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RESEARCH ARTICLE

HAMILTON PRINCIPLE FOR SWCN AND A MODIFIED APPROACH FOR NONLOCAL FREQUENCY ANALYSIS OF NANOSCALE BIOSENSOR

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ABSTRACT

In the present paper, the free vibration response of single-walled carbon nanotubes (SWCNTs) is investigated. The governing equations of motion are derived using a variation approach and the free vibration frequencies are obtained employing two different formulations. In the first part of the paper, the case of the cantilever nanotube with concentrated mass at its free end, in the presence of nonlocal effects, is considered and the Hamilton principle is reformulated, in order to find the equation of motion and the boundary conditions; it turns out that they are the same limit conditions obtained by Reddy and Pang, using a direct approach. In the second one, instead, by employing two different approaches two approximate formulas are deduced the first one is derived by applying the Rayleigh Principle, as defined to Meirovitch, whereas the second approximate formula is derived by a formulation given in energy terms.

Numerical examples end the paper and some comparisons with existing results are offered. Comparisons of the present numerical results with those from the open literature show an excellent agreement.

INTRODUCTION

Carbon nanotubes (CNTs) constitute a prominent example of nonmaterial's and nanostructures and their discovery by Iijima (1991) has stimulated several studies in nanotechnology applications and nano-scale engineering materials. Several studies related with CNTs (Dai *et al*, 1996; Falvo *et al*, 1999; Dharap *et al*, 2004) have shown that the carbon nanotubes have extraordinary mechanical and physical properties and in addition to the large respect ratio and low density have made carbon nanotubes (CNTs) ideal components of nanodevices. The outstanding properties of CNTs have lead to their usage in the emerging field of nanoelectronics, nanosensors and nanocomposites, in which the vibration characteristics of CNTs are significant.

The theoretical approaches such as elastic continuum mechanics, as well as molecular dynamics (MD) simulations are used for simulating vibration behaviours of CNTs. Since the MD simulation involves complex computational processes and is still formidable and expensive, especially for large-sized atomic system, continuum models play an essential role in the study of CNTs. Several researchers implemented the elastic models of beams to study the dynamic problems, such as vibration and wave propagation, of carbon nanotubes (De Rosa and Lippiello, 2014a; Yoon *et al*, 2002; Yoon *et al*, 2003). Although the classical continuum methods are efficient in performing mechanical analysis of CNTs, their applicability to identify the small-scale effects on carbon nanotubes mechanical behaviours is questionable. The importance of size effect has been pointed out in a number of studies where the size dependence of the properties of nanotubes has been investigated. For example, Sun and Zhang (2008) discussed the scarce applicability of continuous models to nanotechnology and proposed a semi-continuum model in studying nano-materials. The authors demonstrated that the values of the Young's modulus and Poisson's ratios depend on the number of atom layers in the thickness direction. These results show that the nanostructures and nanomaterials cannot be homogenized into a continuum. At this point, the non-local elastic continuum models are more pertinent in predicting the structural behaviour of nanotubes because of being capable of taking in to account the small-scale effects. It is well-known that the non-local elasticity theory assumes that the stress state, at a given reference point, is considered to be a function of the strain field at all points of the body. The origins of the non-local theory of elasticity go to pioneering works, published in early 80s, by Eringen (1983). In (Reddy, 2007), Reddy reports a complete development of the classical and shear deformation beam theories using the non-local constitutive differential equations and derived the solutions for bending, buckling and natural frequencies problems of simply supported beams.

In recent years, many researchers have applied the non-local elasticity concept for the bending, buckling and vibration analysis of nanostructures by applying Euler-Bernoulli beam and shell theories and Timoshenko beam theory, in CNTs, (Pieddieson *et al*, 2003; Ghannadpour *et al*, 2013; Pradhan *et al*, 2009; Wang *et al*, 2006; Ansari and Sahmani, 2012; Shakouri *et al*, 2009; Ehteshami and Hajabasi, 2011; Wang *et al*, 2007; Hemmatnezhad and Ansari, 2013). It is worth mentioning that, in literature, most

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of the attention has been focused on deriving the variational formulation of equations and boundary conditions for a multiwalled nanotubes undergoing vibrations with non-local elastic continuum methods (Adali, 2010). Reddy and Pang (2008) reformulated the equation of motion of the Euler-Bernoulli and Timoshenko beam theories, using the non-local differential constitutive relations of Eringen. In Adali (2010), the kinetic energy, due to non local effects, is derived; the natural and geometric boundary conditions are obtained which lead to a set of coupled boundary conditions, due to nonlocal effects. If one considers a cantilever nanotube, the free vibration analysis leads to the boundary conditions which are different by those obtained according to the geometric formulation of Reddy-Pang (2008), or according to the virtual displacement approach, as sketched by Reddy (2007).

