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Orbiting buckyballs inside nanotori

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Abstract

The discovery of carbon nanostructures, such as carbon nanotubes and the so-called buckyballs (or C60 fullerenes), have generated considerable interest for potential nanomechanical device applications. One such device is the high frequency nanoscale gigahertz oscillator. A number of studies investigating these oscillators find that sliding an inner-shell inside an outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies in the gigahertz range. It is found that the oscillation is sensitive to diameter and helicity of the tube and that the inner tube length can be used to tune the frequency, where the buckyball provides the highest frequency. More recently, toroidal carbon nanotubes, termed fullerene "crop circles" were observed in experiments. Researchers observe single continuous toroidal nanotubes with no beginning or end, effectively a single-walled carbon nanotube wrapped around onto itself so that the two open ends join, and are stabilized by van der Waals forces alone, to form a perfect "nanotorus". The question arises as to whether it is possible to create a C60-nanotorus oscillator, whereby a buckyball would orbit around the inside of a nanotorus. As far as the authors are aware, the C60-nanotorus oscillator is yet to be constructed and the aim here is to understand the mechanics and dynamics of this potential nanoscale device. As in previous studies, the Lennard-Jones potential is used to calculate the forces acting on the fullerene due to the non-bonded interactions. A body force diagram is constructed to balance the Lennard-Jones potential with other relevant forces, such as the centrifugal force. Here, we present a synopsis of recent work examining the equilibrium position of a buckyball orbiting inside a nanotorus, followed by investigation into its orbital velocity.

Keywords

orbiting, nanotori, inside, buckyballs

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Orbiting Buckyballs Inside Nanotori

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Abstract—The discovery of carbon nanostructures, such as carbon nanotubes and the so-called buckyballs (or C_{60} fullerenes), have generated considerable interest for potential nanomechanical device applications. One such device is the high frequency nanoscale gigahertz oscillator. A number of studies investigating these oscillators find that sliding an inner-shell inside an outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies in the gigahertz range. It is found that the oscillation is sensitive to diameter and helicity of the tube and that the inner tube length can be used to tune the frequency, where the buckyball provides the highest frequency. More recently, toroidal carbon nanotubes, termed fullerene “crop circles” were observed in experiments. Researchers observe single continuous toroidal nanotubes with no beginning or end, effectively a single-walled carbon nanotube wrapped around onto itself so that the two open ends join, and are stabilized by van der Waals forces alone, to form a perfect ‘nanotorus’. The question arises as to whether it is possible to create a C_{60} -nanotorus oscillator, whereby a buckyball would orbit around the inside of a nanotorus. As far as the authors are aware, the C_{60} -nanotorus oscillator is yet to be constructed and the aim here is to understand the mechanics and dynamics of this potential nanoscale device. As in previous studies, the Lennard-Jones potential is used to calculate the forces acting on the fullerene due to the non-bonded interactions. A body force diagram is constructed to balance the Lennard-Jones potential with other relevant forces, such as the centrifugal force. Here, we present a synopsis of recent work examining the equilibrium position of a buckyball orbiting inside a nanotorus, followed by investigation into its orbital velocity.

Keywords-carbon nanotori; Lennard-Jones potential; buckyball; gigahertz oscillators

I. INTRODUCTION

The discovery of carbon nanotubes by Iijima in 1991 [1] created the opportunity for the invention of several nanoscale devices. Carbon nanotubes, consisting of one or many graphene sheets rolled up into a seamless hollow cylinder to form single-wall (SWNT) or multi-wall (MWNT) carbon nanotubes respectively, hold promise for many new nanoelectronic applications as a result of their fascinating and unique mechanical and electronic properties. The application of carbon nanotubes as high frequency nanoscale oscillators demonstrates one of these exceptional properties. Their ability

to overcome the difficulties faced by micromechanical oscillators in reaching frequencies in the gigahertz range has led to their nickname, “gigahertz oscillators”. Potential applications include ultra-fast optical filters for fiber optic systems and nano-antennae sensitive to high frequency electromagnetic signals.

A number of studies, including mathematical models and molecular dynamical simulations [2, 3], show that sliding an inner-shell inside an outer-shell of a MWNT can generate oscillatory frequencies in the gigahertz range. Legoas *et al.* [2] observe frequencies as high as 38 GHz. By decreasing the length of the inner tube, Zheng and Jiang [3] observe a further increase in oscillation frequency, with the buckyball providing the ultimate inner tube length in terms of realizing the highest oscillation frequency. Cumings and Zettl [4] show that the inner-shell resistance force against sliding of the core is negligibly small, realizing ultra-low friction.

