

Implication of the Exchange-Correlation on Electromagnetic Wave Propagation in Single-Wall Carbon Nanotubes

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Abstract—Using the linearized quantum hydrodynamic model (QHD) and by considering the role of quantum parameter (Bohm's potential) and electron exchange-correlation potential in conjunction with Maxwell's equations, electromagnetic wave propagation in a single-walled carbon nanotubes was studied. The electronic excitations are described. By solving the mentioned equations with appropriate boundary conditions and by assuming the low-frequency electromagnetic waves, two general expressions of dispersion relations are derived for the transverse magnetic (TM) and transverse electric (TE) modes, respectively. The dispersion relations are analyzed numerically and it was found that the dependency of dispersion curves with the exchange-correlation effects (which have been ignored in previous works) in the low frequency would be limited. Moreover, it has been realized that asymptotic behaviors of the TE and TM modes are similar in single wall carbon nanotubes (SWCNTs). The results show that by adding the function of electron exchange-correlation potential lead to the phenomena and make to extend the validity range of QHD model. The results can be important in the study of collective phenomena in nanostructures.

Keywords—Transverse magnetic, transverse electric, quantum hydrodynamic model, electron exchange-correlation potential, single-wall carbon nanotubes.

I. INTRODUCTION

AS we know, CNTs are rolled up graphene sheets, depending on its radius and the geometric angle can be either metallic or semiconducting. Diameter of SWCNTs varies from 1 to several nanometers [1]-[5]. During the past years, some scientist have used some different theoretical models such as the classical hydrodynamic model [6], [7], semi-classical kinetic theory [8], general quantum-mechanical theory [9] and tight-binding model [10] to describe electronic excitations in SWCNTs. On the other hand, in plasmas with low temperature and high electron density, Pauli's principle restricts the electrons not to be more than one in each quantum state; such a system is known as quantum or degenerate plasma [11]. In recent years; however, a huge interest has been developed in the area of quantum plasmas which is motivated by its potential application in modern technology, e.g. metallic and semiconductor nanostructures, metal clusters, thin metal films, nanotubes, quantum well and quantum dots, free-electron lasers, etc. [12]-[15]. A common model to investigate the collective dynamics of degenerate electron gas in plasmas and condensed matter systems is QHD model [16]. When

density of plasma particles is too high, the thermal de Broglie wavelength associated with each plasma particle may exceed the average inter-particle distance [17]. Since electron exchange-correlation effects are very weak; therefore, they are usually ignored in many investigations; however, it has been observed that the electron exchange-correlation effects become significant for high density and low temperature plasmas such as in the ultra-small electronic devices, nanotubes and semiconductor nanostructures (GaAs, GaSb, etc.) [18]-[20]. The electron exchange-correlation potential is a function of electron density and is given by

$$V_{xc} = -0.985 \frac{e^2}{\epsilon} n^{1/3} \left[1 + \frac{0.034}{n^{1/3} a_B} \ln(1 + 18.37 n^{1/3} a_B) \right], \quad (1)$$

which can be obtained via the adiabatic local-density approximation [12], [21]-[24], where $a_B = \epsilon \hbar^2 / m_e e^2$ is the Bohr radius and $\epsilon = 4\pi\epsilon_0$ is the effective dielectric permeability of system. The last equation shows that as density increases, the exchange effects increase, while correlation effects decrease [23].

It is necessary to mention that the quantum effects in the plasma dynamics have been performed in a vast number of studies, during the past years. For example, Wei et al. [3] and then Khosravi et al. [25] studied propagation of electromagnetic waves in SWCNTs. In special, surface excitation modes are one of the most interesting aspects in studies of CNTs. Many experimental realizations [26], [27] and theoretical works [28]-[31] have been done to describe the high-frequency excitations (electron oscillations) in these systems. Wei and Wang, using the QHD model, have studied the quantum ion-acoustic waves in SWCNTs [32]. Additionally, several authors have tried to investigate the effects of a static magnetic field on collective modes in CNTs. Fetter has obtained an acoustic branch in addition to the optical [33]. Chiu et al. [34], [35] studied the low-frequency single-particle and collective excitations of SWCNTs in the presence of a magnetic field. Abdikian et al. by exploiting the QHD model and Maxwell's equations have tried to study the electrostatic waves in CNT which filled by completely electron gas with axial magnetic field [14], [15]. Furthermore, some researchers are interested in TM (Voigt configuration) waves which propagate parallel to the surface of a SWCNT [36], [37].

