10];

$$\prod = e^{\frac{-ikr^2}{2q(r)}}e^{-iP(z)} \tag{54}$$

Since $e^{\frac{-ikr^2}{2q(r)}} = 1$ and P(z) is not a function of r; the phase is changed fast with r and the amplitude remains constant. We have $e^{-iP(z)} = \sqrt{1 + \left(\frac{z}{z_R}\right)^2}e^{i\tan^{-1}\left(\frac{z}{z_R}\right)}$ that

represents amplitude and phase. A Gaussian wave propagating along z-direction in single walled carbon nanotube whose distribution of amplitude on the plane z = 0 is given by

$$|\prod(r,\ z=0)| = e^{-\frac{r^2}{L_0^2}} \tag{55}$$

Where $L_0^2 = \frac{2z_R}{k} = \frac{\lambda_0 z_R}{n\pi} \Rightarrow L_0 = \left(\frac{\lambda_0 z_R}{n\pi}\right)^{\frac{1}{2}}$ and $z_R = \frac{n\pi L_0^2}{\lambda_0}$. The complete expression for the Gaussian wave is

$$\prod(r,z) = \prod_0 \frac{1}{\sqrt{1+\left(\frac{z}{z_R}\right)^2}}\ e^{-\frac{kz_R r^2}{2\left(z^2+z_R^2\right)}}\ e^{-i\frac{kz_R r^2}{2\left(z^2+z_R^2\right)}}\ e^{-i\left(kz-\tan^{-1}\left(\frac{z}{z_R}\right)\right)} \tag{56}$$

This can be also written as

$$\prod(r,z) = \prod_0 \frac{L_0}{L(z)}\ e^{-\frac{r^2}{L^2(z)}} e^{-i\frac{r^2}{2R(z)}}\ e^{-i(kz-\ \varphi(z))} \tag{57}$$

Where $L(z)\left\{= L_0\sqrt{1+\left(\frac{z}{z_R}\right)^2}\right\}$ is called the spot size and L_0 is the minimum spot size at the origin [7] and R(z) is the radius of curvature and equal to $z\left(1+\left(\frac{z}{z_R}\right)^2\right)$ and $\varphi(z)\left\{=\ \tan^{-1}\left(\frac{z}{z_R}\right)\right\}$ is the Guoy phase shift [12]. If $= z_R$, then we have the spot size $L(z) = 1.414\ L_0$. For the propagation of the Gaussian wave through the carbon nano tube, the minimum spot size, L_0, should be less than or equal to the radius of the single walled carbon nanotube.

The minimum diameter in the terms of 1/e field points is shown by $D_0 = 2L_0$. If $z \gg z_R$, the beam waist becomes $\simeq L_0 z/z_R$. In this case, the divergence angle or beam spreading angle is found.

The divergence angle is defind (when the relation of L and z becomes linear) as;

$$\theta_0 \simeq \tan\theta_0 = \frac{L}{z} = \frac{L_0}{z_R} = \frac{\lambda_0}{n\pi L_0} \tag{58}$$

$$\theta = 2\theta_0 = \frac{4}{\pi}\frac{\lambda_0}{n\,D_0} \tag{59}$$

Where θ_0 is the half of the divergence angle, θ, of the beam or wave.

The intensity distribution of Gaussian wave is given by

$$I(r,z) = \frac{I_0}{1+\left(\frac{z}{z_R}\right)^2}\ e^{-\frac{2r^2}{L^2(Z)}} \tag{60}$$

$$\text{Or } I(r,z) = I_0\left(\frac{L_0}{L(z)}\right)^2 e^{-\frac{2r^2}{L^2(Z)}} \tag{61}$$

This represents the transverse intensity distribution. It is measured from the beam centre perpendicular to the direction of propagation. The minimum spot size of the

wave in the carbon nanotube at which the amplitude falls by a factor $\frac{1}{e}$ i.e., the intensity reduces by a factor $\frac{1}{e^2}$.

9. Energy storage capacity of the carbon nanotubes

According to laws of conservation of energy, the kinetic energy of charge particle is equal to the potential energy of charge particle. So, $E - U = U_2 - U_1 = \Delta U$. The Schrödinger wave Eq. (23) is also written as $\left(\nabla^2 + \frac{2m}{2}(U_2 - U_1)\right)\prod = 0$ and compare with the Eq. (49). We have

$$k^2 = \frac{2m}{\hbar^2}\Delta U \tag{62}$$

$$\Delta U = \frac{\hbar^2}{2m}k^2 \tag{63}$$

By work-energy theorem, we have $W = \Delta U$. The distribution of charge on inner wall of nanotube with Gaussian wave is q and Gaussian wave travels in the nanotube with magnetic and electric field explained by Maxwell's equation. So, we have electric potential in terms of the electric Hertz potential $\prod_e$ [11]. The work done by moving charge of wave on the inner wall is given by

$$W = \prod_e q = \frac{1}{2}\, C \prod_e^2 \tag{64}$$

The total energy stored in single walled carbon nanotube is obtained as

$$\frac{1}{2}\, C \prod_e^2 = 4\left(\frac{\pi}{\lambda}\right)^2\left(\frac{2l}{N\pi}\right)^2 \varepsilon_F \tag{65}$$