In the *Additamentum I de curvis elasticis* Euler said:

(…)Cum enim Mundi universi fabrica sit perfectissima, atque a Creatore sapientissimo absoluta nihil omnino in mundo contingit, in quo non maximi minimive ratio quaepiam eluceat:

quamobrem dubium prorfus est nullum, quin omnes Mundi effectus ex causis finalibus, ope Methodi maximorum & minimorum aeque feliciter determinari queant, atque ex ipsis causis efficientibus.(…)

(…) Imprimis autem opera est adhibenda, ut per utramque viam aditus ad Solutionem aperiatur:

sic enim non solum altera Solutio per alteram maxime confirmatur, sed etiam ex sutriusque consensum percipimus voluptatem (…).

Therefore, the study of natural phenomena can be done by following two approaches: the first one through the analysis of the actual causes, the so-called direct method, and the second approach by means of final causes. The two methods should lead to the same results.

Starting from this point of view, in the first part of the present paper, the case of the cantilever nanotube, with concentrated mass at its free end, in the presence of nonlocal effects is considered and the Hamilton principle is reformulated, in order to find the equation of motion and the boundary conditions, which result to be the same limit conditions obtained by Reddy and Pang (2008), using a direct approach.

Because of the CNTs is ultralight and is highly sensitive to its environment changes, many researchers have explored the potential of using CNTs as nanomechanical resonators in atomic-scale mass sensor. For example, Wu *et al* (2006) investigated the resonant frequency and mode shapes of a single-walled carbon nanotube (SWCNT) based mass sensor. Georgantzinos and Anifantis (2010) predicted the vibrational behaviour of single and multiwalled carbon nanotubes (MWCNTs) when a nanoparticle is attached to them by using a spring-mass-based finite element formulation.

Elishakoff *et al* (2013) studied the vibrations of a cantilever double-walled carbon nanotube (DWCNTs) with attached bacterium and the effective stiffness and mass of a DWCNT mass sensor. Mateiu *et al* (2005) developed an approach for building a mass sensor based on MWCNTs. At present, CNTs have been utilized as nanosensors and electromechanical sensing system.

Nanosensors are simple engineering devices designed to detect and convey informations about nanoparticles and biomolecules. The nanosized mass sensors are based on the fact that the resonant frequency is sensitive to the resonator and the attached mass. The change of the attached mass on the resonator causes the resonant frequency to deviate from its original value.

The key challenge in mass detection is in quantifying the changes in the resonant frequencies due to the added masses. Recently, mass detection based on the resonating nanomechanical tools has been subject of growing interests as for example in (Chowdhury *et al*, 2009; Murmu and Adhikari, 2012).

This paper makes the effort to study the resonant frequencies of a SWCNT with an attached nanoparticle, and nonlocal elasticity theory is applied to analyze the vibrational behavior. In (Adhikari and Chowdhury (2010), the Authors examined the potential of single-walled CNTs as biosensors using a continuum mechanics-based approach and derived a closed-form expression to calculate the mass of biological objects from the frequency shift. In the second part of the present paper, by employing two different approaches two approximate formulas: are deduced the first one is derived by applying the Rayleigh Principle, as defined to Meirovitch (2001), whereas the second approximate formula is derived by a formulation given in energy terms.

MATERIALS AND METHODS

Hamilton principle for SWCN

Let us consider a cantilever nanotube (Fig 1) with span L, cross sectional area *A*, second moment of area *I*, Young modulus *E*, mass density ° and concentrated mass M at its free end.

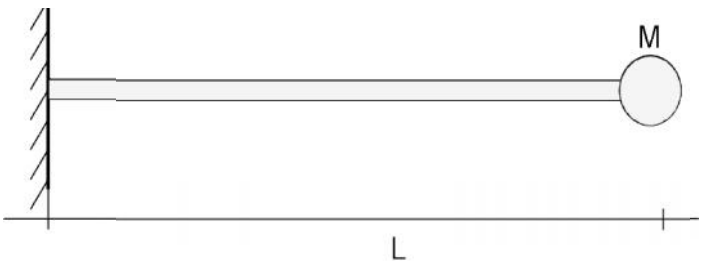

Figure 1 The structural system under consideration

According to Hamilton Principle it is possible to write:

$$\int_{t_1}^{t_2} \left(\delta T(t) - \delta E(t) \right) dt = 0, \tag{1}$$

where

$$T = \frac{1}{2} \int_0^L \rho A \left(\frac{\partial v(z,t)}{\partial t} \right)^2 dz + \frac{1}{2} M \left(\frac{\partial v(L,t)}{\partial t} \right)^2, \tag{2}$$