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In the present study, we use the usual linearized QHD model by using the exchange-correlation effects and focus on the propagation of electromagnetic wave in SWCNTs. And then, we wish to distinguish the difference in the TE and TM modes.

II. MATHEMATICAL MODEL

We consider a quantum electron fluid moving on the surface of an infinitely long and infinitesimally thin SWCNT with radius a . Let us assume that the density of free-electron fluid is $n_0 = 4 \times 38 \text{ nm}^{-2}$, corresponding to four valence electrons per carbon atom. For the following calculations, we use cylindrical coordinates $\mathbf{r} = (\rho, \varphi, z)$. The electromagnetic wave with frequency ω propagating along the nanotube axis z perturbs the homogeneous electron gas. The velocity of the perturbed density (per unit area) $n_1(\mathbf{r}_S, t)$ is considered as $\mathbf{u}(\mathbf{r}_S, t)$ where $\mathbf{r}_S(\varphi, t)$ are the coordinates of a point at the cylindrical surface of the nanotube. The dynamics of the charged particles are governed by the continuity and the momentum-balance equations [3]

$$\frac{\partial n_1(\mathbf{r}_S, t)}{\partial t} + n_0 \nabla_{\parallel} \cdot \mathbf{u}(\mathbf{r}_S, t) = 0, \quad (2)$$

$$\frac{\partial \mathbf{u}(\mathbf{r}_S, t)}{\partial t} = -\frac{e}{m_e} \mathbf{E}_{\parallel}(\mathbf{r}_S, t) - \frac{\alpha}{n_0} \nabla_{\parallel} n_1(\mathbf{r}_S, t) + \frac{\beta}{n_0} \nabla_{\parallel} (\nabla_{\parallel}^2 n_1(\mathbf{r}_S, t)) + \nabla_{\parallel} V_{xc}, \quad (3)$$

where n_1 represents the electron number density, $\mathbf{E}_{\parallel} = E_z \hat{\mathbf{e}}_z + E_{\phi} \hat{\mathbf{e}}_{\phi}$ is the tangential component of the electromagnetic field and m_e is the effective electron mass. The first term of the right-hand side of (3) is the force, on the electron fluid experiences, due to the tangential component of the electric field, and the roots of the second and the third term come from the internal interaction force in the electron gas and the quantum diffraction effect or electron tunneling (Bohm potential) representing the quantum pressure, respectively. Here, $\alpha = v_F^2 / 2$ is the speed of propagation of the density disturbances in the electron gas and $\beta = (a_B v_F)^2 / 4$ describes single-electron excitations in the electron gas (which $v_F = (2\pi n_0 a_B^2)^{1/2} v_B$ being the Fermi velocity of the 2D electron gas, a_B and v_B are the Bohr radius and the Bohr velocity, respectively). By expanding the electric field vector $\mathbf{E}(\mathbf{r}, t)$ and the magnetic field vector $\mathbf{B}(\mathbf{r}, t)$ in the following Fourier forms

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

One may eliminate the velocity $\mathbf{u}(\mathbf{r}_S, t)$ from (1) and (2) and obtain

$$\frac{\partial^2 n_1(\mathbf{r}_S, t)}{\partial t^2} = \frac{e n_0}{m_e} \nabla_{\parallel} \cdot \mathbf{E}_{\parallel}(\mathbf{r}_S, t) + \alpha \nabla_{\parallel}^2 n_1(\mathbf{r}_S, t) - \beta \nabla_{\parallel}^2 (\nabla_{\parallel}^2 n_1(\mathbf{r}_S, t)) + v_{ex}^2 \nabla_{\parallel}^2 n_1(\mathbf{r}_S, t), \quad (5)$$

where $v_{ex}^2 = 0.328 n_0^{1/3} e^2 / m_e \varepsilon [1 + 0.624(1 + 18.37 n_0^{1/3} a_B)]$ [23].

