

Plasma wave propagation in a pair of carbon nanotubes

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Plasma waves which propagate in a pair of parallel metallic carbon nanotubes are studied within the framework of the classical electrodynamics. Electronic excitations over the each nanotube surface are modeled by an infinitesimally thin layer of free-electron gas which is described by means of the linearized hydrodynamic theory. An explicit form of plasmons dispersion in terms of interaction between the bare plasmon modes of the individual surfaces of the nanotubes is presented in this Letter.

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Among outstanding aspects about carbon nanotubes, the study of their collective electronic excitations may be very important in understanding the electron interactions in carbon nanotubes as well as the characteristics of their electronic structures. Collective excitations in the single and multi-walled carbon nanotubes have studied by several authors with various theoretical models [1–19]. Among different theoretical models, hydrodynamic model has found an important place owing to their simplicity and physically intuition. Various versions of the hydrodynamic model of the dielectric response of carbon valence electrons are becoming increasingly used to study collective excitations in such structures [9–19]. The idea to apply a macroscopic hydrodynamic description to the collective dynamics of the many electron systems was suggested by Bloch [20] as a generalization of the hydrostatic Thomas-Fermi theory. Using this simple hydrodynamic model, Fetter found plasma oscillations and screening for electron layers [21].

On the other hands, Schroter and Dereux [22], analyzed the propagation of plasmon on hollow metallic cylinders with a dielectric core, taking into account retardation. Kushawa and Djafari-Rouhani [23], used Green's function theory for calculating dispersion relations for coaxial and multiaxial structures with arbitrary dielectric constants with applications to quantum wire and carbon nanotubes. In the cases mentioned, by contrast with planar and spherical geometries, do not allow independent solutions for TM and TE modes except for the case of modes with no angular dependence. The electromagnetic fields propagating in such geometry are, in general, a linear combination of these two modes.

It is well known that single-walled carbon nanotubes tend to stick into bundles (containing $2 - N$ parallel car-

bon nanotubes) or ropes during their syntheses [24]. Recently, Lien and Lin [6], described the low-energy plasmon excitations in a pair of carbon nanotubes within the tight-binding model. Also, Gumbs and Balassis [7], in the non-retarded limit, studied the collective excitations in a pair of parallel nonoverlapping cylindrical nanotubes by using the random-phase approximation and obtained a high-frequency, corresponds to in-phase longitudinal electron density oscillations along the axes of the nanotubes and a low-frequency that is an out-of-phase collective excitation of the carriers on the two nanotubes. In this Letter, we extend the previous work [17] to describe the plasma waves with the transverse magnetic mode which propagate in a pair of parallel metallic carbon nanotubes.

Let us consider a pair of parallel nanotubes with radii a_1 and a_2 which density free-electron fluid over the each cylindrical surface (per unit area) is n_1^0 and n_2^0 , respectively. The distance between the two axes will be labeled d , where $d > a_1 + a_2$, and the used coordinates are illustrated by Fig.1. The origin of the cylindrical coordinate

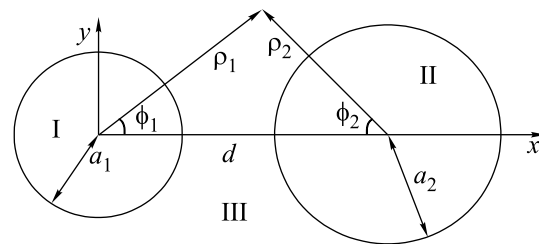


Fig.1. Schematic of a pair of parallel nanotubes with radii a_1 and a_2 , the axis-to-axis separation begin d

$\mathbf{x} = (\rho, \phi, z)$ be located at the point $z = 0$ on the axis of the 1st nanotube. Assuming that the $n_j(\mathbf{x}_j, t)$ be the perturbed density (per unit area) of the homogeneous electron fluid on the j -th wall (with $j = 1, 2$), due to

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propagation of plasma wave with frequency ω , along the axis z .

