Dispersion relation of dust acoustic waves in metallic multi-walled carbon nanotubes

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In this paper, a charged multi-walled carbon nanotube (MWCNT), which is surrounded by charged nanoparticles, is modeled as a cylindrical shell of electron–ion–dust plasma. By employing classical electrodynamics formulations and the linearized hydrodynamic model, the dispersion relation of the dust acoustic wave oscillations in the composed system is investigated. We obtain a new low-frequency electrostatic excitation in the MWCNT, i.e. dust acoustic wave oscillations.

Keywords: dust acoustic wave, dispersion relation

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1. Introduction

Since the discovery of quasi-one-dimensional crystalline structures of carbon atoms, generally referred to as carbon nanotubes (CNTs), by Iijima,[1] several unique physical properties have been predicted theoretically and detected experimentally. Much accumulated information is available in several review papers and monographs.[2,3] CNTs are classified by the dual index (m, n). The two integers m and n represent a vector characterizing the method of turning a planar sheet into a nanotube, with $n = 0$ for zigzag CNTs, $n = m$ for armchair CNTs, and $0 < n \neq m$ for chiral CNTs.

It is well known that CNTs can be metallic or semiconducting, depending on their radius and geometric angle, and their electron and ion components can be regarded as a two-species quantum plasma system. Both the electrons and the ions in CNTs oscillate under low-frequency disturbances. Collective or plasmon excitations of electrons in CNTs have been the focus of intense experimental[4,5] and theoretical[6−9] research over the past several years. Wei and Wang[10] studied the dispersion relation of the low-frequency excitations, i.e. ion-acoustic wave (IAW) oscillations in single wall carbon nanotubes (SWCNTs), with the quantum hydrodynamic model that was developed by Haas *et al.*[11] In the dusty plasma, it is well known that the two normal modes of the unmagnetized weakly coupled plasma are the dust-acoustic (DA) and dust–ion-acoustic (DIA) waves. The DA waves have been theoretically predicted by Rao *et al.*[12] for the multi-component collisionless dusty plasma that constitutes electrons, ions, and negatively charged dust grains. The phase velocity of the DA wave is much smaller than the electrons and the ion thermal speeds. Shukla and Silin[13] were the first to investigate dust-ion acoustic waves (DIAW) theoretically, and they were later observed in laboratory experiments.[14] The phase velocity of the DIA wave is much smaller (larger) than the electron thermal speed (ion and dust thermal speeds). Assuming that metallic CNTs are charged due to the field emission, Shukla[15] considered an ensemble of charged CNTs as charged dust rods surrounded by electrons and ions, and obtained the dispersion relation for the dust acoustic wave (DAW) in the system. Most of the above investigations of DA waves and DIAWs were based on the assumption of constant dust charge. However, dust charge fluctuation is common in the actual environment[16] due to electron and ion collection, secondary electron emission, photoelectron emission, charge exchange with neutral grains, ionization and recombination, etc.

The DAW is a long-wavelength low-frequency collective oscillation mode in the dusty plasma,[17] in which massive charged particles participate in the

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wave motion. The first linear and nonlinear analysis of this mode was presented by Rao *et al.*,[18] who obtained the linear dispersion relation that was verified experimentally by Barkan *et al.*[19] in 1995. DAWs have been observed under a variety of plasma sources and dust conditions in several experiments.[20–22]

In this paper, for simplicity, we model a charged single wall carbon nanotube surrounded by charged nanoparticles[23,24] along with a cylindrical shell of electron–ion–dust plasma. We study the long-wavelength low-frequency collective oscillations. We shall consider modes in which the dust particle dynamics are crucial rather than those that are simply affected by the dust. In particular, we study the collective motion of the negatively charged dust particles in a background of electrons and ions in thermodynamic equilibrium. Thus, we may expect a new low-frequency excitation in the new composed system, i.e. the DAW oscillations.

