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Electron–ion quantum plasma excitations in single-walled carbon nanotubes

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Abstract

The effect of a uniform static external magnetic field in the Voigt configuration on electron–ion quantum plasma oscillations in single-walled carbon nanotubes is discussed using the linearized quantum hydrodynamic model in conjunction with Maxwell's equations. Transverse magnetic waves which propagate parallel to the surface of the nanotubes, in the presence of an external magnetic field, yield a spectrum containing a quantum magnetosonic branch in addition to the magnetoplasmon branch.

In 1928, Langmuir [1] investigated the oscillations of a system composed of a large number of positive ions and free electrons with zero total charge, and he was the first to use the term plasma in this way. The motion of the ions in a plasma, owing to their relatively great mass, may be neglected in comparison with the motion of the electrons. In fact, it is sufficient for many purposes to regard the plasma as an electron gas moving in a positively charged fluid of uniform density, which is called the background of positive charge.

However, in such systems both the positive ions and the electrons oscillate under low-frequency disturbances. For example, Fetter [2] used a simple hydrodynamic model to study the electrodynamics of the electron–ion plasma in a periodic array and obtained an acoustic branch in addition to the optical branch. Wei and Wang [3] studied the dispersion relation of quantum ion acoustic wave (QIAW) oscillations in single-walled carbon nanotubes (SWCNTs) with the quantum hydrodynamic (QHD) model which was developed by Haas *et al* [4, 5]. In particular, Shukla [6] considered SWCNTs as charged dust rods surrounded by electrons and ions and obtained the dispersion relation of the dust acoustic wave (DAW) oscillations using the QHD model.

On the other hand, it is well-known that there exist two types of low-frequency modes in hydromagnetic waves; one is the magnetosonic wave and other the Alfven wave [7]. Thus, in the presence of a static magnetic field, we may expect a new excitation in carbon nanotubes (CNTs), i.e. quantum magnetosonic wave (QMSW) oscillations. Let us note that the effects of a static magnetic field on the plasmon oscillations of an electron gas in CNTs have been investigated by several authors using various methods [8–16]. Shyu *et al* studied the magnetoplasmon of SWCNTs within the tight-binding model [8]. The low-frequency single-particle and collective excitations of SWCNTs were studied in the presence of a magnetic field by Chiu *et al* [9, 10]. Vedernikov *et al* [11] studied the collective oscillations of two-dimensional (2D) electrons in nanotubes in the presence of a magnetic field parallel to the tube axis. The energies of neutral and charged excitons and plasmon frequencies in nanotubes as functions of the magnetic field were analyzed by Chaplik [12]. Gumbs [13], calculated the dispersion relation of the collective magnetoplasmon excitations for an electron gas confined to the surface of a nanotube when a magnetic field is perpendicular to its axis. In particular, by using the hydrodynamic model and Maxwell's equations, Kobayashi [14] studied the magnetoplasma wave oscillations of a SWCNT in the Voigt configuration. Other authors have also reported some interesting results on collective magnetoplasmon excitations in CNTs [15, 16].

Here we are interested in transverse magnetic waves which propagate parallel to the surface of a SWCNT and concentrate on the excitations of the electron–ion system as two fluids confined to its surface. There is assumed to be a static magnetic field $\mathbf{B}_0$ that is normal to the cylindrical surface (Voigt configuration).

We consider an infinitely long and infinitesimally thin SWCNT with a radius a and take the cylindrical polar coordinate $\mathbf{x} = (r, \phi, z)$ for an arbitrary point in space. Let us consider the CNT to consist of electron and ion fluids superimposed at $r = a$ with charges e and Ze, respectively. Charge neutrality requires that the equilibrium densities (per unit area) of electrons n_e^0 and ions n_i^0 satisfy $n_i^0 = n_0$ and

$n_e^0 = Zn_i^0 = Zn_0 = 4 \times 38\ \mathrm{nm}^{-2}$. Assuming that n_e (n_i) is the perturbed density (per unit area) of the homogeneous electron (ion) fluid on the nanotube surface, due to a propagating plasma wave with frequency ω along the nanotube axis z.