Based on the linearized hydrodynamic model, one obtain the linearized continuity equation, for each nanotube,

$$\frac{\partial n_j(\mathbf{x}_j, t)}{\partial t} + n_j^0 \nabla_j \cdot \mathbf{u}_j(\mathbf{x}_j, t) = 0, \quad (1)$$

and the linearized momentum-balance equation,

$$\begin{aligned} \frac{\partial \mathbf{u}_j(\mathbf{x}_j, t)}{\partial t} = & -\frac{e}{m_e} \mathbf{E}_{\parallel}^j(\mathbf{x}_j, t) - \\ & -\frac{\alpha_j}{n_j^0} \nabla_j n_j(\mathbf{x}_j, t) + \frac{\beta}{n_j^0} \nabla_j [\nabla_j^2 n_j(\mathbf{x}_j, t)], \end{aligned} \quad (2)$$

where $\mathbf{E}_{\parallel}^j(\mathbf{x}_j, t) = E_z^j \hat{\mathbf{e}}_z + E_{\phi_j}^j \hat{\mathbf{e}}_{\phi}$ is the tangential component of the electromagnetic field on the j -th cylindrical surface, e is the element charge, m_e is the electron mass, $\mathbf{u}_j(\mathbf{x}_j, t)$ is the velocity of the electrons residing on the j -th shell and $\nabla_j = \hat{\mathbf{e}}_z (\partial/\partial z) + a_j^{-1} \hat{\mathbf{e}}_{\phi} (\partial/\partial \phi_j)$ differentiates only tangentially to that surface. In the right-hand side of Eq. (2), the first term is the force on electrons due to the tangential component of the total electric field, evaluated at the nanotube surface $r = a_j$, the second and third terms arise from the internal interaction force in the electron gas with $\alpha_j = \pi n_j^0 \hbar^2 / m_e^2$ is the square of the speed of propagation of density disturbances in a uniform 2D homogeneous Thomas–Fermi electron fluid and $\beta = \hbar^2 / 4m_e^2$.

In the transverse magnetic wave, the magnetic field component is not in the longitudinal direction ($B_z = 0$) but in the transverse direction ($B_r, B_{\phi} \neq 0$). Using the coordinates illustrated by Fig.1 and Maxwell's equations, we may obtain the following solutions for the longitudinal electric field E_z in the three regions,

$$E_z^1(\mathbf{x}, t) = \sum_{m=-\infty}^{+\infty} A_m \frac{I_m(\kappa \rho_1)}{I_m(\kappa a_1)} e^{im\phi_1} e^{i(qz-\omega t)} \quad (\rho_1 < a_1), \quad (3)$$

$$E_z^2(\mathbf{x}, t) = \sum_{m=-\infty}^{+\infty} D_m \frac{I_m(\kappa \rho_2)}{I_m(\kappa a_2)} e^{im\phi_2} e^{i(qz-\omega t)} \quad (\rho_2 < a_2), \quad (4)$$

and

$$\begin{aligned} E_z^3(\mathbf{x}, t) = & \sum_{m=-\infty}^{+\infty} \left[B_m \frac{K_m(\kappa \rho_1)}{K_m(\kappa a_1)} e^{im\phi_1} + \right. \\ & \left. + C_m \frac{K_m(\kappa \rho_2)}{K_m(\kappa a_2)} e^{im\phi_2} \right] e^{i(qz-\omega t)} \\ & (\rho_1 > a_1 \text{ and } \rho_2 > a_2), \end{aligned} \quad (5)$$

where $I_m(x)$ and $K_m(x)$ are the modified Bessel functions, $\kappa^2 = q^2 - \omega^2/c^2$ and c is the light speed. On the other hands, after eliminating the velocity field $\mathbf{u}_j(\mathbf{x}_j, t)$, from Eq. (1) and (2) and replace the quantity n_j by expression of the form

$$n_j(\mathbf{x}_j, t) = \sum_{m=-\infty}^{+\infty} N_{jm} e^{im\phi_j} e^{i(qz-\omega t)}, \quad (6)$$

we finds

$$N_{jm} = -i \frac{e n_j^0}{m_e} \frac{1}{\Omega_j} \mathbf{q}_m^j \cdot \mathbf{E}_{\parallel}^j, \quad (7)$$