1.1. Formulation of the problem

We consider CNTs with a radius of a. An arbitrary point in space is denoted by $\boldsymbol{X}(r,\phi,z)$ in the cylindrical polar coordinate system. And $\boldsymbol{X}_w(a_w,\phi,z)$ represents the coordinate of a point on the cylindrical surface, $r=a_w$ $(w=1,2,\ldots,N)$. The density perturbations can be obtained from the continuity and the momentum equations as[25,26]

$$\frac{\partial n_{sw1}(\boldsymbol{X}_w,t)}{\partial t}+n_{s0}\boldsymbol{\nabla}_w\cdot\boldsymbol{u}_{sw}(\boldsymbol{X}_w,t)=0, \quad (1)$$

and

$$0=-\frac{q_s}{m_s}\boldsymbol{\nabla}_w\Phi(\boldsymbol{X}_w,t)-\frac{1}{m_s n_{s0}}\boldsymbol{\nabla}_w p_{sw1}(\boldsymbol{X}_w,t)+\frac{\hbar^2}{4m_s^2 n_{s0}}\boldsymbol{\nabla}_w\boldsymbol{\nabla}_w^2 n_{sw1}(\boldsymbol{X}_w,t), \quad (s=\mathrm{e},\mathrm{i}), \quad (2)$$

$$\frac{\partial \boldsymbol{u}_{\mathrm{d}w}(\boldsymbol{X}_w,t)}{\partial t}=-\frac{q_{\mathrm{d}}}{m_{\mathrm{d}}}\boldsymbol{\nabla}_w\Phi(\boldsymbol{X}_w,t), \quad (3)$$

where $n_{sw1}(\boldsymbol{X}_w,t)$, s=e, i, d are the electron, the ion, and the dust density perturbations on the w-th wall, respectively, m_{e}, m_{i}, and m_{d} are the electron, the ion, and the dust masses, respectively, and $\hbar$ is the reduced Planck constant. The second and the third terms on the right-hand side of Eq. (2) are associated with the quantum pressure law[26–28] [(e.g. $p_{sw1}=(3n_{s0}/8\pi)^{2/3}(4\pi^2\hbar^2/3m_s)n_{sw1}$ for nonrelativistic degenerate electrons) and the Bohm potential[28–31] in our metallic plasma, respectively. The electrons and the ions are coupled with the charged dust via the space charge electric field.

According to $\alpha_s=(3n_{s0}/8\pi)^{2/3}(4\pi^2\hbar^2/3m_s^2)$, $\beta_s=\hbar^2/4m_s^2$, and by using Eq. (2), we can obtain

$$0=-\frac{q_s}{m_s}\boldsymbol{\nabla}_w\Phi(\boldsymbol{X}_w,t)-\frac{\alpha_s}{n_{s0}}\boldsymbol{\nabla}_w n_{sw1}(\boldsymbol{X}_w,t)+\frac{\beta_s}{n_{s0}}\boldsymbol{\nabla}_w\boldsymbol{\nabla}_w^2 n_{sw1}(\boldsymbol{X}_w,t), \quad (s=\mathrm{e},\mathrm{i}). \quad (4)$$

The self-consistent potential is given by

$$\Phi(\boldsymbol{X},t)=\sum_{w=1,2,\ldots,N}\int \mathrm{d}^2\acute{X}_w\frac{q_{\mathrm{e}}n_{\mathrm{e}w1}(\acute{\boldsymbol{X}}_w,t)+q_{\mathrm{i}}n_{\mathrm{i}w1}(\acute{\boldsymbol{X}}_w,t)+q_{\mathrm{d}}n_{\mathrm{d}w1}(\acute{\boldsymbol{X}}_w,t)}{|\boldsymbol{X}-\acute{\boldsymbol{X}}_w|}, \quad (5)$$

where $\acute{\boldsymbol{X}}_w=(a_w,\acute{\phi},\acute{z})$, and $\mathrm{d}^2\acute{X}_w=a_w\mathrm{d}\acute{\phi}\mathrm{d}\acute{z}$ is the differential surface element on the w-th nanoshell surface. The Fourier–Bessel transform $\tilde{A}(m,q,\omega)$ of an arbitrary function $A(\phi,z,t)$ is given by

$$A(\phi,z,t)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{(2\pi)^2}\times\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\tilde{A}(m,q,\omega)\,\mathrm{e}^{\mathrm{i}(qz+m\phi-\omega t)}. \quad (6)$$

