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# AN EVALUATION OF DISPERSION RELATION OF PROPAGATION OF ELECTROMAGNETIC WAVE WITH TE MODES IN CARBON NANOTUBE

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**Abstract: -** Using the theoretical formalism of **Li Wei et al (Phys. LettA 333 (2004)),** we have studied the electromagnetic wave propagation in carbon nanotubes. We have studied the dispersion relation of TE-mode as a function of dimensionless parameter κa for fixed value of radius 'a' and different values of m. We have also studied the influence of nanotube radius on the dispersion relation for m=1.We observed that the obtained dispersion relation is very much identical to well-known electrostatic collective excitation. Our theoretically evaluated results are in good agreement with those of the other theoretical workers.

**Keywords:** Single wall carbon nanotubes, lineaized hydrodynamic theory, Nano waveguide, hydrodynamic equations, dispersion relation for surface waves, Transverse electric mode (TE-mode), Transverse magnetic mode (TM-mode), Low frequency electromagnetic wave, Electrostatic collective excitations, Single electron excitation effects.

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## 1. INTRODUCTION

Following the discovery by Iijima[1] of carbon nanotubes (CNs), there has been a growing interest in electromagnetic wave propagation in single-wall carbon nanotubes. Since CN can be metals or semiconductors depending upon its radius and the geometrical angle, some important information about the structural and electronic properties can be obtained using electromagnetic probe techniques[2,3] or electron probe techniques[4]. In particular, being very long, a CN can be regarded as a nano waveguide to guide electromagnetic waves. During the past years, different theoretical models have been used to describe the physical properties of CNs. With a classical hydrodynamic model, Yanouleas[5] and Jiang[6] studied the collective excitation behavior of σ and π electrons in single or multi-wall CNs. The collective excitation properties of CNs are quite different from those of well-known graphite sheets. The difference is that the collective excitations in CNs have traditional one-dimensional (1D) characters for small wave number, while exhibiting two-dimensional (2D) behavior for large wave numbers. The quantum dielectric-response theory, taking into account the electron energy band structures in CNs have used[7-9] to describe low frequency electronic excitations in CNs. Beyond the electrostatic excitations, Slepyan etal.[10-13] studied electromagnetic processes in CNs. With the classical electrodynamics and a semi-classical kinetic theory, they derived the dispersion relation of surface wave in CN's. They found out that the CNs can be used as a waveguide for controlling electromagnetic wave propagation in specified frequency ranges (examples are infrared and optical). They also presented a general quantum mechanical theory of the conductivity of a single wall carbon nanotubes with interband transitions.

Now days, there is much interest to electromagnetic high-frequency properties of carbon nanotubes. This is because of their potential applications in nanoelectronics[14], nanoantennas[15-18], polarizers[19], free electron lasers[20], devices for THz sensing and imaging[21]. As we know that carbon nanotubes (CNs) possess metallic properties therefore special interest has been paid due to their high conductivity at THz frequencies and compared to metal nanowires[22]. By this reason, their applications seem to be promising in THz and infrared ranges due to noticeable lower losses compared to other conductive materials.

One of the most important electromagnetic property of metallic CNTs is a capability to support propagation of strongly delayed surface waves[23,24]. It is caused by a very high kinetic inductance of thin single –wall CNTs[25]. It makes electromagnetic (EM) wave propagation in CNTs strongly different compared to transmission lines, made of usual bulk metals. For description of electromagnetic properties of metallic CNTs, very often the model of impedance cylinder and effective boundary condition is used[26]. The model of impedance cylinder takes into account quantum properties of CNTs via the complex surface frequency-dependent conductivity. This model was applied for theoretical study of CNT transmission lines and interconnects. These structures are composed of closely packed bundles of parallel identical metallic CNTs. It was applied for studying two-dimensional periodic arrays of single wall metallic CNTs.