These exceptional results, in conjunction with the discovery of peapods [5], which are buckyballs (or C_{60} fullerenes) enclosed inside carbon nanotubes, has generated considerable interest into the C_{60} -nanotube oscillator [6, 7]. Using molecular dynamics simulations Liu *et al.* [7] observe frequencies as high as 74 GHz. These studies find that the oscillation is sensitive to the diameter and helicity of the tube (the orientation of their hexagonal units with respect to the tube axis), where the tube length can be used to adjust the oscillation frequency.

Single continuous toroidal carbon nanotubes, termed fullerene “crop circles,” were recently observed in experiments by Liu *et al.* [8]. Researchers regularly observe seamless toroidal carbon nanotubes, with a tube diameter of 10 to 12 Å and a ring diameter of 3000 to 5000 Å. During formation the tube ends align themselves so as to maximize the van der Waals interactions, and then join together seamlessly forming a perfect torus. When formed, the rings are quite stable both chemically and physically [9]. Martel, Shea and Avouris [10] succeed in forming rings using straight SWNT's, where the ring circumference is equal to the initial tube length. Effectively the toroidal nanotube structure can be viewed as a SWNT closed around onto itself into a perfect torus. In this paper these toroidal structures are referred to as nanotori.

The question arises as to whether it is possible to create a C_{60} -nanotorus oscillator. Could we either, close a nanotube

already containing an oscillating buckyball into a torus; or inject a buckyball into the torus just prior to closure; or close a nanotube containing a stationary buckyball to form a torus and subsequently initialize the oscillation by some applied external field (electric, magnetic, chemical doping), inducing a velocity on the enclosed buckyball? These procedures pose numerous practical challenges that need to be overcome before an actual C₆₀-nanotorus oscillator can be realized. The ultra-low friction effect demonstrated by Cumings and Zettl [4] may also be exhibited in the C₆₀-nanotorus oscillator, and if so the buckyball might orbit almost indefinitely inside the nanotorus. A sealed structure is ideal in terms of working devices, and the C₆₀-nanotorus oscillator may well be the ultimate oscillator. As far as the authors are aware, a C₆₀-nanotorus oscillator has yet to be constructed and the aim here is to assess its feasibility by considering the basic mechanics of such a system. Regardless of the speculative nature of these potential nanoscale devices, such a study must inevitably go before any practical implementation.

As a first attempt to model this system, we follow the findings of Cumings and Zettl [4] and ignore any frictional effects. Although we consider the effect of gravity, we find that for a nanotorus lying on a horizontal surface the effects of gravity are considerably less than those arising from both the Lennard-Jones potential and the centrifugal effect, and accordingly may be neglected. The centrifugal potential is shown to cause the position of the fullerene to move further from the centre of rotation and closer to the tube wall. The buckyball equilibrium position depends on the nanotorus tube radius, where the position moves closer to the tube wall as the radius increases. The angular velocity of the buckyball increases as the buckyball moves away from the centre of the nanotorus and with frequencies in the gigahertz range.

In this paper we present a synopsis of recent work by the authors [11] into the mechanics of the motion of a buckyball orbiting inside a single-walled carbon nanotorus. The Lennard-Jones potential, commonly used to find the forces in the modeling of non-bonded interactions, is summarized in Sec II, followed by an overview of the forces acting on the buckyball. In Sec III we outline the Lennard-Jones energy, equilibrium position and frequency of oscillation of the buckyball.

II. POTENTIAL FUNCTIONS AND MECHANICS

A. Lennard-Jones potential

The non-bonded interaction energy is defined by

$$V_1 = \eta_b \eta_t \iint v(\rho) d\Sigma_b d\Sigma_t, \quad (1)$$

where $v(\rho)$ is the potential function for two molecules and ρ is the distance between the two surface elements $d\Sigma_b$ and $d\Sigma_t$ on the buckyball and nanotorus, respectively. The atoms are assumed to be uniformly distributed over the surface of the molecule, where η_b (0.379 atoms/Å²) and η_t (0.382 atoms/Å²) [7] represent the mean surface density of the carbon atoms on the buckyball and nanotorus, respectively. Note that here we

use the mean surface density of graphene as an approximation for the nanotorus.

The inverse power model, the so-called Lennard-Jones potential, is used in this investigation and is given by

$$v(\rho) = -A\rho^{-6} + B\rho^{-12}, \quad (2)$$

where A and B are the attractive and repulsive constants respectively, and here we use $A = 17.4 \text{ eV}\text{\AA}^6$ and $B = 29 \times 10^3 \text{ eV}\text{\AA}^{12}$ for the interaction between C₆₀-graphene [12].

B. Forces on the orbiting buckyball

The three forces acting on the orbiting buckyball are the van der Waals force (resulting from the Lennard-Jones potential), the centrifugal force and the force of gravity and each has an associated potential energy function. We follow the findings demonstrated by Cumings and Zettl [4] and assume ultra-low friction so that friction is negligible when compared to the remaining forces.