The Coulomb potential in the cylindrical coordinate is given by

$$\frac{1}{|\boldsymbol{X}-\acute{\boldsymbol{X}}|}=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{(2\pi)^2}g(r,\acute{r};m,q)\,\mathrm{e}^{\mathrm{i}q(z-\acute{z})+\mathrm{i}m(\phi-\acute{\phi})}, \quad (7)$$

where $g(r,\acute{r};m,q)=4\pi I_m(|q|r_<)K_m(|q|r_>)$, $r_<=\min(r,\acute{r})$, and $r_>=\max(r,\acute{r})$. The Fourier transform of the potential can be expressed as

$$\tilde{\Phi}(r,m,q,\omega)=\sum_{w=1,2,\ldots,N}g(r,a_w;m,q)\times\sum_{s=\mathrm{e},\mathrm{i},\mathrm{d}}\tilde{n}_{sw1}(\acute{m},\acute{q},\omega), \quad (8)$$

where the Fourier transforms of the perturbed electron, ion, and dust densities are

$$\tilde{n}_{sw1}(m,q,\omega)=-\frac{q_s n_{s0}\tilde{\Phi}(a_w,m,q,\omega)}{m_s(\alpha_s+\beta_s q_{mw}^2)}, \quad (s=\mathrm{e},\mathrm{i}), \quad (9)$$

$$\tilde{n}_{\mathrm{d}w1}(m,q,\omega)=\frac{q_{\mathrm{d}}n_{\mathrm{d}0}q_{mw}^2\tilde{\Phi}(a_w,m,q,\omega)}{m_{\mathrm{d}}w^2}, \tag{10}$$

with $q_{mw}^2=q^2+m^2/a_w^2$.

For an N-wall nanotube, by using Eqs. (8)–(10), we can obtain the following equation:

$$|\boldsymbol{H}_{N\times N}-\boldsymbol{I}_{N\times N}|=0, \tag{11}$$

where $\boldsymbol{I}_{N\times N}$ is a unit matrix, and the matrix elements of $\boldsymbol{H}_{N\times N}$ are

$$H_{wl}=a_l g(a_w,a_l;m,q)\sum_{s=\mathrm{e,i}}\frac{-q_s^2n_{s0}}{m_s(\alpha_s+\beta_s q_{mw}^2)}+\frac{q_{\mathrm{d}}^2n_{\mathrm{d}0}q_{mw}^2}{m_{\mathrm{d}}w^2}. \tag{12}$$

We calculated the dispersion relations for the single-wall ($N=1$) and the double-wall ($N=2$) carbon nanotubes. For the SWCNTs ($N=1$), equation (11) can be written as

$$H_{11}-1=0. \tag{13}$$

With

$$G=I_m(|q|a)K_m(|q|a)/a,$$

$$Q=4Ga^2\sum_{s=\mathrm{e,i}}m_s^2\omega_{ps}^2/\hbar^2(k_{\mathrm{F}s}^2+q_m^2),$$

$\omega_{ps}^2=4\pi n_{s0}q_s^2/m_s$, and $k_{\mathrm{F}s}^2=(16\pi^2/3)(3n_{s0}/8\pi)^{2/3}$, the frequency for the SWCNTs is given by

$$\omega=\frac{\sqrt{G}q_m a\omega_{\mathrm{pd}}}{(1+Q)^{1/2}}. \tag{14}$$

For the DWCNTs, equation (11) can be written as

$$(H_{11}-1)(H_{22}-1)-H_{12}H_{21}=0. \tag{15}$$

With

$$G_w=I_m(|q|a_w)K_m(|q|a_w)/a_w,$$
$$Q_w=4G_wa_w^2\sum_{s=\mathrm{e,i}}m_s^2\omega_{ps}^2/\hbar^2(k_{\mathrm{F}s}^2+q_{mw}^2),$$

and $B=I_m(|q|a_1)K_m(|q|a_2)/(K_m(|q|a_1)I_m(|q|a_2))$, the resonant frequencies of the plasmon excitations are obtained as