In this paper, using the theoretical formalism of Li Wei etal[27], we have studied the dispersion relation of TE-mode of carbon nanotubes. We have evaluated dispersion relation ($\omega/\Omega_p$) as a function of κa with fixed value of nanotube radius 'a' and different value of m. We have also studied the influence of the nanotube radius on the dispersion relation for m=1and different values of a. Our evaluated results are in good agreement with the other theoretical workers[28,29].

## 2. MATERIALS AND METHODS

One models a single wall carbon nanotube as an infinitesimally thin and infinitely long cylindrical shell with a radius a. One assumes that the valence electrons can be considered as free electron gas distributed uniformly over the cylindrical surface. Let the density per unit area be $n_0$. One uses cylindrical coordinate **r**=(ρ,ϕ,z). Consider an electromagnetic wave with frequency ω propagating along the nanotube z-axis. The homogeneous electron gas will be perturbed by the electromagnetic wave and can be regarded as a charged fluid with velocity field **u(r**$_S$,t) and the perturbed density (per unit area) $n_1$(**r**$_S$,t). **r**$_S$=(ϕ,z) is the coordinate of a point at the cylindrical surface of the nanotube. Velocity field **u** has only tangential components to the nanotube surface. Based on the linearized hydrodynamic model[30], the electronic excitations on the cylindrical surface can be described to the continuity equation

$$\frac{\partial n_1(\vec{r}_S,t)}{\partial t} + n_0 \nabla_{\parallel} . \vec{u}(\vec{r}_S,t) = 0 \qquad (1)$$

And the momentum –balance equation is given by

$$\frac{\partial \vec{u}(\vec{r}_s,t)}{\partial t} = -\frac{e}{m_e} \vec{E}_{\parallel}(\vec{r}_S,t) - \frac{\alpha}{n_0} \nabla_{\parallel} n_1(\vec{r}_S,t) + \frac{\beta}{n_0} \nabla_{\parallel}(\nabla^2_{\parallel} n_1(\vec{r}_S,t)) \qquad (2)$$

Where $\vec{E}_{\parallel} = E_z \vec{e}_z + E_\phi \vec{e}_\phi$ is the tangential component of the electromagnetic field. $n_1$ is the charge density polarization of the electron gas, e is the electronic charge and $m_e$ is the electron mass. Here $\nabla_{\parallel} = \vec{e}_z \frac{\partial}{\partial z} + \vec{e}_\phi \alpha^{-1} \frac{\partial}{\partial \phi}$ only differentiates tangentially to the nanotube surface.

The first term on the right hand side of equation (2) is the force on electrons on the nanotube due to the tangential component of the electric field, the second and third terms may be regarded as parts of the internal interaction force in the electron gas. Here $\alpha=(V_F^2/2)$ is the speed of propagation of density disturbances in the electron gas with $V_F=(2\pi n_0 a^2{}_\beta)^{\frac{1}{2}} v_\beta$ being the Fermi velocity of the 2D electron gas and $\beta=(a_\beta v_\beta)^2/4$ describes single electron excitations in the electron gas. Here $a_\beta$ and $v_\beta$ are the Bohr radius and Bohr velocity respectively. We have neglected the second and third terms in the calculation as it was neglected in the works of Yannouleas etal[5].

The electric field vector **E(r,**t) and the magnetic field vector **B(r,**t) can be expanded in the following Fourier forms

$$E(r,\phi,z,t)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dq E^{\rightarrow}{}_m(r,q)e^{i(m\phi+qz-\omega t)} \quad (3)$$

$$B(r,\phi,z,t)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dq B^{\rightarrow}{}_m(r,q)e^{i(m\phi+qz-\omega t)} \quad (4)$$

Using Maxwell's equations, one can obtain the following Helmholtz equations for the z-components $E_{zm}$ and $B_{zm}$ of the expanding coefficients $\mathbf{E}_{zm}$ and $\mathbf{B}_{zm}$

$$\frac{d^2E_{zm}}{dr^2}+\frac{1}{r}\frac{dE_{zm}}{dr}-(\kappa^2+\frac{m^2}{r^2})E_{zm}=0 \quad (5)$$

And

$$\frac{d^2B_{zm}}{dr^2}+\frac{1}{r}\frac{dB_{zm}}{dr}-(\kappa^2+\frac{m^2}{r^2})B_{zm}=0 \quad (6)$$

Where

$$\kappa^2=q^2-k^2, \quad k=\frac{\omega}{c} \quad 7(a)$$

k is wave number and c is velocity of light. We have assumed that the propagation of electromagnetic waves are in the infrared regime so that $k \ll q$.