By means of the space-time Fourier transforms for the induced density $n_1(\mathbf{r}_S, t)$ on the cylindrical surface,

$$n_1(\varphi, z, t) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dq N_m(q) e^{i(m\varphi + qz - \omega t)}, \quad (6)$$

where

$$N_m = -i \frac{e n_0}{m_e} \frac{1}{W_m} \mathbf{q}_m \cdot \mathbf{E}_m, \quad (7)$$

where

$$\mathbf{q}_m = q \hat{\mathbf{e}}_z + (m/a) \hat{\mathbf{e}}_{\phi} \quad \text{and}$$

$W_m = \omega^2 - \alpha q_m^2 - \beta q_m^4 - v_{ex}^2 q_m^2$. By combining the Maxwell's equations, one may obtain the well-known Helmholtz equations for the z -components E_{zm} and B_{zm} of the expanding coefficients \mathbf{E}_{zm} and \mathbf{B}_{zm}

$$\frac{d^2 E_{zm}}{dr^2} + \frac{1}{r} \frac{d E_{zm}}{dr} - \left(\kappa^2 + \frac{m^2}{r^2} \right) E_{zm} = 0, \quad (8)$$

and

$$\frac{d^2 B_{zm}}{dr^2} + \frac{1}{r} \frac{d B_{zm}}{dr} - \left(\kappa^2 + \frac{m^2}{r^2} \right) B_{zm} = 0, \quad (9)$$

where $\kappa^2 = q^2 - \omega^2 / c^2$ and c is the light speed. In the following two sections, we have tried to derive the plasmon dispersion of low-frequency electromagnetic wave (so $\omega/c \ll q$ [3]) with the TM and TE modes, of course, by solving (8) and (9) by providing appropriate boundary conditions. With the induced density, these boundary conditions can be written as

$$E_{rm}(a) \Big|_{r>a} - E_{rm}(a) \Big|_{r<a} = -\frac{e N_m}{\varepsilon_0}, \quad (10)$$

$$\mathbf{E}_{\parallel m}(a) \Big|_{r>a} - \mathbf{E}_{\parallel m}(a) \Big|_{r<a} = 0, \quad (11)$$

and

$$B_{rm}(a) \Big|_{r>a} - B_{rm}(a) \Big|_{r<a} = 0, \quad (12)$$

As be seen from (10) and (11), by considering the

polarization of the electron fluid on the nanotube surface, the radial component of the electric field E_{rm} is discontinuous whereas the azimuthal component $E_{\varphi m}$ of the electric field is continuous at the cylinder $r = a$.

III. TM MODE

For the TM mode, the longitudinal magnetic field is zero, i.e., $B_z = 0$. From (8), the longitudinal electric field can be expressed by

$$\begin{cases} E_{zm}(r) = C_m I_m(\kappa r) & (r < a) \\ E_{zm}(r) = C_m K_m(\kappa r) & (r > a) \end{cases}, \quad (13)$$

where $I_m(x)$ and $K_m(x)$ are the modified Bessel functions, and coefficients C_m and D_m will be determined by the boundary conditions. With Maxwell's equations $\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t$ and $\nabla \times \mathbf{B} = -c^{-2} \partial \mathbf{E} / \partial t$, the radial component E_{rm} and the azimuthal component $E_{\varphi m}$ of the electric field and the radial component B_{rm} of the magnetic field can be expressed as

$$E_{rm}(r) = -\frac{i q}{\kappa^2} \frac{dE_{zm}(r)}{dr}, \quad (14)$$

$$E_{\varphi m}(r) = \frac{m q}{\kappa^2 r} E_{zm}(r), \quad (15)$$

and

$$B_{rm}(r) = \left(1 - \frac{q^2}{\kappa^2}\right) \frac{m}{\omega r} E_{zm}(r). \quad (16)$$

Using (7), (14) and (16), the Fourier coefficient N_m of the induced density is turned into

$$N_m = -i \frac{en_0}{m_e} \frac{1}{W_m} \left(q E_{zm} + \frac{m}{a} E_{\varphi m} \right), \quad (17)$$

By substituting (14)-(17) into the boundary conditions, we can obtain the following dispersion relation of the TM mode

$$\omega^2 = \alpha (\kappa^2 + \omega^2 / c^2 + m^2 / a^2) + \beta (\kappa^2 + \omega^2 / c^2 + m^2 / a^2)^2 + v_{ex}^2 (\kappa^2 + \omega^2 / c^2 + m^2 / a^2) + \Omega_p^2 (\kappa^2 a^2 + m^2) I_m(\kappa a) K_m(\kappa a) \quad (18)$$

where $\Omega_p^2 = (e^2 n_0 / \epsilon_0 m_e a)$. For derivation the above equation, 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 and with introducing the dimensionless variable $y = \omega / \Omega_p$ and $x = \kappa a$, the dispersion relation of the TM mode in the low

frequency case can be reduced to the following equation

$$y^2 = (\alpha_1 + \lambda_1) (x^2 + m^2) + \beta_1 (x^2 + m^2)^2 + (x^2 + m^2) I_m(\kappa a) K_m(\kappa a), \quad (19)$$

where $\alpha_1 = \alpha / (\Omega_p a)^2$, $\beta_1 = \beta / (\Omega_p^2 a^4)$, $\lambda_1 = v_{ex}^2 / (\Omega_p a)^2 = 2\alpha_1 \delta^2$ and $\delta = v_{ex} / v_F$.

