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Interaction of charged particles with nanotubes

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ABSTRACT

We have studied the interaction of charged particles with single-walled metallic nanotubes by solving Poisson's equation with appropriate boundary conditions. Numerical results for the energy dispersion relations as a function of the wave vector are presented when the charged particle is inside or outside the nanotube.

1. Introduction

Interaction of charged particles with nanoscale systems has attracted much interest in the past several years. These processes play an important role in a variety of recent studies of charged particle interactions with nanotubes due to applications in both fundamental and applied physics, such as, the electron energy loss spectroscopy of nanotubes [1–4] and plasmon excitations [5,6], channeling of ion or electron beams through the nanotubes [7,8] and very recently in nanoelectronics and nanophotonics [9]. In addition, recent technological developments in the area of plasmonic devices, which are considered as a route of subwavelength instruments, have produced a wide field of research in studies of small systems [10,11].

Surface plasmons are collective motions of electrons at the surface of a metal that excited by charged particles and can amplify local electromagnetic fields [12–15]. On the other hand, surface plasmons are waves that propagate along the surface of a conductor. Surface plasmons are being explored for their applications in optics, magneto-optic data storage, microscopy and solar cells, biophotonics, as well as being used to construct biosensors for detecting biologically interesting molecules [16]. Plasmonic excitations in nanotubes has been studied by different authors. Zabala et al. studied the energy spectroscopy of nanostructures based on classical descriptions of the medium [17]. Electron energy loss spectrum of an electron passing near a locally anisotropic nanotube has been reported by Taverna and co-workers [18]. The self energy and the energy loss of charged particles in solids, and plasmon excitations in cylindrical wires by external charged particles has been investigated by Arista et al. and stopping force of the charged particle in cylindrical wires studied by Aligia et al. [19–22]. Wang and Mišković [23,24] and Mowbray et al. [25] studied the interaction of fast ions with carbon nanotubes. Furthermore, the use of nanotubes as templates for the formation of nanowires has been realized by experimentalists for many different metals, as described by Guerret-Piecourt and co-workers that were able to produced nickle nanowire coating of nanotubes more than 1 μm in length [26]. Gumbs and Balassis presented a model and theory within random phase approximation for electron energy loss spectroscopy and the image potential in cylindrical nanotubes [27]. They considered the motion of a charged particle near the surface of a single-walled cylindrical nanotube of radius *R*. Segui et al. studied the Plasmon excitation in nanostructures and impact of charged particles and the stopping force on an electron following trajectory parallel to the tube axis [28,29].

In this work we have considered a single-walled metallic nanotube (SWMNT) with internal and external radii ρ_1 and ρ_2 ($\rho_2 > \rho_1$), respectively. By using Drude model for dielectric function Poisson's

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equation have been solved and energy dispersion relations for interaction of nanotube with charged particle while it is located inside or outside of the SWMNT are obtained in matrix form. The dispersion relations for both cases, the charged particle is inside and outside the nanotube, are solved numerically and plasmon energies as a function of the wave number are plotted for comparison.

2. Theoretical formulation

Since plasmon excitations play important and dominant role in electrostatical interactions of charged particles with nanostructures, elementary excitations on a nanotube may be modelled by a thin layer of quasi-free electron gas, uniformly distributed over long cylindrical surface of a tubule. Thus, to begin with, theoretical analysis formalism, we consider a method based on classical electrostatic that describe the interaction between charged particles and SWMNTs with a finite thickness and definite dielectric constant. We use cylindrical coordinates and assume that a charge, is located at cylindrical coordinates $(\acute{\rho},\acute{\varphi},\acute{z})$. The electrostatic potential Φ, for a cylindrical nanotube with internal radius ρ_1 and external radius ρ_2, can be obtained by the Green expansion method [30]:

$$\nabla^2 G(\rho,\varphi,z) = -\frac{4\pi}{\rho}\delta(\rho-\acute{\rho})\delta(\phi-\acute{\phi})\delta(z-\acute{z}) \tag{1}$$

where the delta function has been expressed in cylindrical coordinates. The ϕ and z delta functions can be written in terms of orthonormal functions. We expand the Green function in similar fashion:

$$G(\rho,\varphi,z) = \frac{1}{\pi}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dk e^{im(\varphi-\acute{\varphi})}\cos(k(z-\acute{z}))g_m(k,\rho) \tag{2}$$

where the radial Green function $g_m(k,\rho)$ can be expressed in term of the modified Bessel functions.