The behavior of the quantum plasma under consideration may be described by the following two-fluid equations: equations of linearized continuity

$$\frac{\partial n_e(\mathbf{x},t)}{\partial t} + Zn_0\nabla_\parallel \cdot \mathbf{u}_e(\mathbf{x},t) = 0, \tag{1}$$

$$\frac{\partial n_i(\mathbf{x},t)}{\partial t} + n_0\nabla_\parallel \cdot \mathbf{u}_i(\mathbf{x},t) = 0, \tag{2}$$

and equations of linearized momentum,

$$\frac{\partial \mathbf{u}_e(\mathbf{x},t)}{\partial t} = -\frac{e}{m_e}\left[\mathbf{E}_\parallel(\mathbf{x},t) + \mathbf{u}_e(\mathbf{x},t)\times\mathbf{B}_0\right] - \frac{\alpha}{Zn_0}\nabla_\parallel n_e(\mathbf{x},t) + \frac{\beta}{Zn_0}\nabla_\parallel\left[\nabla_\parallel^2 n_e(\mathbf{x},t)\right], \tag{3}$$

$$\frac{\partial \mathbf{u}_i(\mathbf{x},t)}{\partial t} = \frac{Ze}{m_i}\left[\mathbf{E}_\parallel(\mathbf{x},t) + \mathbf{u}_i(\mathbf{x},t)\times\mathbf{B}_0\right] \tag{4}$$

where $\mathbf{E}_\parallel(\mathbf{x},t) = E_z\hat{\mathbf{e}}_z + E_\phi\hat{\mathbf{e}}_\phi$ is the tangential component of the electromagnetic field, m_e (m_i) is the electron (ion) mass, $\mathbf{u}_e$ ($\mathbf{u}_i$) is the velocity of the electron (ion) fluid and $\nabla_\parallel = \hat{\mathbf{e}}_z(\partial/\partial z) + a^{-1}\hat{\mathbf{e}}_\phi(\partial/\partial\phi)$ differentiates only tangentially to the nanotube surface. In the right-hand side of equation (3), the first term is the force on the electron fluid due to the tangential component of the electric field and drift, $\mathbf{u}_e \times \mathbf{B}_0$, evaluated at the nanotube surface $r = a$, and the second term is the force due to the internal interaction in the electron species, with $\alpha = \pi Zn_0\hbar^2/m_e^2$ that is the square of the speed of propagation of density disturbances in a uniform 2D homogeneous Fermi electron fluid. This term can be considered to be the classical pressure of the electron fluid, whereas the third term with $\beta = \hbar^2/4m_e^2$ comes from the quantum diffraction effect contained in the $\hbar$-dependent term (sometimes called the Bohm potential) that represents the quantum pressure.

The electric current density flowing on the surface of the cylinder is given by

$$\mathbf{J}_e(\mathbf{x},t) = -Zen_0\mathbf{u}_e(\mathbf{x},t) = \hat{\sigma}_e\mathbf{E}_\parallel(\mathbf{x},t), \tag{5}$$

$$\mathbf{J}_i(\mathbf{x},t) = Zen_0\mathbf{u}_i(\mathbf{x},t) = \hat{\sigma}_i\mathbf{E}_\parallel(\mathbf{x},t), \tag{6}$$

where $\hat{\sigma}_e$ ($\hat{\sigma}_i$) is the conductivity tensor of the electron (ion). We define the Fourier–Bessel (FB) transform $A_m(q)$ of an arbitrary function $A(\phi,z,t)$ by

$$A(\phi,z,t) = \sum_{m=-\infty}^{+\infty}\int_{-\infty}^{+\infty} \mathrm{d}q\, A_m(q)\exp\left[\mathrm{i}(m\phi + qz - \omega t)\right], \tag{7}$$

By eliminating the induced density $n_e(\mathbf{x},t)$ and $n_i(\mathbf{x},t)$ from equations (1)–(4) and applying equations (5)–(7), we find

$$\hat{\sigma}_e = \frac{\mathrm{i}n_0Ze^2}{m_e\omega\Omega_m^2} \times \begin{pmatrix} \omega^2 - \frac{m^2}{a^2}(\alpha+\beta q_m^2) & \frac{m}{a}q(\alpha+\beta q_m^2) + \mathrm{i}\omega\omega_{ce} \\ \frac{m}{a}q(\alpha+\beta q_m^2) - \mathrm{i}\omega\omega_{ce} & \omega^2 - q^2(\alpha+\beta q_m^2) \end{pmatrix}, \tag{8}$$

$$\hat{\sigma}_i = \frac{\mathrm{i}n_0Z^2e^2}{m_i(\omega^2-\omega_{ci}^2)}\begin{pmatrix} \omega & -\mathrm{i}\omega_{ci} \\ \mathrm{i}\omega_{ci} & \omega \end{pmatrix}, \tag{9}$$

where $\omega_{ce} = eB_0/m_e$ ($\omega_{ci} = ZeB_0/m_i$) is the cyclotron frequency of the electron (ion), $\Omega_m^2 = \omega^2 - \omega_{ce}^2 - \alpha q_m^2 - \beta q_m^4$ and $q_m^2 = q^2 - m^2/a^2$.