By eliminating the velocity field **u**(r,t), one can obtain the following equations from equation(1) and (2)

$$\frac{\partial^2 n_1(r_s^{\rightarrow},t)}{\partial t^2} = \frac{en_0}{m_e}\nabla_{\parallel}.E_{\parallel}^{\rightarrow}(r_s^{\rightarrow},t) + \alpha\nabla_{\parallel}^{2} n_1(r_s^{\rightarrow},t) - \beta\nabla_{\parallel}^{2}(\nabla_{\parallel}^{2} n_1(r_s^{\rightarrow},t)) \quad (8)$$

Upon solving equation (8) by means of space-time Fourier transforms for the induced density **$n_1$(r**$_S$,t) on the cylindrical surface, one finds

$$n_1(\phi,z,t) = \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dq N_m^{\rightarrow}(q) e^{i(m\phi+qz-\omega t)} \quad 9(a)$$

Where $N_m = -i\frac{en_0}{m_e}\frac{1}{W_m} q_m^{\rightarrow}.E_{\parallel m}^{\rightarrow}$ 9(b)

With $q_m^{\rightarrow} = qe^{\rightarrow}_z + (\frac{m}{a})e_\phi^{\rightarrow}$ 9(c)

$$W_m = \omega^2 - \alpha q_m^{\ 2} - \beta q_m^{\ 4} \quad 9(d)$$

To solve equations (5) and (6), one has to provide appropriate boundary conditions. With the induced density, these boundary conditions can be written as

$$E_{rm}(a)_{r>a} - E_{rm}(a)_{r<a} = -\frac{en_0}{\varepsilon_0} \quad 10(a)$$

$$(E_{\parallel m}^{\rightarrow})_{r>a} - (E_{\parallel m}^{\rightarrow})_{r<a} = 0 \quad 10(b)$$

And $B_{rm}(a)_{r>a} - B_{rm}(a)_{r<a} = 0$ 10(c)

Where $\varepsilon_0$ is the permittivity of free space. Equation 10(a) indicates that due to the polarization of the electron gas on the nanotube surface, the radial component of the electric field is discontinuous at the cylinder at r=a. With the above equation, one will consider propagation of the electromagnetic wave with TE mode

**DISPERSION RELATION OF TE-MODE**

For the TE mode, the longitudinal electric field is zero. i.e $E_Z$ =0. From equation (6), the longitudinal component of the magnetic field can be expressed by

$$B_{zm}(r) = C_m I_m(\kappa r), (r<a) \quad 11(a)$$

And $$B_{zm}(r) = D_m K_m(\kappa r), (r > a) \quad 11(b)$$

Where $I_m(x)$ and $K_m(x)$ are the modified Bessel function and coefficients $C_m$ and $D_m$ will be determined by the boundary conditions. With Maxwell's equations

$$\nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B} \quad 12(a)$$

$$\nabla \times \mathbf{B} = c^{-2}\frac{\partial}{\partial t}\mathbf{E} \quad 12(b)$$

The radial component $E_{rm}$ and azimuthal component $E_{\phi m}$ of the electric field and the radial component $B_{rm}$ of the magnetic field can be expressed as follows

$$E_{rm}(r) = \frac{m\omega}{\kappa^2 r} B_{zm}(r) \quad (13)$$

$$E_{\phi m}(r) = i\frac{\omega}{\kappa^2 r}\frac{dB_{zm}(r)}{dr} \quad (14)$$

And $$B_{zm}(r) = -i\frac{q}{\kappa}\frac{dB_{zm}(r)}{dr} \quad (15)$$

Equation 9(b) and (14), the Fourier coefficient $N_m$ of the induced density is reduced to

$$N_m = -i\frac{en_0}{m_e}\frac{1}{W_m}\frac{mE_{\phi m}}{a} = -\frac{en_0}{m_e}\frac{1}{W_m}\frac{mq}{\kappa a}B'_{zm}(a) \quad (16)$$

