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ON THE NANO TORSIONAL PENDULUM

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A torsional nano-pendulum based on a single molecule suspended on a carbon nanotube with a single wall is considering in this paper. The molecule is rotated, resulting in large elastic torsional deformations of the nanotube. The motion equation of this system leads to the sine-Gordon equation. The closed solutions of the sine-Gordon equation, which are expressed in terms of Jacobi elliptic functions (cnoidal solutions) are analyzed by applying the variable separation method.

Key Words: Nano torsional pendulum, Carbon nanotube, Torsional deformation, Cnoidal solutions.

1. INTRODUCTION

Eliminating vibrations and controlling dynamics in nano-world are subjects must address to applications in nano-electromechanical structures. One of the major obstacles to miniaturization and to build useful micro- and nano-sized devices involves changes to mechanical properties that can occur as the size of a system are below the macroscale toward the atomic scale. Mechanical devices with molecular-scale components are potential building blocks for nanoelectromechanical systems and may also serve as sensors or actuators (Meyer, Paillet and Roth [1]).

An interested point of view with respect to mechanical behavior of molecular scale devices is presented by Ortega and Spong in [2]. The dynamical systems are viewed as energy transformation systems which require shaping of the total energy to globally stabilize the motion. The idea of energy shaping has the root in the control of robots, where controllers are derived with simple potential energy shaping (Takegaki and Arimoto [3]). For nanoscopic scales, the quasi-continuum method can be applied as an approximation theory to atomistic, which reduces to the exact atomistic theory when all the atomic degrees of freedom are considered (Chiroiu *et al*. [4], Teodorescu *et al.* [5], Teodorescu, Chiroiu and Munteanu [6], Chiroiu *et al*. [7]). In this paper we study a torsional nano-pendulum consisted of a rotating molecule of mass M suspended on an individual single wall carbon nanotube. The carbon nanotube is used as a torsional spring for moving suspended molecule. Although the key motion-enabling element here is a single molecule from the carbon nanotube, the suspended molecule is large enough to be visible in an optical microscope. The suspended molecule is rotating by an electric field and as a result of the extremely small restoring force associated with the torsional deformation of molecules of carbon nanotube, unusually large oscillations are excited by the energy of the pendulum.

The motion equation of this system leads to the sine-Gordon equation. The closed solutions of the sine-Gordon equation, which are expressed in terms of Jacobi elliptic functions (cnoidal solutions) are analysed by applying the variable separation method.

2. MODEL

Consider the problem of free torsional oscillations of a pendulum consisting of a molecule suspended from a carbon nanotube with a single wall (fig.1). A carbon nanotube is a cylindrical molecule composed of carbon atoms. A typical section of a single-walled carbon nanotube is illustrated in Fig.2, each node being a carbon atom and lines the chemical bonds (Ruoff, Qian and Liu [8]). Fig.2 represents a damaged carbon nanotube with missing atoms in a region of the wall (Belytschko *et al.* [9]).

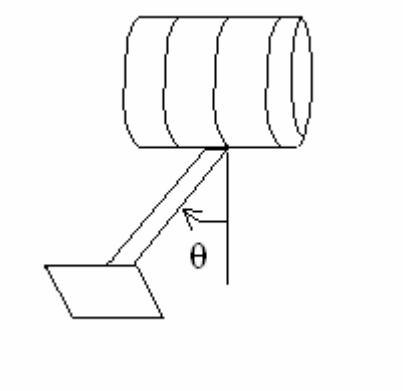

Fig. 1. The model.

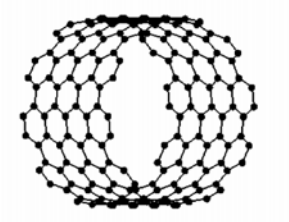

Fig. 2. A section through a carbon nanotube viewed from the side [7].