The behavior of dispersion relation by assuming the two cases of $x \gg |m|$ or $x \ll |m|$ will be different and we can distinguish two different dimensionality regimes. For $x \gg |m|$, we may use the well-known asymptotic expressions of the Bessel functions $I_m(x) \rightarrow e^x / \sqrt{2\pi x}$, $K_m(x) \rightarrow \sqrt{\pi / 2x} e^{-x}$ (with the finite m). Thus, the dispersion relation can be written approximately as

$$y^2 = (\alpha_1 + \lambda_1) x^2 + \beta_1 x^4 + \frac{x}{2}, \quad (20)$$

For large-radius nanotubes, the parameters α_1 , β_1 and λ_1 approached zero and dispersion relation in this case becomes

$$\omega^2 = \Omega_p^2 \frac{x}{2}, \quad (21)$$

which corresponds to a proper 2D behavior. On the other hand, for $x \ll |m|$, we use other well-known expressions of Bessel functions, i.e. $I_m(x) \rightarrow a_m x^m$, $K_m(x) \rightarrow b_m x^{-m}$ (for non-zero m) in where $a_m = 2^{-m} / \Gamma(m+1)$, $b_m = 2^{m-1} \Gamma(m+1)$, and $K_0(x) \rightarrow \ln(1.23/x)$. Then for $m \neq 0$, the dispersion relation turns into

$$\omega^2 = \left[(\alpha_1 + \lambda_1) m^2 + \beta_1 m^4 + \frac{m}{2} \right] \Omega_p^2, \quad (22)$$

By comparing (21) and (22), we understand that the former is independent of the dimensions of the tube, while the latter depends strongly on the radius of the tube, and for $m = 0$, we have $\omega = 0$ implying that no wave could propagate under this condition.

In Fig. 1, the influence of the exchange-correlation potential on the dispersion relation of the TM mode for $a = 3a_B$ with different azimuthal quantum numbers is depicted. As we see, the exchange-correlation effect causes to shift up the curves.

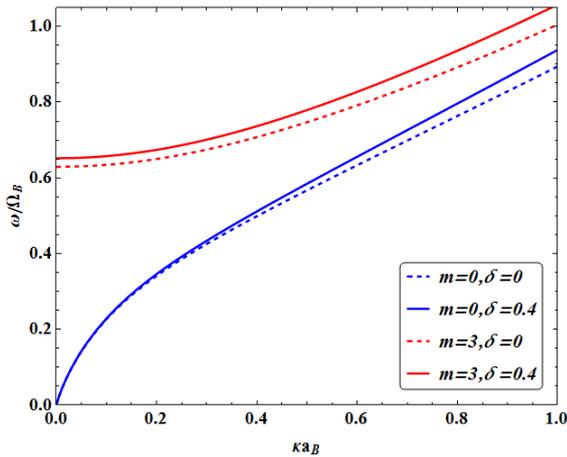


Fig. 1 Dispersion curves ω/Ω_B versus the variable κa_B of TM mode for some m and δ of a CNT with $a = 3a_B$

IV. TE MODE

For the TE mode, the longitudinal electric field is zero, i.e., $E_z=0$. From (9), the longitudinal electric field can be expressed by

$$\begin{cases} B_{zm}(r) = C_m I_m(\kappa r) & (r < a) \\ B_{zm}(r) = C_m K_m(\kappa r) & (r > a) \end{cases}, \quad (23)$$