is the kinetic energy of the nanotube, and

$$E = L_e - P = \frac{1}{2} \int_0^L EI \left(\frac{\partial^2 v(z,t)}{\partial z^2} \right)^2 dz - \int_0^L (e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \frac{\partial^2 v(z,t)}{\partial z^2} dz, \tag{3}$$

is the total potential energy, L_e is the strain energy of the nanotube, and P is the potential energy of the inertial force $\left(\rho A \frac{\partial^2 v(z,t)}{\partial t^2} \right)$ due to the additional displacement $(e_0 a)^2 \frac{\partial^2 v(z,t)}{\partial z^2}$, where e_0 is a constant which has to be experimentally determined for each material, a is an internal characteristic length.

The first variation of these two energies can be easily calculated as:

$$\delta T = \int_0^L \rho A \frac{\partial v(z,t)}{\partial t} \delta \frac{\partial v(z,t)}{\partial t} dz + M \frac{\partial v(L,t)}{\partial t} \delta \frac{\partial v(L,t)}{\partial t}, \tag{4}$$

$$\delta E = \int_0^L EI \frac{\partial^2 v(z,t)}{\partial z^2} \delta \frac{\partial^2 v(z,t)}{\partial z^2} dz - \int_0^L (e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta \frac{\partial^2 v(z,t)}{\partial z^2} dz, \tag{5}$$

so that eq. (1) gives:

$$\int_{t_1}^{t_2} \left(\int_0^L \rho A \frac{\partial v(z,t)}{\partial t} \delta \frac{\partial v(z,t)}{\partial t} dz + M \frac{\partial v(L,t)}{\partial t} \delta \frac{\partial v(L,t)}{\partial t} \right) dt -$$
$$\int_{t_1}^{t_2} \left(\int_0^L EI \frac{\partial^2 v(z,t)}{\partial z^2} \delta \frac{\partial^2 v(z,t)}{\partial z^2} dz - \int_0^L (e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta \frac{\partial^2 v(z,t)}{\partial z^2} dz \right) dt = 0. \tag{6}$$

A series of integration by part can be conducted on the terms of eq. (6), leading to:

$$\int_0^L \int_{t_1}^{t_2} \rho A \frac{\partial v(z,t)}{\partial t} \delta \frac{\partial v(z,t)}{\partial t} dt\, dz =$$
$$\int_0^L \left[\rho A \frac{\partial v(z,t)}{\partial t} \delta v(z,t) \right]_{t_1}^{t_2} dz - \int_0^L \int_{t_1}^{t_2} \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta v(z,t)\, dt\, dz; \tag{7}$$

$$\int_{t_1}^{t_2} M \frac{\partial v(L,t)}{\partial t} \delta \frac{\partial v(L,t)}{\partial t} dt = \left[M \frac{\partial v(L,t)}{\partial t} \delta v(L,t) \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} M \frac{\partial^2 v(L,t)}{\partial t^2} \delta v(L,t)\, dt; \tag{8}$$

$$\int_{t_1}^{t_2} \int_0^L (e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta \frac{\partial^2 v(z,t)}{\partial z^2} dz\, dt = \int_{t_1}^{t_2} \left[(e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta \frac{\partial v(z,t)}{\partial z} \right]_0^L dt -$$
$$\int_{t_1}^{t_2} \int_0^L (e_0 a)^2 \rho A \frac{\partial^3 v(z,t)}{\partial t^2 \partial z} \delta \frac{\partial v(z,t)}{\partial z} dz\, dt = \int_{t_1}^{t_2} \left[(e_0 a)^2 \rho A \frac{\partial^2 v(z,t)}{\partial t^2} \delta \frac{\partial v(z,t)}{\partial z} \right]_0^L dt - \tag{9}$$
$$\int_{t_1}^{t_2} \left[(e_0 a)^2 \rho A \frac{\partial^3 v(z,t)}{\partial t^2 \partial z} \delta v(z,t) \right]_0^L dt + \int_{t_1}^{t_2} \int_0^L (e_0 a)^2 \rho A \frac{\partial^4 v(z,t)}{\partial t^2 \partial z^2} \delta v(z,t)\, dz\, dt,$$

and

$$-\int_{t_1}^{t_2}\int_0^L EI\frac{\partial^2 v(z,t)}{\partial z^2}\¢\frac{\partial^2 v(z,t)}{\partial z^2}dz\,dt=\int_{t_1}^{t_2}-\left[EI\frac{\partial^2 v(z,t)}{\partial z^2}\¢\frac{\partial v(z,t)}{\partial z}\right]_0^L dt+$$

$$\int_{t_1}^{t_2}\int_0^L EI\frac{\partial^3 v(z,t)}{\partial z^3}\¢\frac{\partial v(z,t)}{\partial z}dz\,dt=\int_{t_1}^{t_2}-\left[EI\frac{\partial^2 v(z,t)}{\partial z^2}\¢\frac{\partial v(z,t)}{\partial z}\right]_0^L dt+ \tag{10}$$

$$\int_{t_1}^{t_2}\left[EI\frac{\partial^3 v(z,t)}{\partial z^3}\¢v(z,t)\right]_0^L dt-\int_{t_1}^{t_2}\int_0^L EI\frac{\partial^4 v(z,t)}{\partial z^4}\¢v(z,t)\,dz\,dt.$$