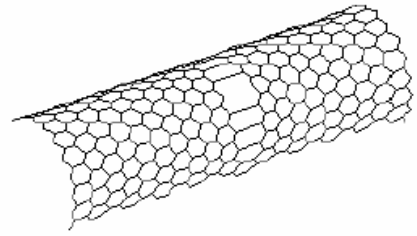

Fig. 3. A damaged carbon nanotube by missing atoms [8].

For the carbon nanotube the modified Morse potential function is used

$$E = E_{stretch} + E_{angle},$$
$$E_{strech} = D\{[1-\exp(-\beta(r-r_0)]^2 - 1\},\ E_{angle} = \frac{1}{2}k_\varphi(\varphi-\varphi_0)^2[1+k_s(\varphi-\varphi_0)^4], \tag{2.1}$$

where $E_{stretch}$ is the bond energy due to bond stretch, E_{angle} is the bond energy due to bond angle-bending, D,β,k_s and k_φ are constants, r is the length of the bond, r_0 a given constant and φ is the current angle of the adjacent bond related to the standard deformation measure in molecular mechanics with φ_0 a given value. The restoring torque Γ exerted by suspended molecule when rotated through an angle θ is assumed to be given by the linear relation $\Gamma = k_\theta\theta$, where k_θ is a constant called the torque constant of the molecule. If the angle made with the downward vertical by the pendulum is θ then the angular velocity ω is $\ddot{\theta}$. The Newtonian equation of motion for nano-pendulum is

$$J\omega = \Gamma - Mhg\sin\theta, \tag{2.2}$$

where Γ is the torque spring, the second terms in the right-side represents the torque due to the gravity, J is moment of inertia of pendulum, h is the distance of the center of mass from the central axis, g the gravity acceleration constant. The torque due to the rotating molecule is given by $k\theta$. To obtain a continuous model for pendulum, a limiting process is considered, by introducing new space and time variable

$$X = \sqrt{\frac{Mhg}{k_\theta}}\frac{x}{L}, \quad T = \sqrt{\frac{Mhg}{J}}t, \tag{2.3}$$

where L is the length of carbon nanotube. The equation (2.2) is reduced to the sine-Gordon equation

$$\theta_{TT} - \theta_{XX} + m^2\sin\theta = 0, \tag{2.4}$$

with

$$m = \frac{1}{2}\frac{\alpha_2}{\alpha_1}, \ \alpha_2 = D\{[1-\exp(-\beta(r-r_0)]^2 - 1\}, \ \ \alpha_1 = \frac{1}{2}k_\varphi(\varphi-\varphi_0)^2[1+k_s(\varphi-\varphi_0)^4].$$

We impose that the sine-Gordon equation (2.4) must admit a first integral for the Hamiltonian of the system

$$H = E_{stretch} + E_{angle} = E, \tag{2.5}$$

with E given by (2.1). The sine-Gordon equation such as other evolution equations with solitonic behavior, admits infinitely many exact solutions and conservation laws (Dodd *et al*. [10], Drazin [11], Drazin and Johnson [12], Munteanu and Donescu [13]). The first conservation law is related to the symmetry group of the equations (2.4) and (2.1) and it is given by

$$H = \alpha_2\cos\theta - 1 + \frac{\alpha_1}{2}(\theta_x^2 + \theta_t^2). \tag{2.6}$$

For new variables $\xi = m\gamma(x-vt)+\delta$ and $\gamma^2 = (1-\nu^2)^{-1}$, the equation (2.4) becomes

$$\theta_{\xi\xi} = \sin\theta. \tag{2.7}$$

Multiplying the equation (2.7) by θ_ξ and integrating, we have

$$\theta_\xi^2 = -\cos\theta + C. \tag{2.8}$$

Assuming the boundary conditions of the form $\theta \to 0(\mathrm{mod}\,2\pi)$, the integration constant C is zero and it results

$$\xi = \int\frac{d\theta}{\sqrt{2\sin^2\frac{\theta}{2}-1}} = \ln\tan\frac{\theta}{4}, \tag{2.9}$$

or

$$\tan\frac{\theta}{4} = \exp\xi. \tag{2.10}$$

It is easy to show from $\theta_{\xi\xi} = -2\,\mathrm{sech}\xi\tanh\xi$, $\sin\theta = -2\,\mathrm{sech}\xi\tanh\xi$, that the solution of (2.10) is given by

$$\theta = 4\arctan\exp[m\gamma(x-vt)+\delta], \ \gamma^2 = (1-\nu^2)^{-1}. \tag{2.11}$$