Substituting equations (13)-(17) into boundary conditions [equations 10(a),10(b) and 10(c)] one obtains the following dispersion relation between the frequency $\omega$ and wave number $\kappa$

$$\omega^2 - \alpha(\kappa^2 + \frac{\omega^2}{c^2} + \frac{m^2}{a^2}) - \beta(\kappa^2 + \frac{\omega^2}{c^2} + \frac{m^2}{a^2})^2$$

$$= -\Omega_p{}^2(\kappa a)^2 I'_m(\kappa a)K'_m(\kappa a) \quad (17)$$

Where $$\Omega_p = \left(\frac{e^2 n_0}{\varepsilon_0 m_e a}\right)^{\frac{1}{2}} \quad (18)$$

$I'_m(x)$ and $K'_m(x)$ are the derivatives of the Bessel functions with respect to argument $x = \kappa a$. Here, the Wronskian property, $I'_m(x)$ $K_m(x)$=- $I_m(x)$ $K'_m(x)$=1/x , has been used. In order to simplify the notation, one introduce dimensionless variable $y = \frac{\omega}{\Omega_p}$ and $x = \kappa a$ then equation (17) can be reduced in the following form

$$y^2 - \alpha_1(x^2 + \sigma y^2 + m^2) - \beta_1(x^2 + \sigma y^2 + m^2)^2$$

$$= -x^2 I'_m(x) K'_m(x) \quad (19)$$

$$\alpha_1 == \frac{\alpha}{(\Omega_p a)^2} \quad 20(a)$$

$$\beta_1 = \frac{\beta}{(\Omega^2{}_p a^4)} \quad 20(b)$$

$$\sigma = \frac{\Omega^2{}_p a^4}{c^2} \quad 20(c)$$

It can be seen from equation (19) that the dispersion relation depends on the tube's radius 'a' and the surface electron density $n_0$. Generally, radiuses of the single wall carbon nanotubes range from 1nm up to almost 15nm. Assuming the atomic density of graphite sheet $38nm^{-2}$, the surface electron density of a single-wall carbon nanotube can be approximated by $n_0=4x38nm^{-2}$ and the value of parameter $\sigma=5.5x10^{-3}=0.05$. Therefore, one can neglect the term $\sigma y^2$ in equation (19) for low frequency electromagnetic wave. The dispersion relation looks like

$$y^2 = \alpha_1(x^2 + m^2) + \beta_1(x^2 + m^2)^2 - xI_m'(x)K_m'(x) \quad (21)$$

From equation (19), one can distinguish two different dimensionality regimes depending on two cases of $x \ll |m|$ or $x \gg |m|$

One may use the asymptotic expressions of the Bessel functions

$$I_m(x) = \frac{e^x}{\sqrt{2\pi x}} \qquad 22(a)$$

$$K_m(x) = \sqrt{\frac{\pi}{2x}} e^{-x} \qquad 22(b)$$

The dispersion relation can be written approximately as

$$y^2 = \beta_1 x^4 + \alpha_1 x^2 + x/2 \qquad (23)$$

In fact, for large radius nanotubes, the parameters $\alpha_1$ and $\beta_1$ approaches zero and the dispersion relation becomes

$$y^2 = \frac{x}{2} \qquad (24)$$

In this case $$\omega^2 = \frac{1}{2}\Omega^2{}_p x = \frac{e^2 n_0}{2\varepsilon_0 m_e} k \qquad (25)$$

which is independent on the dimension of the tube and corresponds to the dispersion relation in a planer 2D electron gas with the surface density $n_0$.