Collecting all the terms in the previous equations allows us to write:

$$\int_{t_1}^{t_2}\int_0^L\left(-\circ A\frac{\partial^2 v(z,t)}{\partial t^2}-EI\frac{\partial^4 v(z,t)}{\partial z^4}+(e_0a)^2\circ A\frac{\partial^4 v(z,t)}{\partial t^2\partial z^2}\right)\¢v(z,t)\,dz\,dt=0, \tag{11}$$

$$\int_{t_1}^{t_2}\left(\left[(e_0a)^2\circ A\frac{\partial^2 v(z,t)}{\partial t^2}\¢\frac{\partial v(z,t)}{\partial z}\right]_0^L-\left[(e_0a)^2\circ A\frac{\partial^3 v(z,t)}{\partial t^2\partial z}\¢v(z,t)\right]_0^L-\right.$$
$$\left.\left[EI\frac{\partial^2 v(z,t)}{\partial z^2}\¢\frac{\partial v(z,t)}{\partial z}\right]_0^L+\left[EI\frac{\partial^3 v(z,t)}{\partial z^3}\¢v(z,t)\right]_0^L-M\frac{\partial^2 v(L,t)}{\partial t^2}\¢v(L,t)\right)dt=0. \tag{12}$$

Consequently, the equation of motion will be:

$$EI\frac{\partial^4 v(z,t)}{\partial z^4}-(e_0a)^2\circ A\frac{\partial^4 v(z,t)}{\partial t^2\partial z^2}+\circ A\frac{\partial^2 v(z,t)}{\partial t^2}=0, \tag{13}$$

together with the following general boundary conditions

$$\left((e_0a)^2\circ A\frac{\partial^3 v(z,t)}{\partial t^2\partial z}-EI\frac{\partial^3 v(z,t)}{\partial z^3}\right)\¢v(z,t)=0\qquad z=0, \tag{14}$$

$$\left(-(e_0a)^2\circ A\frac{\partial^2 v(z,t)}{\partial t^2}+EI\frac{\partial^2 v(z,t)}{\partial z^2}\right)\¢\frac{\partial v(z,t)}{\partial z}=0\qquad z=0, \tag{15}$$

$$\left(-(e_0a)^2\circ A\frac{\partial^3 v(z,t)}{\partial t^2\partial z}+EI\frac{\partial^3 v(z,t)}{\partial z^3}-M\frac{\partial^2 v(z,t)}{\partial t^2}\right)\¢v(z,t)=0\qquad z=L, \tag{16}$$

$$\left((e_0a)^2\circ A\frac{\partial^2 v(z,t)}{\partial t^2}-EI\frac{\partial^2 v(z,t)}{\partial z^2}\right)\¢\frac{\partial v(z,t)}{\partial z}=0\qquad z=L. \tag{17}$$

At the left end (z=0) the boundary geometric conditions of the cantilever nanotube impose $v(z=0,t)=0$ and $\frac{\partial v(z=0,t)}{\partial z}=0$, and at right end z = L the boundary equilibrium conditions are entirely coincident with the conditions given by Reddy and Pang (2008), in the absence of concentrated mass, using a direct approach.

Rayleigh quotient - first approach

Let us start with the differential eq. (13), where the variables can be separate as follows:

$$v(z,t)=v(z)\ \mathrm{Cos}(\mu t) \tag{18}$$

Eq. (18) can be inserted in the equation of motion (eq. (13)), which in turn can be integrated between 0 and L. Finally, it is possible to insert a trial function y(z), leading to:

$$\int_0^L EI\frac{\partial^4 v(z)}{\partial z^4}y(z)\,dz+\mu^2\int_0^L(e_0a)^2\circ A\frac{\partial^2 v(z)}{\partial z^2}y(z)\,dz-\mu^2\int_0^L\circ Av(z)y(z)dz=0. \tag{19}$$