In the space above and below the 2D electron–ion cylinder, the transverse electric wave, satisfies the solution

$$E_{zm}(r) = E_{0z}K_m(\kappa a)I_m(\kappa r) \qquad (r < a), \tag{10}$$

and

$$E_{zm}(r) = E_{0z}I_m(\kappa a)K_m(\kappa r) \qquad (r > a), \tag{11}$$

where $I_m(x)$ and $K_m(x)$ are the modified Bessel functions and $\kappa^2 = q^2 - \omega^2/c^2$ and c is the speed of light. Due to the polarization of the electron–ion fluid on the nanotube surface, the radial component of the electric field is discontinuous at the cylinder $r = a$ and we have

$$E_{rm}(a)|_{r>a} - E_{rm}(a)|_{r<a} = \frac{1}{\epsilon_0\omega}\left[q(j_{ez}+j_{iz}) + \frac{m}{a}(j_{e\phi}+j_{i\phi})\right], \tag{12}$$

where ϵ_0 is the permittivity of free space and the radial component E_{rm} and the azimuthal component $E_{\phi m}$ of the electric field are given in [17]. For the particular case when the speed of light can be taken to be infinitely large, i.e. $c \longrightarrow \infty$, we have

$$\begin{aligned}\omega^4 - \omega^2\Bigg[&(\alpha+\beta q_m^2)q_m^2 + \left(1+\frac{Z^2m_e^2}{m_i^2}\right)\omega_{ce}^2 \\ &+ \frac{e^2Zn_0a}{\epsilon_0m_e}\left(1+\frac{Zm_e}{m_i}\right)q_m^2I_m(qa)K_m(qa)\Bigg] \\ &+ \frac{Zm_e}{m_i}\left[(\alpha+\beta q_m^2)q_m^2 + \left(1+\frac{Zm_e}{m_i}\right)\omega_{ce}^2\right] \\ &\times \frac{e^2Zn_0a}{\epsilon_0m_e}q_m^2I_m(qa)K_m(qa) \\ &+ \frac{Z^2m_e^2}{m_i^2}\omega_{ce}^2\left[\omega_{ce}^2 + (\alpha+\beta q_m^2)q_m^2\right] = 0,\end{aligned} \tag{13}$$

which determines the normal electrostatic modes. In the limit $Zm_e/m_i \ll 1$, the roots of equation (13) become

$$\omega_+^2(m,q) \approx \omega_{ce}^2 + \alpha q_m^2 + \beta q_m^4 + \frac{e^2Zn_0a}{\epsilon_0m_e}q_m^2I_m(qa)K_m(qa), \tag{14}$$

$$\omega_-^2(m,q) \approx \frac{Zm_e}{m_i}\left[\omega_{ce}^2 + (\alpha+\beta q_m^2)q_m^2\right] \times \left[1 + \frac{\omega_{ce}^2 + (\alpha+\beta q_m^2)q_m^2}{\frac{e^2Zn_0a}{\epsilon_0m_e}q_m^2I_m(qa)K_m(qa)}\right]^{-1} \tag{15}$$

representing a high frequency (magnetoplasmon dispersion) and a low frequency (QMSW dispersion), respectively.

By setting $m = 0$ and $\alpha = \beta = 0$, from equation (14) we obtain the result in [14] that it is known as the upper hybrid mode in gas plasma physics [7]. Formally speaking, the dispersion curves ω_+ for the nanotube continue to increase with increasing value of q for all m. On the other hand, when one turns off the external magnetic field, equation (15) describes the QIAW oscillations in the SWCNTs [3]. Let us note here that the terms with β do not affect in any substantial way the long-wavelength properties of the dispersion relations, equations (14) and (15) [18–20]. Thus, in the following discussion, we may neglect the term β for the long-wavelength limit. The dispersion of QMSW oscillations, equation (15), has interesting limits:

(1) In the long-wavelength limit, i.e. $qa \longrightarrow 0$, by using the well-known expressions of Bessel functions, $I_m(x) = a_m x^m$, $K_0(x) = \ln(1.123/x)$ and $K_m(x) = b_m x^{-m} (m \neq 0)$, where here $a_m = 2^{-m}/\Gamma(m+1)$ and $b_m = 2^{m-1}\Gamma(m)$, we may obtain for $m = 0$

$$\omega_-^2(m=0, q\approx 0) \approx \frac{Zm_e}{m_i}\frac{Ze^2n_0a}{\epsilon_0 m_e}\left|\ln\frac{qa}{2}\right| q, \tag{16}$$

where $(\frac{Zm_e}{m_i}\frac{Ze^2n_0a}{\epsilon_0 m_e}|\ln\frac{qa}{2}|)^{1/2}$ is the propagating velocity of the magnetosonic mode and dose not depends on the magnitude of external magnetic field. For $m \neq 0$, one obtains

$$\omega_-^2(m, q=0) \approx \frac{Zm_e}{m_i}\left[\omega_{ce}^2 + \alpha\frac{m^2}{a^2}\right]\left[1 + \frac{\omega_{ce}^2 + \alpha\frac{m^2}{a^2}}{\frac{e^2n_0}{\epsilon_0 m_e a}\frac{m}{2}}\right]^{-1}, \tag{17}$$

which is quite sensitive to an external magnetic field and the radius of the tube. It is easy to find that as the values of the nanotube radius a increases the values of ω_- decrease.