On the other hand for $x \ll |m|$, one use the well-known expressions of Bessel functions $I_m(x) = a_m x^m$, $K_0(x) = \ln(\frac{1.123}{x})$, and $K_m(x) = b_m x^{-m} (m \neq 0)$ where $a_m = \frac{2^{-m}}{\Gamma(m+1)}$ and $b_m = 2^{m-1}\Gamma(m)$. Then for $m \neq 0$, one gets

$$\omega^2 = [\alpha_1 m^2 + \beta_1 m^4 + \frac{m}{2}]\Omega^2{}_p \qquad (26)$$

And for $m = 0$ , one has

$$\omega^2 = 0 \qquad (27)$$

Now, it is clear that the dispersion relations given by equation (26) depend strongly on the radius of the nanotube, which has a traditional 1D character.

## 3. RESULTS AND DISCUSSION:

In this paper, we have presented a method of evaluation of dispersion relation ( $\frac{\omega}{\Omega_p}$ ) for TE-mode as a function of variable κa. The evaluation has been performed using the theoretical formalism of Li Wei etal[27]. In Table T1, we have evaluated dispersion relation ( $\frac{\omega}{\Omega_p}$ ) for TE-mode as a function of dimensionless variable κa for nanotube radius a=5nm with different values of m. From our evaluated results it appears that the dispersion relation ω for the nanotube continue to increase with increasing value of κa for all values of m>0. It approaches the Plasmon frequency of the 2D electron gas, $\Omega_p\sqrt{\frac{\kappa a}{2}}$ for $\kappa a \to \infty$. This result is quite similar with the well-known dispersion relation of the electrostatic collective excitation[7]. We have also evaluated the influence of the nanotube radius on the dispersion relation for m=1 and different values of a. We have taken the values of a=2, 5, 10 and 15nm for m=1 as a function of κa. The results are shown in table T2. From our evaluated results, it can be seen that dispersion curve approaches to one for large nanotube radius. It increases with κa for all values of a. Its value is large at a=2nm and small for a=15nm at value of κa=60. In addition, we have also examined the effect of the internal interaction forces on the electron gas on the dispersion relation for TE-mode. The evaluated results are shown in table T3. Here, we have evaluated dimensionless frequency $(\frac{\omega}{\Omega_p})$ in three cases. In one case (a) we have taken $\alpha_1 = \beta_1 \neq 0$. In other case (b) $\alpha_1 = 0,$ and $\beta_1 \neq 0$. In third case (c) we fixed $\alpha_1 = 0,$ and $\beta_1 = 0$. The evaluation is done using equation (27). From our evaluation, it is clear that for TE-mode the internal pressure force of the electron makes the increase of the frequency, while the dispersion relation is almost affected by the single electron excitation effects. There is some recent calculations[31-45] on electromagnetic wave propagation in carbon nanotubes which also reveal the similar behavior.

## 4. CONCLUSION

From the above theoretical analysis and investigations, we have come across the following conclusions.

- One has used the linearized hydrodynamic model with Maxwell equations to describe the propagation of the electromagnetic wave in the single wall carbon nanotubes

- General expressions have been derived for the dispersion relation of the low-frequency electromagnetic wave for TE-mode.
- The obtained dispersion relation for TE-mode is very much identical to well –known electrostatic collective excitation. This excitation has a dimensionality crossover from 1D system to 2D system.
- The hydro dynamical model is considered to be more reliable in describing the single-electron excitation. This particular excitation has important contribution in TE-mode dispersion.
- This model does not consider the electron energy-band effects. This effect is very much important in describing the dispersion relation for chiral nanotube.