Two successive integrations by part can be performed:

$$\int_0^L EI\frac{\partial^4 v(z)}{\partial z^4}y(z)dz=\left[EI\frac{\partial^3 v(z)}{\partial z^3}y(z)\right]_0^L-\int_0^L EI\frac{\partial^3 v(z)}{\partial z^3}\frac{\partial y(z)}{\partial z}dz=$$
$$\left[EI\frac{\partial^3 v(z)}{\partial z^3}y(z)\right]_0^L-\left[EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial y(z)}{\partial z}\right]_0^L+\int_0^L EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial^2 y(z)}{\partial z^2}dz; \quad (20)$$

and:

$$\mu^2\int_0^L(e_0a)^2\circ A\frac{\partial^2 v(z)}{\partial z^2}y(z)dz=\left[\mu^2(e_0a)^2\circ A\frac{\partial v(z)}{\partial z}y(z)\right]_0^L-$$
$$\int_0^L\mu^2(e_0a)^2\circ A\frac{\partial v(z)}{\partial z}\frac{\partial y(z)}{\partial z}dz=\left[\mu^2(e_0a)^2\circ A\frac{\partial v(z)}{\partial z}y(z)\right]_0^L-$$
$$\left[\mu^2(e_0a)^2\circ Av(z)\frac{\partial y(z)}{\partial z}\right]_0^L+\int_0^L\mu^2(e_0a)^2\circ Av(z)\frac{\partial^2 y(z)}{\partial z^2}dz; \quad (21)$$

so that eq. (19) becomes:

$$\int_0^L EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial^2 y(z)}{\partial z^2}dz+\int_0^L\mu^2(e_0a)^2\circ Av(z)\frac{\partial^2 y(z)}{\partial z^2}dz-\mu^2\int_0^L\circ Av(z)y(z)dz+$$
$$\left[EI\frac{\partial^3 v(z)}{\partial z^3}y(z)\right]_0^L-\left[EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial y(z)}{\partial z}\right]_0^L+ \quad (22)$$
$$\left[\mu^2(e_0a)^2\circ A\frac{\partial v(z)}{\partial z}y(z)\right]_0^L-\left[\mu^2(e_0a)^2\circ Av(z)\frac{\partial y(z)}{\partial z}\right]_0^L=0.$$

The boundary conditions at the right end permit to simplify the previous equation:

$$\int_0^L EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial^2 y(z)}{\partial z^2}dz+\int_0^L\mu^2(e_0a)^2\circ Av(z)\frac{\partial^2 y(z)}{\partial z^2}dz-\mu^2\int_0^L\circ Av(z)y(z)dz+$$
$$EI\frac{\partial^3 v(L)}{\partial z^3}y(L)-EI\frac{\partial^2 v(L)}{\partial z^2}\frac{\partial y(L)}{\partial z}+\mu^2(e_0a)^2\circ A\frac{\partial v(L)}{\partial z}y(L)- \quad (23)$$
$$\mu^2(e_0a)^2\circ Av(L)\frac{\partial y(L)}{\partial z}=0;$$

whereas the free end will be subjected to the following equilibrium conditions:

$$\mu^2(e_0a)^2\circ A\frac{\partial v(L)}{\partial z}+EI\frac{\partial^3 v(L)}{\partial z^3}+\mu^2Mv(L)=0, \quad (24)$$

$$-\mu^2(e_0a)^2\circ Av(L)-EI\frac{\partial^2 v(L)}{\partial z^2}=0. \quad (25)$$

Finally, eq. (23) reduces to:

$$\int_0^L EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial^2 y(z)}{\partial z^2}dz+\int_0^L \mu^2(e_0a)^2\circ Av(z)\frac{\partial^2 y(z)}{\partial z^2}dz-$$
$$\mu^2\int_0^L \circ Av(z)y(z)dz-\mu^2 Mv(L)y(L)=0, \tag{26}$$

and the frequency μ^2 can be written down, putting y(z) = v(z), as:

$$\mu^2=\frac{\int_0^L EI\frac{\partial^2 v(z)}{\partial z^2}\frac{\partial^2 y(z)}{\partial z^2}dz}{-\int_0^L (e_0a)^2\circ Av(z)\frac{\partial^2 v(z)}{\partial z^2}dz+\int_0^L \circ Av^2(z)dz+Mv^2(L)}. \tag{27}$$

Nonlocal resonance frequency of CNT with attached mass - first method

In the following, an approximate displacement is assumed:

$$v(z)=\frac{z^2(3L-z)}{2L^3}, \tag{28}$$

So that eq. (27) gives the approximate frequency value:

$$\mu^2=\frac{\frac{3EI}{L^3}}{\left(\frac{33}{140}Lm+M-\frac{3¦^2Lm}{10}\right)}, \tag{29}$$

