A Phase Plane Analysis of Discrete Breathers in Carbon Nanotube

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Abstract— *We study the nonlinear dynamics of anharmonic oscillations in a carbon nanotube (CNT). The problem consists of solving a perturbation Hamiltonian using Brenner potential. A dispersion relation has been obtained, which predicts the formation of discrete breather below a lower frequency limit. Equations of motion in cylindrical coordinates predict that spatially localized nonlinear modes may exist in the form of discrete breathers. The mathematical model takes into consideration the chiralities of CNT. As in earlier studies twisting breathers have been found to exist.*

Key Words— Brenner potential, carbon nanotube, discrete breather, dispersion relation, nonlinear dynamics, spatially localized nonlinear modes, twisting breathers

1.Introduction

Carbon nanotubes were synthesised by thermal decomposition of carbon oxide by Iijma[1]. Obtained as a by-product of the synthesis of fullerene C_{60}, their unique properties make them a good candidate for a wide range of applications due to their unique physical properties which are experimentally verified [2]. They are found to exhibit superior mechanical strength [3] and better heat conductance[4]. In addition, C_{60} fullerene is found to support large amplitude oscillations[5]. Such oscillations are excited and controlled by laser pulses[6]. These are macromolecules having cylindrical geometry and diameter having of the order of a nanometer and length of the order of several microns.

It was observed by Anderson that localized oscillations may take place due to defects in crystal lattices. This phenomenon is known as Anderson localization. However, Ovehimnikov, Takeno and Sievers [7,8] observed that intrinsic localized modes are found in perfectly periodic but strongly nonlinear systems. These were called discrete breathers.

The discrete breather (DB) excitations have been observed in a large variety of lattice systems, in lattice vibrations and spin excitations, in molecules and and charge flow in coupled Josephson junctions, in light propagation in interacting optical waveguides[9], cantilever vibrations in micromechanical arrays, in Bose-Einstein condensates and cold atom dynamics in optical lattices, in composite metamaterials, in nonlinear protein molecules etc.

Particularly, large-amplitude oscillations of discrete breathers in nanotubes with chiralities (m,0) and (m,m) have been observed by Savin and Kivshar[10]. They predict the existence of spatially localized nonlinear modes in the form of discrete breathers which may be in the form of longitudinal, radial and torsion anharmonic vibrations. However, they found that only the twisting breathers are actually the nonradiating nonlinear modes.

We carry out a phase plane analysis of discrete breathers. An analysis of resulting exact equations is carried out so as to determine the existence and stability of different types of breathers.

2 THE STRUCTURE OF CARBON NANOTUBE (CNT)

We consider a carbon nanotube (CNT) with chirality (m,m). The nanotube is characterized by its radius r and longitudinal dimension z. There are two layers of nanotube. Each layer has m atoms separated by angular distance. Each atom of CNT is characterized by a set of indices (i,j,k) where (i,j) defines an elementary cell $i:0,1,2,\ldots$; k defines the atom number of the cell: k=0,1. The geometrical model follows from [10].

3 MATHEMATICAL MODEL

In this paper, we apply an extended Brenner bond order dependent potential, following the empirical equations derived in to the calculation of fullerene and nanotube properties. The implementation of long-range interactions in this potential allows the consistent treatment of all types of long-range nonbond non- bonding interactions. Binding energy in Abell-Tersoff [13,14] formalism is given as

$$V_i = \frac{1}{2}\sum_{i,j(\neq i)}\left[V_R(r_{ij}) - \bar{B}_{ij}V_A(r_{ij})\right] \quad (1)$$

$$V_R(r_{ij}) = f_{ij}(r_{ij})\frac{D_{ij}^{(e)}}{S_{ij}-1}\exp[-\sqrt{2S_{ij}}\,\zeta] \quad (2a)$$

and

$$V_R(r_{ij}) = f_{ij}(r_{ij})\frac{D_{ij}^{(e)}S_{ij}}{(S_{ij}-1)}\exp[-\sqrt{2/S_{ij}}\,\zeta] \quad (2b)$$

where $\zeta = \beta_{ij}(r - R_{ij}^{(e)})$, $D_{ij}^{(e)}$ is the well depth, $R_{ij}^{(e)}$ is the equilibrium distance , β_{ij} are the Morse parameters.