$$\omega_{\pm}^2=\frac{\omega_1^2(1+Q_1)[1+Q_2(1-B)]+\omega_2^2(1+Q_2)[1+Q_1(1-B)]}{2(1+Q_1+Q_2+(1-B)Q_1Q_2)}\pm\frac{1}{2}\left(\left\{\frac{\omega_1^2(1+Q_1)[1+Q_2(1-B)]+\omega_2^2(1+Q_2)[1+Q_1(1-B)]}{(1+Q_1+Q_2+(1-B)Q_1Q_2)}\right\}^2-4\frac{\omega_1^2\omega_2^2(1+Q_1)(1+Q_2)(1-B)}{1+Q_1+Q_2+(1-B)Q_1Q_2}\right)^{1/2}, \tag{16}$$

where

$$\omega_1=\sqrt{G_1}q_{m1}a_1\omega_{\mathrm{pd}}/(1+Q_1)^{1/2}$$

and

$$\omega_2=\sqrt{G_2}q_{m2}a_2\omega_{\mathrm{pd}}/(1+Q_2)^{1/2}$$

are the frequencies of the oscillations on cylinders 1 and 2 of the metallic SWCNTs, respectively.

2. Numerical results and discussion

In order to clearly see the character of the dispersion relation, the dependence of dimensionless frequency ω/ω_{pd} on dimensionless variable $q\Delta a$ for an SWCNT characterized with a diameter of 8.82 Å and different values of m is illustrated in Fig. 1(a). It is shown that ω for the nanotube continuously increases with the increasing value of $q\Delta a$ for all $m\geq 0$.

To illustrate the effect of two layers on resonant frequency, we set an example of a DWCNT with the inner and outer cylinders having radii of $a_1=5.43$ Å and $a_2=8.82$ Å, respectively. To see the behaviors of the two groups of resonant plasmon dispersions from Eq. (16) clearly, we plot dimensionless frequency $\omega_{\pm}/\omega_{pd}$ versus dimensionless variable $q\Delta a$ in Fig. 1(b) for $m=0,1,2$, and 3. We note that all the curves in Fig. 1(b) tend to the same limit for large q. The upper group of plasmon dispersions exhibit a characteristic dimensional crossover from a one-dimensional electron system to a two-dimensional electron system,[10] and the lower group of plasmon dispersions exhibit weaker dispersions, which are consistent with the results found for SWCNTs and MWCNTs in Ref. [32].

To better understand the behavior of the DAW oscillations in the system, in Fig. 2 we plot dimensionless frequency $\omega/\omega_{\mathrm{pd}}$ versus dimensionless variable

$q\Delta a$ for SWCNTs and DWCNTs using Eqs. (14) and (16), respectively. As can be seen, the DAW oscillation frequencies continuously increase with the increasing value of $q\Delta a$ for all m. It is important to note that equations (14) and (16) are in qualitative agreement with the low frequency excitations obtained theoretically for SWCNTs[33] and DWCNTs,[27] as shown in Figs. 1 and 2.