Where $¦^2=\frac{(e_0a)^2}{L^2}$, m = °A and the resonant frequency can be approximated as:

$$f_{n1}=\frac{\mu}{2®}=\frac{1}{2®}\sqrt{\frac{\frac{3EI}{L^3}}{\left(\frac{33}{140}Lm+M-\frac{3¦^2Lm}{10}\right)}}, \tag{30}$$

It is also possible to express the resonant frequency as a function of three calibration constants C_k, C_{n1}, C_m. It will be:

$$f_{n1}=\frac{1}{2®}\sqrt{\frac{\frac{3EI}{L^3}\frac{140}{33Lm}}{\left(1+\frac{M}{Lm}\frac{140}{33}-\frac{3¦^2Lm}{10}\frac{140}{33Lm}\right)}}, \tag{31}$$

so that:

$$f_{n1}=\frac{1}{2®}\frac{C_k}{\sqrt{1+C_m\Delta M-C_{n1}¦^2}}, \tag{32}$$

where

$$\Delta M=\frac{M}{Lm};\qquad =\sqrt{\frac{EI}{L^4m}}$$
$$C_k=\sqrt{\frac{140}{11}};\quad C_{n1}=\frac{14}{11};\quad C_m=\frac{140}{33}. \tag{33}$$

Nonlocal resonance frequency of CNT with attached mass - Second method

In this case, let us start from the energy terms:

$$T = \frac{1}{2}\int_0^L \circ A\left(\frac{\partial v(z,t)}{\partial t}\right)^2 dz + \frac{1}{2}M\left(\frac{\partial v(L,t)}{\partial t}\right)^2, \tag{34}$$

$$E = L_e - P = \frac{1}{2}\int_0^L EI\left(\frac{\partial^2 v(z,t)}{\partial z^2}\right)^2 dz - \int_0^L (e_0 a)^2 \circ A\frac{\partial^2 v(z,t)}{\partial t^2}\frac{\partial^2 v(z,t)}{\partial z^2}dz \tag{35}$$

and let us assume the separation of variables

$$v(z,t) = v(z)\,\mathrm{Cos}(\mu t) \tag{36}$$

so that the energies read:

$$T = \frac{\mu^2}{2}\int_0^L \circ Av(z)^2\,dz\,\mathrm{Sin}^2(\mu t) + \frac{\mu^2}{2}Mv(L)^2\,\mathrm{Sin}^2(\mu t), \tag{37}$$

$$E = L_e - P = \frac{1}{2}\int_0^L EI\left(\frac{\partial^2 v(z)}{\partial z^2}\right)^2 dz\,\mathrm{Cos}^2(\mu t) + \mu^2\int_0^L (e_0 a)^2 \circ Av(z)\frac{\partial^2 v(z)}{\partial t^2}dz\,\mathrm{Cos}^2(\mu t). \tag{38}$$

The maximum kinetic energy will be equal to the maximum total potential energy, so that:

$$\frac{1}{2}\int_0^L EI\left(\frac{\partial^2 v(z)}{\partial z^2}\right)^2 dz + \mu^2\int_0^L (e_0 a)^2 \circ Av(z)\frac{\partial^2 v(z)}{\partial t^2}dz = \frac{\mu^2}{2}\int_0^L \circ Av(z)^2\,dz + \frac{\mu^2}{2}Mv(L)^2, \tag{39}$$

and the frequency μ^2 can be deduced as:

$$\mu^2 = \frac{\frac{1}{2}\int_0^L EI\left(\frac{\partial^2 v(z)}{\partial z^2}\right)^2 dz}{\frac{1}{2}\int_0^L \circ Av(z)^2\,dz + \frac{1}{2}Mv^2(L) - \int_0^L (e_0 a)^2 \circ Av(z)\frac{\partial^2 v(z)}{\partial z^2}dz}. \tag{40}$$

Nonlocal resonance frequency of CNT with attached mass

The same approximate displacement is assumed:

$$v(z) = \frac{z^2(3L - z)}{2L^3} \tag{41}$$

which leads to the following approximate frequency value:

$$\mu^2 = \frac{\frac{3EI}{L^3}}{\left(\frac{33}{140}Lm + M - \frac{3|^2 Lm}{5}\right)} \tag{42}$$

and the approximate resonant frequency is now given by:

$$f_{n2} = \frac{\mu}{2®} = \frac{1}{2®}\sqrt{\frac{\frac{3EI}{L^3}}{\left(\frac{33}{140}Lm + M - \frac{3|^2 Lm}{5}\right)}}, \tag{43}$$

or:

$$f_{n2} = \frac{1}{2®} \frac{C_k}{\sqrt{1 + C_m \Delta M - C_{n2}\,¦^2}} \tag{44}$$

where the three calibration constants C_k, C_{n2}, C_m are given by:

$$C_k = \sqrt{\frac{140}{11}}; \quad C_{n2} = \frac{28}{11}; \quad C_m = \frac{140}{33}. \tag{45}$$