When a charged particle is located at coordinates $(\acute{\rho},\acute{\phi},\acute{z})$ inside or outside of the nanotube, it polarized its surface and induced a scalar potential. The total scalar potential $\Phi = \Phi_0 + \Phi_{\text{ind}}$ is the sum of potential due to the charged particle Φ_0, and the induced potential Φ_{ind} [31]. Therefore, the total potential is given by:

$$\Phi(\rho,\varphi,z) = \frac{Q}{|\rho-\acute{\rho}|} + \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))g_m(k,\rho) \tag{3}$$

where the first term is the external potential of the charged particle (Coulomb potential), while the second term is the induced potential expressed radial Green function and Q is the particle charge.

The Coulomb potential is given in cylindrical coordinates by the following expression [30]:

$$\frac{1}{|\rho-\acute{\rho}|} = \frac{1}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))I_m(k\rho_<)K_m(k\rho_>) \tag{4}$$

In the region $\rho_1 < \rho < \rho_2$, the solution is given by a linear combination of the two modified Bessel function and in the regions $0 < \rho < \rho_1$ and $\rho > \rho_2$ the nanotube, the solution is given by a function of one of the Bessel functions. If one expands the Coulomb term is cylindrical coordinates, the potential for case that the charge is outside the nanotube, as follows:

$$\Phi^{\text{out}}_{0<\rho\leqslant\rho_1}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))A_{1m}I_m(k\rho) \tag{5}$$

$$\Phi^{\text{out}}_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))(A_{2m}I_m(k\rho) + A_{3m}K_m(k\rho)) \tag{6}$$

$$\Phi^{\text{out}}_{\rho_2\leqslant\rho}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))(A_{4m}K_m(k\rho) + I_m(k\rho_<)K_m(k\rho_>)) \tag{7}$$

and the potential for case that the charge is inside the nanotube, as follows:

$$\Phi^{\text{in}}_{0<\rho\leqslant\rho_1}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))(B_{1m}I_m(k\rho) + I_m(k\rho_<)K_m(k\rho_>)) \tag{8}$$

$$\Phi^{\text{in}}_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))(B_{2m}I_m(k\rho) + B_{3m}K_m(k\rho)) \tag{9}$$

$$\Phi^{\text{in}}_{\rho_2\leqslant\rho}(\rho,\varphi,z) = \frac{Q}{\pi}\sum_{m=-\infty}^{\infty} e^{im(\varphi-\acute{\varphi})}\int_{-\infty}^{\infty} dk\cos(k(z-\acute{z}))B_{4m}K_m(k\rho) \tag{10}$$

where $I_m(k\rho)$ and $K_m(k\rho)$ are the modified Bessel functions of the first and second kinds, k is a wave vector along z, and $\rho_<(\rho_>)$ is the smaller (larger) of ρ and $\acute{\rho}$.

The unknown coefficients A_{im} and B_{im} in Eqs. (5)–(7) and Eqs. (8)–(10) can be determined by the following boundary conditions at $\rho=\rho_1$ and $\rho=\rho_2$

$$\Phi_{\rho\leqslant\rho_1}(\rho,\varphi,z)|_{\rho=\rho_1} = \Phi_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z)|_{\rho=\rho_1} \tag{11}$$

$$\Phi_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z)|_{\rho=\rho_2} = \Phi_{\rho\geqslant\rho_2}(\rho,\varphi,z)|_{\rho=\rho_2} \tag{12}$$