(2) In the short-wavelength limit, i.e. $qa \longrightarrow \infty$, we may use the asymptotic expressions of the Bessel functions $I_m(x) = e^x/\sqrt{2\pi x}$ and $K_m(x) = \sqrt{\frac{\pi}{2x}}e^{-x}$, so that the dispersion relation can be written approximately as

$$\omega_-^2(q) \approx \frac{Zm_e}{m_i}\left[\alpha + \beta q^2\right] q^2 \left[1 + \frac{\alpha + \beta q^2}{\frac{e^2n_0}{\epsilon_0 m_e}\frac{1}{2q}}\right]^{-1}. \tag{18}$$

Comparing the long-wavelength and short-wavelength limits, it can be seen that the internal interaction forces play an important role in the dispersion relation, in the short-wavelength limit. Also, it is clear that the external static magnetic field increases the frequencies only in the long-wavelength limit.

In the following, let us consider the cold plasma approximation in the long-wavelength limit [21, 22]. Then equations (14) and (15) yield

$$\omega_+^2(m, q) \approx \omega_{ce}^2 + \frac{e^2Zn_0a}{\epsilon_0 m_e} q_m^2 I_m(qa)K_m(qa), \tag{19}$$

$$\omega_-^2(m, q) \approx \frac{Zm_e}{m_i}\omega_{ce}^2\left[1 + \frac{\omega_{ce}^2}{\frac{e^2Zn_0a}{\epsilon_0 m_e} q_m^2 I_m(qa)K_m(qa)}\right]^{-1}. \tag{20}$$

At this stage it is easy to make sure that, in the presence of a static magnetic field, when one turns off the internal interaction in the electron fluid magnetosonic wave (MSW), oscillations may be found in the CNTs. We expect that one will obtain similar MSW oscillations in the random phase approximation (RPA) approach, since the hydrodynamic model gives results equivalent to the RPA method in the long-wavelength limit. This long-wavelength agreement between hydrodynamic and RPA theories is well known in the literature [23].

To see clearly the character of the dispersion relation for the MSW oscillations, we illustrate in figure 1 the dependence

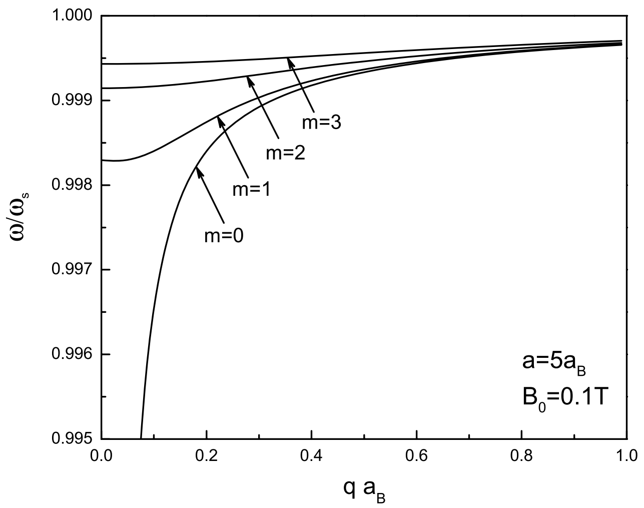

Figure 1. Dispersion curves ω_-/ω_s versus the variable qa_B, from equation (20), for a single-walled carbon nanotube with the radius $a = 5a_B$, where $\omega_s = (Zm_e\omega_{ce}^2/m_i)^{1/2}$ and $B_0 = 0.1$ T.

of the dimensionless frequency ω/ω_s on the dimensionless variable qa_B for a nanotube characterized by $a = 5a_B$ and different values of m, where $\omega_s = (Zm_e\omega_{ce}^2/m_i)^{1/2}$ and $B_0 = 0.1$ T. Let us note here that the magnetic field strength is chosen in a range that is experimentally accessible. However, the second term of equation (19) overwhelms the first term in the region of a magnetic field of $B = 0.1$ T [14]. It can be seen that for the MSW oscillations, the frequencies becomes fixed for all m modes when the wavenumber approaches infinity.

In conclusion, we have used the two-fluid quantum hydrodynamic model in conjunction with Maxwell's equations to investigate the QMSW oscillations in SWCNTs. General expressions have been derived for the dispersion relation of the electrostatic modes oscillations. In particular, in the cold plasma approximation, we have discussed the possibility of MSW oscillations in CNTs.

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