Nonlocal sensor equation

In this section one will derive the general expression of the added mass on the relative frequency-shift of the SWCNT (Murmu and Adhikari, 2012). Using eq.(32) and eq. (44) the resonant frequency, without the added mass, is given by:

$$f_{n0} = \frac{C_k}{2®}, \tag{46}$$

the frequency shift can be written as:

$$\Delta f = f_{n0} - f_{ni} - \frac{f_{n0}}{\sqrt{1 + C_m \Delta M - C_{ni}\,¦^2}}, \quad i = 1, 2, \tag{47}$$

or the relative frequency shift:

$$\frac{\Delta f}{f_{n0}} = 1 - \frac{1}{\sqrt{1 + C_m \Delta M - C_{ni}\,¦^2}}, \tag{48}$$

So that the relative added mass is defined:

$$\Delta M = \frac{1}{C_m \left(1 - \left(\frac{\Delta f}{f_{n0}}\right)^2\right)} - ¦^2 \frac{C_{ni}}{C_m} - \frac{1}{C_m} \tag{49}$$

Using equation (33) it is possible to calculate:

$$M = \frac{L m}{C_m} \frac{C_k{}^2}{\left(C_k - 2® \Delta f\right)^2} - ¦^2 \frac{C_{ni}}{C_m} L m - \frac{L m}{C_m}. \tag{50}$$

This is the general equation for the calculation of the added mass, where the nonlocal calibration constants are given by:

$$C_{n1} = \frac{14}{11}; \quad C_{n2} = \frac{28}{11} \tag{51}$$

they depend on the first or second method.

Numerical examples

As a matter comparisons, the nanotube given by (Mehdipour *et al*, 2011) will be studied, whose geometrical and material properties are given in Table 1:

Table 1 Geometrical and material properties of the nanotube under consideration

SWCNT properties density	Symbol	Value	Unit
Inner diameter	D_1	$18.8\ 10^{-9}$	m
Outer diameter	D_2	$33\ 10^{-9}$	m
Length	L	$5.5\ 10^{-6}$	m
Density	°-	1300	Kg/m^3
Young's modulus	E	$32\ 10^9$	Pa

In the Table 2 the resonant frequency values $f_n = \frac{\mu}{2®}$ are given, for increasing values of the attached concentrated mass and in the absence of nonlocal effects. The first and second column of (Mehdipour *et al*, 2011) gives the exact values, as obtained by solving the boundary value problem; the third column refers to the approximate method CDM, the well-known Cell Discretization Method, (De Rosa and Lippiello, 2014b). Increasing values of the attached concentrated mass lead to decreasing values of the first frequency value.

Table 2 First resonant frequency for various values of the attached mass

M (fg)	(30)	Exact value ¦=0	CDM ¦=0
0		861556.099	861553.410
20	190401.785	190401.785	190401.630
22	181934.726	181934.727	181934.547
24	174505.207	174505.207	174504.928
26	167917.297	167917.297	167917.161
28	162023.235	162023.236	162023.048
30	156709.208	156709.202	156709.003
35	145419.280	145419.280	145419.165
40	136263.504	136263.504	136263.382
50	122175.371	122175.371	122175.239

In the following Tables 3 and 4, the frequency values fn are given, for increasing values of the attached concentrated mass. The second column gives the exact values, as obtained by solving the boundary value problem, the third column refers to the approximate formula eq. (32), and finally the fourth column refers to the approximate formula eq. (44). The Table 3 assumes a nonlocal parameter $\eta = 0.1$, whereas the Table 4 has been obtained for $\eta = 0.5$. As obvious, the approximate values are always greater than the true frequencies, but the approximate frequencies given by eq. (32) are always better than their counterparts given by eq. (44).

Table 3 First resonant frequency for various values of the attached mass and $\eta = 0.1$

M (fg)	Exact	Eq. (32)	Eq. (44)
20	190458	190465	190523
22	181984	181990	182040
24	174549	174553	174598
26	167956	167960	168000
28	162058	162061	162097
30	156741	156744	156776
35	145445	145447	145472
40	136284	136286	136307
50	122190	122191	122206

Table 4 First resonant frequency for various values of the attached mass and $\eta = 0.5$.

M (fg)	Exact	Eq. (32)	Eq. (44)
20	191851	191862	193349
22	183198	183207	184500
24	175619	175626	176765
26	168909	168915	169927
28	162914	162919	163827
30	157515	157519	158339
35	146063	146065	146718
40	136792	136794	137331
50	122556	122557	122943

Let us consider a zigzag (5,0) single-walled carbon nanotube (SWCNT), in Fig 2, as a biosensor. The length of SWCNT is equal to 8.52 nm.

