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# Nonlocal Effects on the Dynamics of Carbon Nanotubes

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**Abstract:** The present work is devoted to the study of dynamics of single-walled carbon nanotube (SWCNT). The study invokes Sanders-Koiter's thin shell theory in modelling the CNT. Eringen's theory is considered to incorporate nonlocal effects. Closed-form normal mode solutions are presented for varying aspect ratios, boundary conditions and chiralities. Atomistic simulations are considered to corroborate the nonlocal effects on normal modes of SWCNTs.

**Keywords:** SWCNT, Sanders-Koiter's shell theory, Eringen's nonlocal theory

## 1. Introduction

With the discovery of CNTs in the mid 1990s [1], the synthesis and characterization of CNTs have attracted the attention of physicists, material scientists and chemical engineers. CNTs find applications, to name a few [2], in material strengthening, hydrogen storage, FETs. The mechanical properties of CNTs are orders of magnitude higher than those of the bulk materials. To this end, the structural and dynamical properties of these structures are important in predictive design of systems using these nano structures. Due to the spatial scale of nano structures, the experimental study poses a challenge. However, mechanics of CNTs has been studied invoking the density functional theory (DFT), atomistic simulations and continuum theory [3]. Computational studies are expensive as well owing to their response time scales of the order of nanoseconds or lower. It is obvious that these contrasting modelling techniques are better applicable at different length/time scales. Many researchers have studied the vibration of CNTs using 1-D, 2-D (beam, rod) models. These models are accurate at low frequencies, whereas high frequency responses are seen to be affected by the nonlocal effects. To explore the behaviour of SWCNTs at intermediate/high frequencies, a 3-D continuum model [5] is considered here.

Relatively few analytical works have dwelled on the 3-D structural dynamics of the CNTs. Recent studies by Strozzi et. al. [5] consider reduced-order shell model by neglecting the normal and tangential shear strain of the shell's mid surface thereby limiting its applicability for wider frequency range. The objective herein is to study the behaviour of SWCNTs in a broad frequency range and by incorporating nonlocal effects due to Eringen [6]. The nondimensional evolution equations of a cylindrical thin shell (Fig. 1) is [5, 6]

$$\alpha u_{xx} + \frac{(4+\beta^2)(1-\mu)}{8} u_{\theta\theta} + \alpha \left\{ \left( \frac{(1+\mu)}{2} + \frac{3\beta^2(\mu-1)}{8} \right) v_{x\theta} + \mu w_x + \frac{\beta^2(1-\mu)}{2} w_{\theta\theta x} \right\} = u_{tt} + \gamma \left( \frac{u_{\theta\theta tt}}{\alpha^2} + u_{xxtt} \right) \tag{1a}$$

$$\alpha \left( \frac{(1+\mu)}{2} + \frac{3\beta^2(\mu-1)}{8} \right) u_{x\theta} + \alpha^2 \left( \frac{1}{2} + \frac{9\beta^2}{8} \right) (1-\mu) v_{xx} + (1+\beta^2) v_{\theta\theta} + w_\theta - \beta^2 w_{3\theta} + \frac{(\mu-3)\,\beta^2\alpha^2}{2} w_{xx\theta} = v_{tt} + \gamma \left( \frac{v_{\theta\theta tt}}{\alpha^2} + v_{xxtt} \right) \tag{1b}$$

$$\alpha\mu u_x + \frac{\alpha\beta^2(1-\mu)}{2} u_{\theta\theta x} + v_\theta - \beta^2 v_{3\theta} + \frac{(\mu-3)\,\beta^2\alpha^2}{2} v_{xx\theta} + w + \beta^2(\alpha^4 w_{4x} + 2\alpha^2 w_{xx\theta\theta} + w_{4\theta}) = -w_{tt} - \gamma \left( \frac{w_{\theta\theta tt}}{\alpha^2} + w_{xxtt} \right) \tag{1c}$$

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where $u, v, w$ are axial, angular and radial deformation respectively, $\alpha = R/L$, $R$ is the radius, $L$ is the characteristic macroscopic length, $\beta = h/\left(R\sqrt{12}\right)$, $h$ is the effective thickness, $\mu$ is the Poisson's ratio, $\gamma = (e_0 a/L)^2$ is the parameter describing the nonlocal effects, $e_0$ is the nonlocal constant [6], $a$ is the characteristic atomistic length and $u_{4\theta} = u_{\theta\theta\theta\theta}, u_{x\theta} = \partial^2 u/\partial x \partial \theta$ … .

## 2. Results and Discussion

We herein explore normal mode solutions, i.e., time periodic synchronous oscillations. Additionally, imposing periodic boundary condition (BC) with periodicity $m \in \mathbb{Z}$ in the circumferential direction, Eq. (1) are reduced to a set of ordinary differential equations in $x$. Upon solving the eigenvalue problem with appropriate BCs, an eighth order polynomial equation in axial wavenumber $k$ is obtained. One among the eight wavenumbers is shown in Fig. 2 as function of frequency and revealing the effect of increasing nonlocal parameter. The nonlocal effects on the normal modes for various boundary conditions are considered in this work and will be presented in the full version of the paper with exhaustive comparison with the full-scale atomistic simulations.

## 3. Concluding Remarks

In this work, we study the nonlocal effects on the normal modes of a finite CNT. The nonlocality has significant effect on the characteristics of the normal modes. Exact analytic solutions for a wide frequency range are obtained. The analytic solutions obtained form the basis for exploring nonlinear modal interaction of CNTs and energy localization thereof. Further analysis and comparisons with full-scale atomistic simulations will be reported in the full version of the paper.

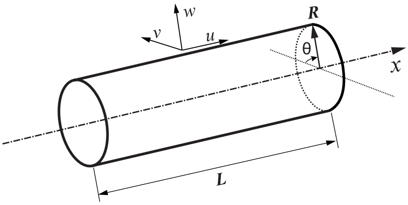

**Fig. 1.** Kinematics of a flexible CNT of radius $R$ and length $L$

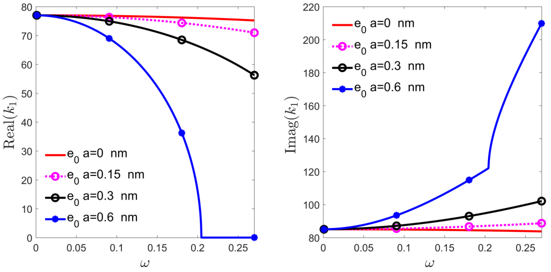

**Fig. 2.** Wave number v/s natural frequency for varying nonlocal parameter for $\alpha = 0.0392, \beta = 0.048, \mu = 0.19$

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