Similar to the TM mode, with Maxwell's equations, we find the expressions of E_{rm} , $E_{\phi m}$ and B_{rm} as follows

$$E_{rm}(r) = -\frac{m\omega}{\kappa^2 r} B_{zm}(r), \quad (24)$$

$$E_{\phi m}(r) = i \frac{\omega}{\kappa^2 r} \frac{dB_{zm}(r)}{dr}, \quad (25)$$

and

$$B_{rm}(r) = -i \frac{q}{\kappa} \frac{dB_{zm}(r)}{dr}. \quad (26)$$

Using (7) and (25), the Fourier coefficient N_m of the induced density is reduced to

$$N_m = -i \frac{en_0}{m_e} \frac{1}{W_m} \frac{m}{a} E_{\phi m} = \frac{en_0}{m_e} \frac{1}{W_m} \frac{m\omega}{\kappa a} B'_{zm}(a), \quad (27)$$

Substituting (24)–(27) into boundary conditions (10)–(12), we can obtain the following dispersion relation between the frequency ω and the wave number κ

$$\omega^2 = \alpha(\kappa^2 + \omega^2/c^2 + m^2/a^2) + \beta(\kappa^2 + \omega^2/c^2 + m^2/a^2)^2 + v_{ex}^2(\kappa^2 + \omega^2/c^2 + m^2/a^2) + \Omega_p^2(\kappa a)^2 I'_m(\kappa a) K'_m(\kappa a) \quad (28)$$

where $I'_m(x)$ and $K'_m(x)$ are the derivatives of the modified Bessel functions with respect to argument $x = \kappa a$. With the dimensionless variable $y = \omega/\Omega_p$ and $x = \kappa a$, the dispersion relation of the TE mode in the low-frequency case can be turned into

$$y^2 = (\alpha_1 + \lambda_1)(x^2 + m^2) + \beta_1(x^2 + m^2)^2 + (x^2 + m^2)I'_m(\kappa a)K'_m(\kappa a), \quad (29)$$

Considering the two different regimes mentioned above (i.e. $x \gg |m|$ and $x \ll |m|$), one may derive the equations which are quite similar with TM [35], so it does not need to be repeated again.

The impact of the exchange-correlation potential on the dispersion relation of the TE mode for $a = 3a_B$ with different azimuthal quantum numbers is illustrated in Fig. 2.

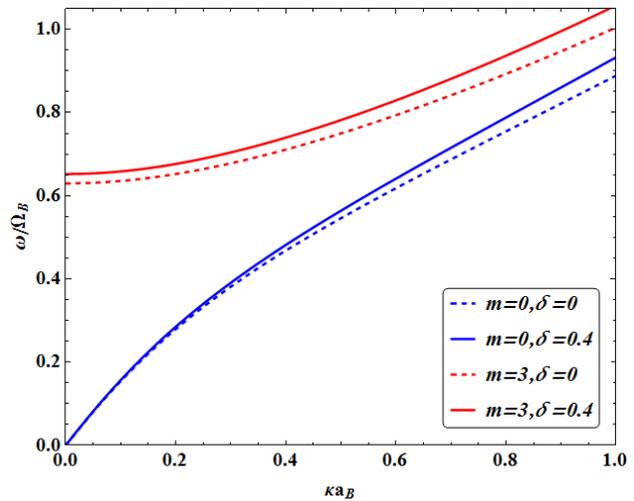


Fig. 2 Dispersion curves ω/Ω_B versus the variable κa_B of TE mode for some m and δ of a CNT with $a = 3a_B$

Comparing curves with and without the exchange-correlation potential, it can be seen that this effect plays an important role on the dispersion relation for the both modes.

V. CONCLUSION

To summarize, we studied the propagation of the electromagnetic wave in the SWCNs in the framework of QHD model by considering the role of quantum parameters (Bohm's potential) and electron exchange-correlation potential. By using the Fourier transformation of the linearized set of equations on the electron time scale by neglecting the ion dynamics in conjunction with Maxwell's equations, the general expressions have been derived for the dispersion relations of the low-frequency electromagnetic waves with TE and TM modes, respectively. The transcendental dispersion relation (TDR) derived in Sections III and IV are based on the

same method as a TDR derived by Wei *et al.* [3]. The asymptotic behaviors of the TE and TM modes were found to be similar in SWCNTs. The dispersion relations were analyzed numerically with typical data of SWCNT. Our calculations have shown the dependency of dispersion curves on the exchange-correlation effects (which were ignored in previous works) in the low frequency limit. The impact of azimuthal quantum number and CNT's radius on dispersion relation were also discussed. Adding the function of electron exchange-correlation potential V_{xc} led to the novel phenomena and extended the validity range of QHD model.

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