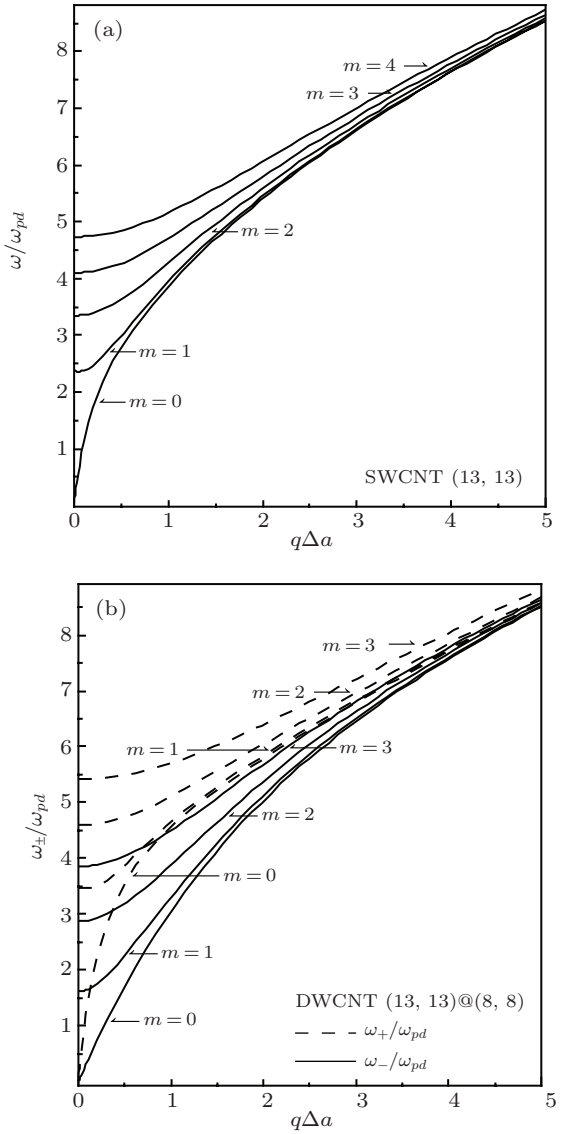


Fig. 1. Dispersion relations for (a) an SWCNT with diameter $a = 8.82$ Å and (b) a DWCNT with diameters $a_1 = 5.43$ Å and $a_2 = 8.82$ Å.

We then investigated the DAW. The dust acoustic wave is an acoustic wave in which the dust does participate in the wave motion. It is really a dust mode in which the dynamics of the dust is the essential feature.

In the DAW, the dust participates directly in the wave motion. This means that the wave is propagating because of the dust oscillation. Meanwhile, in the DIAW, the ions play the main role, the wave is propagating due to ion oscillations, and the dust is immobile, neutralizing the background. By considering the fact that the dust is much heavier than the ion, we can understand why the DAW frequency is much smaller than the DIAW frequency.

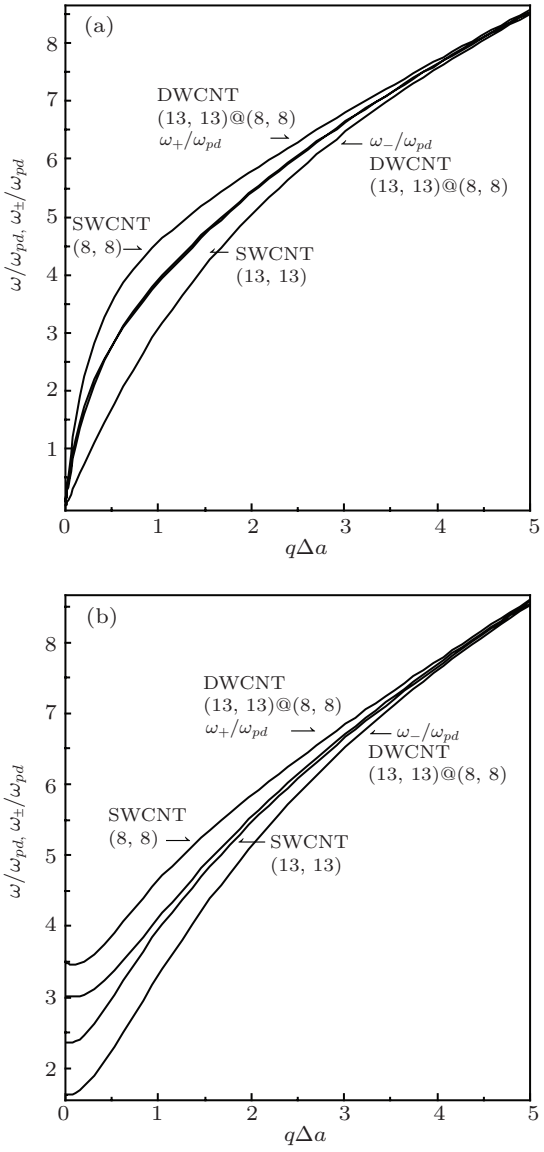


Fig. 2. Dispersion relations for (a) $m = 0$ and (b) $m = 1$.

3. Conclusion

In this work, we have discussed the possible excitation of DAW oscillations in metallic plasma composed of charged MWCNTs. We derived an analytical expression for the dispersion relation of the DAW in the composed system by employing classical electrodynamics formulation and the linearized hydrodynamic

model. The new excitation, i.e. DAW oscillations, is found theoretically.

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