Here, i is the atom site, j is the nearest neighbor of atom i , E_i is the contribution due to each atom site, V_R and V_A are respectively the pair additive repulsive and attractive interactions. $\bar{B}_{ij}$ represent many body coupling between the bond from atom i to atom j . For diamond and graphite, it can be written as $\bar{B}_{ij} = (B_{ij} + B_{ji})/2$ where $B_{ij} = \Omega^{-\delta}$ and Ω is the local coordination number depending on the orientation of bonds and δ depends on the particular system.

$$\Omega = 1 + \sum_{k(\neq i,j)} G(\theta_{ijk})f(r_{ik}) \quad (3)$$

$$G(\theta) = a_o\left[1 + \frac{c_o^2}{d_o^2} - \frac{c_o^2}{d_o^2 + (1+\cos\theta)^2}\right] \quad (4)$$

The lattice parameters are as follows[11]

$r_o = 1.315\,\overset{o}{A}$, $D = 6.325\,eV$, $\beta = 1.5\,\overset{o}{A}^{-1}$, $S = 1.29$,

$a_o = 0.011304$, $c_o = 19$, $d_o = 2.5$, $\delta = 0.80469$, $\theta = 2\pi/3$.

We transform the coordinates from the cartesian coordinates (x,y,z) to the radial coordinates (r_i,ϕ_i,z_i). We consider a plane wave propagating along the z axis

$$\psi_i = \psi_i^o(r_i,\phi_i)\exp[i(qz_i - \omega t)] \quad (5)$$

The Hamiltonian for the problem takes the following form

$$H = \sum_i\left\{\frac{1}{2}M\left[\dot{r}_i^2 + (r_1 + r_i)^2\dot{\phi}_i^2 + \dot{z}_i^2\right]\right\} + \sum_i V_i \quad (6)$$

The prime indicates differentiation with respect to time.

The potential term can be simplified using specific values of constants in the empirical relations Eq.(1)-(4):

$$\sum_i V_i = D\left[\exp\{-\alpha(r - r_o) - 1\right]^2 + \gamma(g + \frac{1}{\cos\theta})^s + k_1 z^2 \quad (7)$$

where D, g, s, k_1 and γ are constants.

For slowly varying envelope approximation, we obtain the dispersion for the longitudinal phonons,

$\omega^4 M^2 - 2\omega^2 M(K_1 + K_2) + 4K_1K_2\sin^2 q = 0$ with

$K_1 = V_1^{''}(0) = 2D\alpha^2$ and

$K_2 = V_2^{''}(0) = \dfrac{27(\gamma s)}{2r_o^{\,2}} + D\alpha^2$

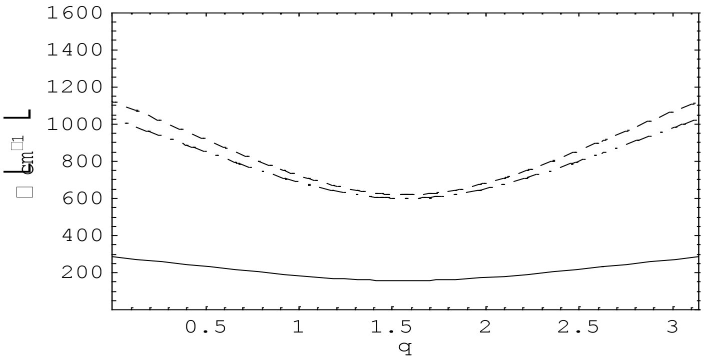

Fig.1: Dispersion curves for (a) longitudinal modes (soli line),
(b) radial modes(dash) and (c) torsion oscillations (dash-dot)

3.1 Discrete Breathers

For $r = r_{i+1} - r_i$, $\phi = \phi_{i+1} - \phi_i$ and $z = z_{i+1} - z_i$ we obtain the localized nonlinear modes of longitudinal oscillations shown in Fig. 2.

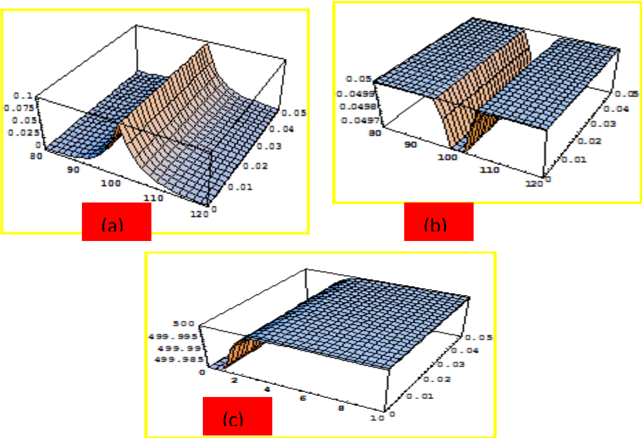

Fig.2: (a) Transverse nonlinear breathing mode, (b) twisting breather and (c) longitudinal breathing modes.