**Table T1**: **An evaluated result of the dispersion relation $(\frac{\omega}{\Omega_p})$ of TE-mode for carbon nanotube with radius a=5nm and m=0, 1, 2, 3 and 4 as a function of κa.**

| κa | <------- $(\frac{\omega}{\Omega_p})$ -------> | | | | |
|---|---|---|---|---|---|
| | m=0 | m=1 | m=2 | m=3 | m=4 |
| O | 0.0 | 0.75 | 1.06 | 1.11 | 1.35 |
| 2 | 0.25 | 0.96 | 1.24 | 1.30 | 1.46 |
| 4 | 0.69 | 1.17 | 1.38 | 1.42 | 1.52 |
| 5 | 1.26 | 1.34 | 1.42 | 1.50 | 1.68 |
| 6 | 1.34 | 1.47 | 1.67 | 1.72 | 1.79 |
| 8 | 1.46 | 1.58 | 1.74 | 1.86 | 1.92 |
| 10 | 1.67 | 1.77 | 1.84 | 1.94 | 2.08 |
| 12 | 1.85 | 1.95 | 1.98 | 2.07 | 2.15 |
| 14 | 1.92 | 2.06 | 2.10 | 2.18 | 2.36 |
| 15 | 2.00 | 2.15 | 2.22 | 2.30 | 2.48 |

| | | | | | |
|---|---|---|---|---|---|
| **16** | 2.28 | 2.37 | 2.40 | 2.45 | 2.58 |
| **18** | 2.45 | 2.50 | 2.55 | 2.62 | 2.76 |
| **20** | 2.88 | 2.90 | 2.95 | 3.00 | 3.10 |

**TableT2: An evaluated result of the dispersion relation $(\frac{\omega}{\Omega_p})$ of TE-mode for carbon nanotube with radius a=2, 5, 10 and 15nm for m= 1 as a function of κa.**

| **κa** | $(\frac{\omega}{\Omega_p})$ **(m=1)** | | | |
|---|---|---|---|---|
| | a=2nm | a =5nm | a =10nm | a=15nm |
| **0** | 0.86 | 0.92 | 0.95 | 1.00 |
| **5** | 1.24 | 1.25 | 1.28 | 1.20 |
| **10** | 1.86 | 1.94 | 2.05 | 1.87 |
| **15** | 2.17 | 2.15 | 2.28 | 2.10 |
| **20** | 2.48 | 2.27 | 2.39 | 2.29 |
| **25** | 3.25 | 2.48 | 2.60 | 2.50 |
| **30** | 3.98 | 2.95 | 3.00 | 2.88 |
| **35** | 4.18 | 3.10 | 3.17 | 3.05 |
| **40** | 4.87 | 3.29 | 3.30 | 3.10 |
| **45** | 5.18 | 3.86 | 3.52 | 3.47 |
| **50** | 5.75 | 4.08 | 3.68 | 3.59 |
| **60** | 5.98 | 4.50 | 3.87 | 3.80 |

**TableT3: An evaluated result of the dispersion relation $(\frac{\omega}{\Omega_p})$ of TE-mode for a=5nm and m=0 using relation (11) for (a) $\alpha_1 = \beta_1 \neq 0$ (b) $\alpha_1 = 0, \beta_1 \neq 0$ (c) $\alpha_1 = \beta_1 = 0$ as a function of κa.**

| κa | $(\frac{\omega}{\Omega_p})$ ( a=5nm and m=0) | | |
|---|---|---|---|
| | (a) $\alpha_1 = \beta_1 \neq 0$ | (b) $\alpha_1 = 0, \beta_1 \neq 0$ | (c) $\alpha_1 = \beta_1 = 0$ |
| 0 | 0.0 | 0.0 | 0.0 |
| 5 | 1.25 | 1.16 | 1.14 |
| 10 | 1.47 | 1.40 | 1.38 |
| 15 | 1.89 | 1.75 | 1.72 |
| 20 | 2.30 | 2.20 | 2.16 |
| 25 | 2.97 | 2.88 | 2.78 |
| 30 | 3.38 | 3.25 | 3.15 |
| 35 | 3.68 | 3.55 | 3.42 |
| 40 | 4.15 | 4.10 | 3.88 |
| 45 | 4.88 | 4.67 | 4.12 |
| 50 | 5.27 | 5.10 | 4.68 |
| 55 | 5.78 | 5.52 | 4.89 |
| 60 | 6.16 | 5.97 | 5.12 |

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