Applying the eq. (30), one gets:

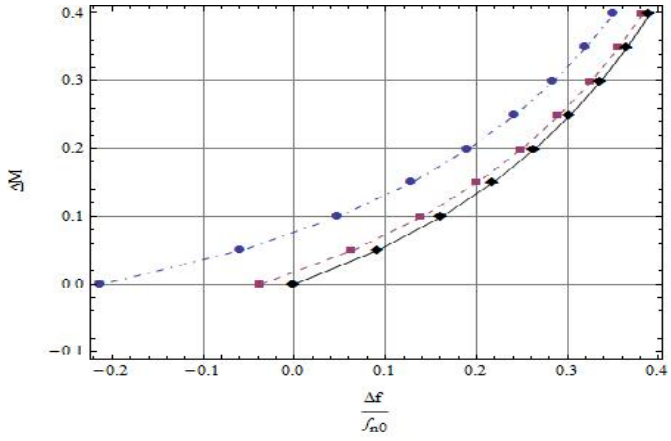

Figure 2 The relative frequency shift for various values of the attached mass and ¦ = 0, $\dagger = \frac{2\times10^{-9}}{8.52\times10^{-9}}$, ¦ = 0.5, applying to the calibration constants eq. (33).

$$\frac{\Delta f}{f_{n0}} = 1 - \frac{1}{\sqrt{1 + \Delta M\, C_m - \mu^2\, C_{n1}}}, \tag{52}$$

which is nearer to the exact values and, varying the ΔM parameter, it is possible to obtain the relative frequency shift $\frac{\Delta f}{f_{n0}}$.

Generally, for carbon nanotubes, it is observed that the nonlocal parameter ($e_0 a$) is considered within the range $0.0\ \text{nm} \le e_0 a \le 2.0\ \text{nm}$ and, in the example under consideration, this parameter corresponds to the nondimensional factors whose range is $0 \le \mu \le 2.34742$ and for a length of the nanotube L = 8.52 nm. In Fig 2 three curves are reported corresponding to a values of ΔM between $0 \le \Delta M \le 0.4$ and μ = 0, μ = 0.234742 and finally, for a higher value of the non-dimensional nonlocal effect, μ = 5.

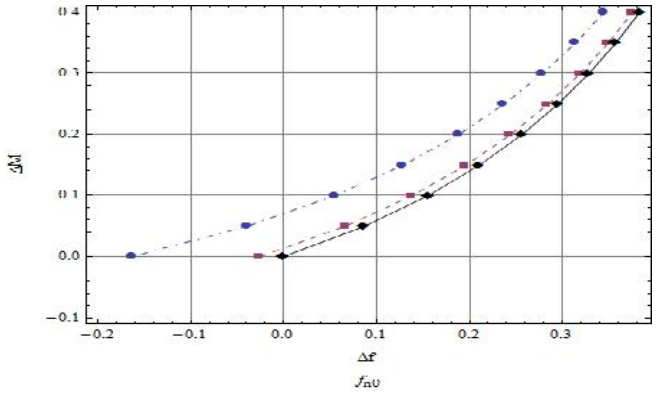

Figure 3 The relative frequency shift for various values of the attached mass and μ =0, $\mu = \frac{2\times10^{-9}}{8.52\times10^{-9}}$, μ = 0.5, applying to the exact formula.

The plot shows that if the nonlocal effect is introduced the relative frequency shift decreases and the curves are located to the left of that obtained to setting μ = 0.

Solving the eq. (13) and calculating the relative frequency shift, $\Delta f / f_{n0}$ where f_{n0} is the value obtained to a clamped nanotube, in the absence of mass and nonlocal effect, and by means exact method, in Fig 3 are reported the relative curves.

As one can see the plots are coincident and confirm the exactness of the approximated method.

CONCLUSION

In the first part of the present paper, the exact formulation of Hamilton Principle for a SWCNT, in presence of nonlocal effects, is presented. Interestingly, this energy approach gives the same boundary problem is obtained by using the geometric method (Reddy and Pang, 2008). Of course, the approach is extendable to nanotubes that are based upon the Timoshenko theory.
In a second phase of the present paper the approximate method of the Rayleigh quotient has been applied in order to obtain the first approximate frequency; finally using the definitions of kinetic and potential energies, an approximate method has been employed, which also provides the first approximate frequency value depending on the particular coefficients of caliber. Finally, on the basis of the theory already developed in (Murmu and Adhikari, 2012), it is possible to deduce the value of the added mass.

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