where $\mathbf{q}_m^j = q \hat{\mathbf{e}}_z + (m/a_j) \hat{\mathbf{e}}_{\phi}$ and $\Omega_j = \omega^2 - \alpha_j (\kappa^2 + \omega^2/c^2 + m^2/a_j^2) - \beta (\kappa^2 + \omega^2/c^2 + m^2/a_j^2)^2$. Now, we apply the boundary conditions [17] at the surface of the first wall, at $\rho_1 = a_1$ and express the term depending on ρ_2 and ϕ_2 in the outer cylinder in terms of ρ_1 and ϕ_1 , using an addition theorem for modified Bessel functions [25],

$$K_m(\kappa \rho_2) e^{im\phi_2} = \sum_{l=-\infty}^{+\infty} K_{l+m}(\kappa d) I_l(\kappa \rho_1) e^{il\phi_1}.$$

After doing some algebra, in the low-frequency electromagnetic wave region ($\kappa \approx q \gg \omega/c$), at $\rho_1 = a_1$, we obtain the matrix form,

$$\mathbf{B} = \mathbf{M}\mathbf{C}, \quad (8)$$

where \mathbf{B} and \mathbf{C} are vectors whose components are B_m and C_m , respectively and the matrix \mathbf{M} has the elements

$$M_{mn} = (\kappa^2 + m^2/a_1^2) \frac{a_1^2 \omega_{1p}^2}{\omega^2 - \omega_1^2} \frac{K_{m+n}(\kappa d) K_m(\kappa a_1) I_m^2(\kappa a_1)}{K_n(\kappa a_2)}. \quad (9)$$

In an analogous way, we use the boundary conditions at the surface of the second wall, at $\rho_2 = a_2$. We obtain,

$$\mathbf{C} = \mathbf{N}\mathbf{B}. \quad (10)$$

We note that the matrix \mathbf{N} is obtained from \mathbf{M} through permutation of the index 1 and 2, where $\omega_{jp}^2 = e^2 n_j^0 / \varepsilon_0 m_e a_j$ and

$$\begin{aligned} \omega_j^2(m, \kappa) = & \alpha_j (\kappa^2 + m^2/a_j^2) + \beta (\kappa^2 + m^2/a_j^2)^2 + \\ & + \omega_{jp}^2 a_j^2 (\kappa^2 + m^2/a_j^2) I_m(\kappa a_j) K_m(\kappa a_j), \end{aligned} \quad (11)$$

are the squares of the plasmon dispersion on the cylinders $j = 1$ and 2 . From Eq. (8) and (10), one obtains

$$(\mathbf{M}\mathbf{N} - \mathbf{I})\mathbf{B} = 0. \quad (12)$$

The zeros of the determinant of the matrix $(\mathbf{M}\mathbf{N} - 1)$ correspond to normal mode frequencies of the plasmon excitations on the surfaces of the two coupled cylinders, where the determinant is of infinite dimension. To obtain a simple form of plasmons dispersion in terms of interaction between the bare plasmon modes of the individual surfaces of the tubes and compare with two-walled carbon nanotubes, in the following we consider plasma wave which propagate parallel to an axial direction (z -direction) of the two parallel nanotube, so that from Eq. (12), by set $m = 0$ and $n = 0$, we obtain two branches for ω defining the resonant frequencies of the plasmon excitations which are clearly separated into a high-frequency, $\omega_+(0, \kappa)$, and a low-frequency, $\omega_-(0, \kappa)$,

$$\omega_{\pm}^2(0, \kappa) = \frac{\omega_1^2 + \omega_2^2}{2} \pm \sqrt{\left(\frac{\omega_1^2 - \omega_2^2}{2}\right)^2 + \Delta^2}, \quad (13)$$

where

$$\Delta^2 = \omega_{1p}^2 \omega_{2p}^2 (\kappa a_1)^2 (\kappa a_2)^2 [K_0(\kappa d) I_0(\kappa a_1) I_0(\kappa a_2)]^2, \quad (14)$$