This total energy also expressed as

$$\epsilon_{total} = 16\left(\frac{l}{N\lambda}\right)^2 \varepsilon_F \tag{66}$$

The capacitance of the carbon nanotube is expressed as

$$C = 32\left(\frac{l}{N\lambda}\right)^2 \varepsilon_F / \prod_e^2 \tag{67}$$

10. Conclusions

The crystal structure of graphene with lattice and chiral vector gives the metallic and semiconducting character that is represented by various graphs and equation with energy dispersion relation and density of state which are found by Bloch theorem,

Fourier series and Schrödinger wave equation. The solution of Helmholtz equation gives the plane monochromatic transverse wave and also Gaussian profile. We have found the minimum spot size of Gaussian wave that ensures the propagation of wave through the single walled carbon nanotube along the z-direction and verified by various graphs. The Gaussian beam within the low divergence has better wave quality. We have also found the relation between the energy and wave vector by using Helmholtz and Schrödinger equation that gives us energy storage capacity of the carbon nanotubes with the electric Hertz potential.

Summarizing, the plane monochromatic transvers Gaussian wave with minimum spot size propagates through the hollow cylindrical carbon nanotube and the energy is stored on the inner wall (or in Fermi surface of nanotube) as a capacitor. The charges are accumulated on the surface with Hertzian potential. The stored energy is inversely proportional to the square of the wavelength and directly proportional to the Fermi energy. At minimum wavelength we have the higher energy.

A. Derivation of Helmholtz Wave Equation

We have $\nabla^2 \prod = \mu_0 \varepsilon_0 \frac{\partial^2 \prod}{\partial t^2}$The plane wave along z-direction, thus, $\prod$ will be the function of z and t i.e.,

$$\prod = \prod(z, t) = \prod_0 \cos \omega \left(t - \frac{z}{C}\right)$$

Where $\omega = \frac{2\pi c}{\lambda}$ then

$$\frac{\partial \prod}{\partial t} = -\omega \prod_0 \sin \omega \left(t - \frac{z}{c}\right)$$

or

$$\frac{\partial^2 \prod}{\partial t^2} = -\omega^2 \prod_0 \cos \omega \left(t - \frac{z}{C}\right) = -\omega^2 \prod$$

$$= -\left(\frac{2\pi c}{\lambda}\right) \prod = -c^2 k^2 \prod$$

We have $\nabla^2 \prod = \mu_0 \varepsilon_0 \left(-c^2 k^2 \prod\right) \nabla^2 \prod = -k^2 \prod since, \mu_0 \varepsilon_0 = \frac{1}{c^2}$

or $\left(\nabla^2 + k^2\right) \prod = 0$This required wave equation is called the Helmholtz wave equation.

B. Solution of Helmholtz wave equation

Let the origin of the cylindrical coordinate system (r_m, θ_m, z) be located at the point $z = 0$ on the axis of the m^{th} carbon nanotube in a bundle. So, the Helmholtz wave equation in cylindrical coordinate system written as

$$\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}+k^2\right)\prod_m(r)=0$$

Since $\prod_m$ is a function of only r then $\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$ and $\frac{\partial^2}{\partial z^2}$ are neglected and let us consider the solution of the above equation written as

$$\prod_m(r)=R(r)=R$$

Now, the Helmholtz wave equation is also written as

$$\frac{\partial^2}{\partial r^2}(R)+\frac{1}{r}\frac{\partial}{\partial r}(R)+k^2(R)=0$$

Let $R=e^{\alpha r}$ and differentiate it with respect to r then we have

$$\frac{\partial R}{\partial r}=\frac{\partial}{\partial r}(e^{\alpha r})=\alpha e^{\alpha r}$$

and

$$\frac{\partial^2 R}{\partial r^2}=\alpha^2 e^{\alpha r}$$

Putting these in the above equation and we can write

$$\alpha^2 e^{\alpha r}+\frac{1}{r}\alpha e^{\alpha r}+k^2 e^{\alpha r}=0$$
$$\text{or } e^{\alpha r}\left\{\alpha^2+\frac{\alpha}{r}+k^2\right\}=0$$

We have a bundle of carbon nanotubes, so, $r\to\infty$ and consider $\frac{\alpha}{r}$ has negligible value. Above equation, therefore, written as

$$e^{\alpha r}\left\{\alpha^2+k^2\right\}=0$$
$$\alpha^2=-k^2 \implies \alpha=\pm ik$$

Now, we have

$$R=e^{\pm ikr}$$
$$\prod_m(r)=e^{\pm ikr}$$

In vector form

$$\prod_m(r)=\hat{e}_z e^{i\vec{k}\cdot\vec{r}}$$

This is solution of the Helmholtz wave equation and indicates the plane wave. It is true for all type of the carbon nanotube. $\hat{e}_z$ is the unit vector along the carbon nanotube axis and at the right angles to the direction of propagation and shows the transverse character of wave.

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