The solution (2.11) represents a twist in the variable $\theta(x,t)$, which takes the system from one solution $\theta = 0$ to an adjacent solution with $\theta = 2\pi$. We are interested in finding the cnoidal solutions of (2.4) expressed in Jacobi elliptic functions (Munteanu [14]). Consider the change of function (Hoenselaers and Micciché [15]).

$$\theta = 4\arctan d \ . \tag{2.12}$$

Substituting (2.12) into (2.4) for $m = 1$ we obtain

$$(d_{xx} - d_{tt})(1 + d^2) - 2d(d_x^2 - d_t^2) + d(d^2 - 1) = 0 \ . \tag{2.13}$$

Applying the variable separation method, we set $d(x,t) = \dfrac{a(x)}{b(t)}$ and denoting $a_x^2 = A(a)$ and $b_t^2 = B(b)$, equation (2.13) is rewritten as

$$(a^2 + b^2)(bA_a - aB_b) - 2ab(A + B) + ab(a^2 + b^2) = 0 \ . \tag{2.14}$$

It is easy to show that (2.14) is verified only and if only the followings equations are verified

$$a_x^2 = c_1 a^4 + c_2 a^2 + c_3 \ , \quad b_t^2 = -c_1 a^4 + (c_2 - 1)a^2 - c_3 \ , \tag{2.15}$$

where c_i, $i = 1,2,3$ are arbitrary constants. We recognize in (2.15) the Weierstrass equations with polynomials of fourth degrees. The boundary conditions and initial conditions on θ require that the function a satisfies the conditions

$$a(0) = a_0 \ , \ a_x(0) = a_x(L) = a_1 \ , \ b(0) = b_0 \ , \ \ b_t(0) = b_1 \ .$$

If either c_1 or c_3 vanishes, the solution becomes one of the two-soliton solutions (Munteanu [14], Chiroiu *et al.* [16], Munteanu *et al.* [17]). We consider that neither c_1 nor c_3 is zero. In this case the solutions are represented by cnoidal functions. The Hamiltonian (2.6) takes the form

$$H = \frac{8}{(a^2 + b^2)^2}(b^2 a_x^2 + a^2 b_t^2 + a^2 b^2) \ . \tag{2.16}$$

We mention that the Hamiltonian does not distinguish between soliton and antisolitons (Hoenselaers and Micciché [15]). The form of a and b are determined by the zeros of the equations

$$c_1 a^4 + c_2 a^2 + c_3 \ , \ -c_1 a^4 + (c_2 - 1)a^2 - c_3 \ .$$

These equations can have four real zeros, two real and two purely imaginary zeros, four purely imaginary zeros or four complex zeros ($c_1 = 1$).

3. RESULTS

In all simulations, the dimensionless space $0 \le x \le 1$ and time $0 \le t \le 1$ variables are used. Consider a single-walled nanotube of $L = 0.58\mu\text{m}$ ($0.58 \times 10^{-6}\,\text{m}$) length, with a diameter of d_t satisfying $\dfrac{L}{d_t} = 10$. The moment inertia with respect to the tube axis is $J = 7 \times 10^{-30}\,\text{kgm}^2$. Others parameters of carbon nanotube are $r_0 = 1.39 \times 10^{-10}\,\text{m}$, $D = 6.03 \times 10^{-19}\,\text{Nm}$, $\beta = 2.63 \times 10^{10}\,\text{m}^{-1}$, $\theta_0 = 2.09\text{rad}$, $k_\varphi = 3 \times 10^{-18}\,\text{Nm/rad}$ and $k_s = 0.75\text{rad}^{-4}$. The molecule is modelled as a rigid sphere of diameter d_b given by $\dfrac{d_b}{d_t} = 5$. The mass ration of the wire carbon nanotube to the molecule is 3. Plots are made for two cases:

Case 1 Four real zeros for a_x^2 and four imaginary zeros for b_t^2 (fig.4);

Case 2 Four imaginary zeros for a_x^2 (and two real and two imaginary zeros for b_t^2 (fig.5).

The both cases correspond to two-soliton solutions (Munteanu and Donescu [13]). The first case displays a train of solitons moving to the right while the antisolitons move to the left, or vice versa. The second case consists of two solitons interaction.

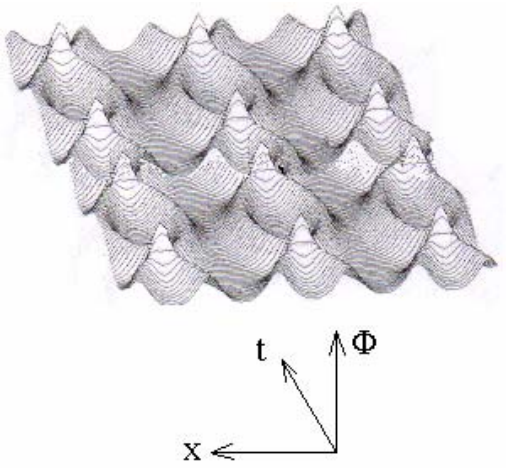

Fig. 4 The interaction between a soliton and a antisoliton (*case* 1).

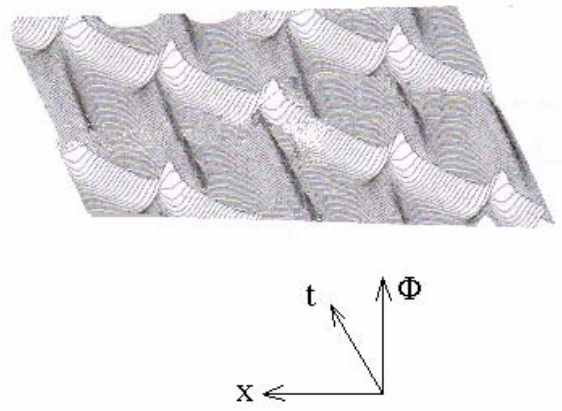

Fig. 5 The interaction between two solitons (*case* 2).

The torsional pendulum built on a single wall carbon nanotube can be turned by extremely small forces. For a rotation of 1°, a torque of 6×10^{-20} Nm is necessary. More interesting is the possibility that the nanotube itself could be used to sense the deformation, because a torsional deformation is expected to change the electronic structure of the tube (Meyer, Paillet and Roth [1]). The resonance frequency for torsional oscillations is calculated to be $f=\frac{1}{2\pi}\sqrt{\frac{k_{\varphi}}{J}}\approx 0.1\text{MHz}$. Next we consider that the nanotube is damaged by missing of some atoms in a portion of the wall (fig. 3). In this case, free decay oscillations of the system are observed. Its equilibrium position is shifting during oscillations. After oscillations died out, the equilibrium position remains shifted.

4. CONCLUSIONS

We have studied a torsional pendulum consisted from a single-walled carbon nanotube, which is used as a torsional spring for rotating suspended molecule. It results large but fully elastic torsional deformations of the nanotube. As a result of the extremely small restoring force associated with the torsional deformation of a single molecule of the carbon nanotube, unusually large oscillations are excited by the energy of the pendulum. Mechanical devices with molecular-scale components are potential building blocks for nanoelectromechanical systems and may also serve as sensors or actuators.

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