gives the interaction between two parallel nanotubes. This interaction leads to shifts of the plasmon energies between the two free plasmon modes. When d decreases, the interaction will be strong and the splitting of the plasmon will be large. When $d \rightarrow \infty$, the tubules decouple (i.e., $\Delta \approx 0$) and oscillate independently of each other with frequencies ω_1 and ω_2 [see Eq. (11)]. The dispersion relations given by Eq. (13) has a structure similar to that of resonant frequencies of the plasmon excitations in two-walled carbon nanotubes and metallic nanotubes [17, 26]. In particular, in the long-wavelength limit, when each nanotube has the same radius, if we neglect the retardation effects, we obtain

$$\omega_{\pm}^2(0, \kappa \approx 0) \approx \frac{e^2 a \kappa^2}{2 \epsilon_0 m_e} (n_1^0 + n_2^0) \left| \ln \frac{\kappa a}{2} \right| \pm \frac{e^2 a \kappa^2}{\epsilon_0 m_e} \times \left\{ \frac{1}{4} (n_1^0 - n_2^0)^2 \left| \ln \frac{\kappa a}{2} \right|^2 + n_1^0 n_2^0 \left| \ln \frac{\kappa d}{2} \right|^2 \right\}^{1/2}, \quad (15)$$

where the lower-energy plasmon exhibits a quasi-acoustic (linear) dispersion that is quite similar with the result obtained in random-phase approximation [7]. This quasi-acoustic plasmon mode seems to be a common occurrence when a splitting of plasmon energies happens due to the tubule interactions [7, 17]. To illustrate the effect of two parallel walls on resonant frequency and compare with two-walled carbon nanotubes, we choose an example of a pair of carbon nanotubes with radii $a_1 = 4\Delta a$ and $a_2 = 6\Delta a$ with $d = 12\Delta a$, where $\Delta a = 3.4\text{\AA}$. To see clearly behavior

of the two groups of resonant plasmon dispersions we plot dimensionless frequency ω/ω_p , versus dimensionless variable $\kappa\Delta a$ in Fig.2, where $n_1^0 = n_2^0 = n_0$ and

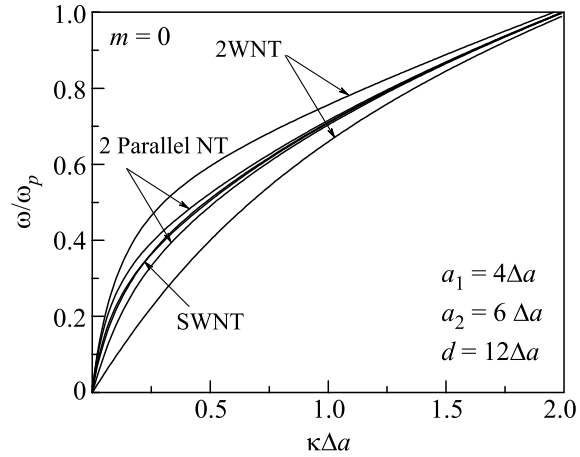


Fig.2. The dimensionless plasmon frequencies ω/ω_p versus dimensionless variable $\kappa\Delta a$ in a pair of parallel nanotubes with radii $a_1 = 4\Delta a$ and $a_2 = 6\Delta a$ are compared with the two-walled nanotubes from Ref. 17

$\omega_p = (e^2 n_0 / \epsilon_0 m_e \Delta a)^{1/2}$. It is clear that in two-walled carbon nanotubes the splitting of the plasmons is large compared with a pair of parallel carbon nanotubes. It can be seen that the dispersion curves will approach one for small wavelengths.

In summary, we have used the linearized hydrodynamic model in conjunction with Maxwell's equations to describe the plasmonic response of a pair of metallic carbon nanotubes. We have found an analytical formalism of plasmons dispersion, at low frequencies, in terms of interaction between the bare plasmon modes of the individual surfaces of the nanotubes. In long wavelength limit, if we neglect the retardation effects, the result obtained in this way is quite similar with the result obtained in random-phase approximation.

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