$$\frac{\partial\Phi_{\rho\leqslant\rho_1}(\rho,\varphi,z)}{\partial\rho}|_{\rho=\rho_1} = \epsilon(\omega)\frac{\partial\Phi_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z)}{\partial\rho}|_{\rho=\rho_1} \tag{13}$$

$$\epsilon(\omega)\frac{\partial\Phi_{\rho_1\leqslant\rho\leqslant\rho_2}(\rho,\varphi,z)}{\partial\rho}|_{\rho=\rho_2} = \frac{\partial\Phi_{\rho\geqslant\rho_2}(\rho,\varphi,z)}{\partial\rho}|_{\rho=\rho_2} \tag{14}$$

The method of matrix algebra prove to be very useful in solving a system of linear equations in some unknown. Thus, substituting Eqs. (5)–(7) and Eqs. (8)–(10) into boundary conditions (11)–(14), we can obtain the system of linear equations in the matrix form for a charge outside SWMNT as follows:

$$\begin{pmatrix} I_m(k\rho_1) & -I_m(k\rho_1) & -K_m(k\rho_1) & 0 \\ \epsilon_0\dot{I}_m(k\rho_1) & -\epsilon(\omega)\dot{I}_m(k\rho_1) & -\epsilon(\omega)\dot{K}_m(k\rho_1) & 0 \\ 0 & I_m(k\rho_2) & K_m(k\rho_2) & -K_m(k\rho_2) \\ 0 & \epsilon(\omega)\dot{I}_m(k\rho_2) & \epsilon(\omega)\dot{K}_m(k\rho_2) & -\epsilon_0\dot{K}_m(k\rho_2) \end{pmatrix} \times \begin{pmatrix} A_{1m} \\ A_{2m} \\ A_{3m} \\ A_{4m} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ K_m(k\acute{\rho})I_m(k\rho_2) \\ \epsilon_0 K_m(k\acute{\rho})\dot{I}_m(k\rho_2) \end{pmatrix} \tag{15}$$

and for a charge inside SWMNT is given by:

$$\begin{pmatrix} -I_m(k\rho_1) & I_m(k\rho_1) & K_m(k\rho_1) & 0 \\ -\epsilon_0\dot{I}_m(k\rho_1) & \epsilon(\omega)\dot{I}_m(k\rho_1) & \epsilon(\omega)\dot{K}_m(k\rho_1) & 0 \\ 0 & I_m(k\rho_2) & K_m(k\rho_2) & -K_m(k\rho_2) \\ 0 & \epsilon(\omega)\dot{I}_m(k\rho_2) & \epsilon(\omega)\dot{K}_m(k\rho_2) & -\epsilon_0\dot{K}_m(k\rho_2) \end{pmatrix} \times \begin{pmatrix} B_{1m} \\ B_{2m} \\ B_{3m} \\ B_{4m} \end{pmatrix} = \begin{pmatrix} I_m(k\acute{\rho})K_m(k\rho_1) \\ \epsilon_0 I_m(k\acute{\rho})\dot{K}_m(k\rho_1) \\ 0 \\ 0 \end{pmatrix} \tag{16}$$

where $I_m(k\rho)$ and $I_m(k\rho)$ are the modified Bessel functions of order m and $\dot{I}_m(k\rho) = \frac{dI_m(k\rho)}{d\rho}$ and $\dot{K}_m(k\rho) = \frac{dK_m(k\rho)}{d\rho}$.

To obtain the dispersion relation of the modes, we solve the system of Eqs. (15) and (16). For each m, there is an eigenmode corresponding to the electromagnetic field supported by the system and characterized with a dispersion relation $\omega_m(k)$. Such modes are of collective character, since they describe the combined effect from the collective electron excitations through the dielectric function. Thus, we obtain two modes for each m and k value. The most simple approximation to the dielectric function is given by $\epsilon(\omega) = 1 - \omega_p^2/\omega(\omega+i\gamma)$ (Drude model), where ω_p is the plasma