Table 1: Displacements of CNT due to Anharmonic and Brenner Potential

Chirality	Transverse (r_i)	Torsion (φ_i)	Longitudinal (z_i)
(m,0)	Radial long lived nonlinear modes can appear [560, 585] cm^{-1}	Twisting breathers due to Brenner Potential [1140, 1640] cm^{-1}	Exact nonlinear modes (planar) [1160, 1205] cm^{-1}
(m,m)	Radial long lived nonlinear modes can appear in window [430.5, 436] cm^{-1} (Not exact solutions. Radiation leads to decay).		

4 PHASE PLANE ANALYSIS

We solve the Hamiltonian for the equations of motion in (r_i, ϕ_i, z_i) coordinates:

$$M\ddot{r}_i - M(r_1+r_i)\dot{\phi}^2 + \frac{\partial}{\partial r_i}\sum_i V_i = 0 \qquad 8(a)$$

$$M(r_1+r_i)^2\ddot{\phi} + 2M(r_1+r_i)\dot{\phi}\dot{r}_i + \frac{\partial}{\partial \phi_i}\sum_i V_i = 0 \qquad 8(b)$$

$$M\ddot{z} + \frac{\partial}{\partial z_i}\sum_i V_i = 0 \qquad 8(c)$$

The prime indicates differentiation with respect to time.

We assume

$\dot{r}_i = R, \dot{\phi} = \Phi$ and $\dot{z} = Z$ so that we obtain the equations in the following form:

$$M\dot{R} - M(r_1+r)\Phi^2 - D\alpha^2 r = 0 \qquad 9(a)$$

$$M(r_1+r)^2\dot{\Phi} + 2M(r_1+r)\Phi\dot{R} - \gamma s(g+1/\cos\theta)(1/\cos\theta)^2 = 0 \qquad 9(b)$$

$$M\dot{Z} + 2k_1 z = 0 \qquad 9(c)$$

We obtain a system of the following three nonlinear autonomous equations

$$\dot{R} = (r_1+r)\Phi^2 - \frac{D\alpha^2 r}{M} \qquad 10(a)$$

$$\dot{\Phi} = \frac{\gamma s(g+1/\cos\theta)(1/\cos\theta)^2}{M\{(r_1+r)^2+2R^2\}} \qquad 10(b)$$

$$\dot{Z} = -\frac{2k_1}{M}z \qquad 10(c)$$

A phase plane analysis of the above set of equations shows the following results:

1. The Hamiltonian, Eq.(6), is derived using the Brenner empirical potential and classical mechanics. It helps us to obtain the dispersion relation to carry out the nonlinear dynamics. The results obtained are similar to the case of diatomic lattices and as obtained in [10] with slight cnange in the cut-off frequency. The

improved results, shown in Table 1, predict the existence of discrete breathers with the frequencies below the lowest frequency of the longitudinal phonons.

2. The breathers are studied numerically by drawing phase plane trajectories. The 3D plot of breather form is shown in Fig. 1. The breather frequency is inside the band [1160, 1205] cm^{-1} near the lowest edge of the longitudinal optical oscillations. As the angular frequency ω is decreased, both the energy and and amplitude grow monotonically, and the breather width decreases.
3. The equations of motion have been obtained in cylindrical coordinates by canonical method from the Hamiltonian (6). These equations have been studied numerically, drawing the phase plane curves. It was observed that these equations support three types of strongly localized nonlinear modes – discrete breathers:

(i) The first type are the radial breathers, These trajectories describe transverse localized nonlinear modes with the frequency band [560, 585] cm^{-1}. The evolution curve for radial breather has been shown in Fig. 1(a). The lifetime of these breathers can be of the order of several nanoseconds.

(ii) The second type of breathers are the twisting breathers.These are have the charactistics of localized torsion oscillations of the nanotube with the frequency spectrum, [1440, 1640] cm^{-1} using the Brenner potential and are associated with the torsion oscillations of the nanotube. These breathers have wider the frequency spectra of the breathers. The evolution curve is as per Fig. 1(b). The twisting breathers are associated with the torsion oscillations of the nanotube. In a sharp contrast to other two breathing modes, the twisting breather is an exact solution of the motion equations of the nanotube, and it does not radiae phonons. An example of this genuine discrete breather is shown in fig. 4. These oscillations are stable and have the largest frequency spectrum.

(iii) The third type of breathers is called the longitudinal breathers. They exist in planar carbon structures, such breathers exist in the frequency range [1160, 1205] cm^{-1}. Fig. 1(c) shows the respective evolution curve. The longitudinal breathers become coupled to the transverse phonon modes. They do not have a finite lifetime and therefore they have localized discrete modes associated with the energy self-rapping of torsion oscillations of the carbon nanotubes.

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