Using the Lennard-Jones potential we derive the van der Waals interaction force, given as $F_1 = -\nabla V_1(x, y, z)$, where x, y, z refer to the coordinates of the buckyball and V_1 is the Lennard-Jones potential defined by (1). As the buckyball orbits inside the nanotorus it experiences a centrifugal force, which is the force experienced by a body spinning on an axis and is directed away from the centre of rotation. The centrifugal force is $F_2 = -mR\omega^2$, where m is the mass of the buckyball taken to be $1.196 \times 10^{-24} \text{ kg}$, with corresponding energy $V_2 = -\frac{1}{2}mR^2\omega^2$. The buckyball also experiences a gravitational effect as it rotates, defined by $F_3 = mg$, where g is acceleration due to gravity (9.81 m/s^2). The corresponding potential energy is $V_3 = -mgh$, where h is the height above some datum level and we assume the plane of the nanotorus is positioned in the horizontal. The total energy becomes $V = V_1 + V_2 + V_3$, and the position of the buckyball is located where this energy is a minimum.

III. ORBITING BUCKYBALL

In this section we summarize results of work recently presented by the authors [11]. A brief overview of the Lennard-Jones energy and the equilibrium position of the buckyball are given followed by a discussion of the orbital velocity of a buckyball orbiting inside a carbon nanotorus. We assume that it is possible to close a C₆₀-nanotube oscillator around onto itself so as to form the C₆₀-nanotorus seamlessly. The vacuum effect, where a buckyball is sucked into one end of the nanotube [12, 13], generating an initial velocity, is presumed to occur just prior to closure of the nanotorus.

A. Equilibrium position

The position of the buckyball is illustrated in Fig. 1 and its centre is defined by

$$x = (c + \varepsilon \cos \phi_1) \cos \theta_1, \quad y = (c + \varepsilon \cos \phi_1) \sin \theta_1, \quad z = \varepsilon \sin \phi_1, \quad (3)$$

where c is the nanotorus ring radius taken as $1500 \text{ \AA}$ [8], b is the nanotorus tube radius and the centre of the buckyball is a distance ε from the cross-sectional tube centre, at an angle ϕ_1

from the horizontal. The radius of the buckyball, a , is taken to be $3.55 \text{ \AA}$ [12].

Figure 1. Torus and its coordinates.

Using (1) and (2) we can evaluate the Lennard-Jones energy between the buckyball and the nanotorus, to be

$$V_1 = 256\pi^3 abc \eta_i \eta_t \left[\frac{-5Aa^3 c^3 (c + \epsilon)^3}{2[\delta(4c(c + \epsilon) + \delta)]^{7/2}} F_1\left(\frac{1}{2}; \frac{7}{2}, \frac{7}{2}; 1; \alpha, \beta\right) + \frac{155584Ba^9 c^9 (c + \epsilon)^9}{[\delta(4c(c + \epsilon) + \delta)]^{9/2}} F_1\left(\frac{1}{2}; \frac{19}{2}, \frac{19}{2}; 1; \alpha, \beta\right) \right] \quad (4)$$

where $\delta = (b + \epsilon)^2 - a^2$, $\alpha = 4b\epsilon/\delta$ and $\beta = 4b\epsilon/[4c(c + \epsilon) + \delta]$. Note that the energy potential given above is only valid for $|\epsilon| \leq |b - a|$ and $F_1(\alpha; \beta, \beta_1; \gamma; x, y)$ is an Appell's hypergeometric function of two variables [14, 15, 16].

Using the algebraic package, MAPLE, we plot the Lennard-Jones energy against buckyball position, shown in Fig. 2 for both a nanotorus created from closing a (10, 10) ($b = 6.784 \text{ \AA}$) and a (16, 16) ($b = 10.856 \text{ \AA}$) nanotube. The gravity potential is found to be negligible when compared to the centrifugal and Lennard-Jones potentials, hence we assume $\phi_1 = 0$. The buckyball's minimum energy or equilibrium position is found to depend on the nanotorus tube radius b , where the buckyball moves closer to the nanotorus wall as the radius increases. For example, the equilibrium position for the (10, 10) nanotorus is $\epsilon = 0.9 \text{ \AA}$, while for the (16, 16) nanotorus we obtain $\epsilon = 5.25 \text{ \AA}$. These represent distances from the tube wall of $2.334 \text{ \AA}$ and $2.056 \text{ \AA}$, respectively. A similar observation is made by Cox, Thamwattana and Hill [17]. The inclusion of the centrifugal potential moves the minimum energy position further from the centre of rotation. The amount it moves depends on the nanotorus tube radius, for example the (10, 10) nanotorus moves 7% closer to the tube wall and the (16, 16) nanotorus 2% closer. The position also depends on the angular velocity, where it is more dominant for larger velocities.

In the limit as c tends to infinity for Eq. (4), we obtain overall agreement with Cox, Thamwattana and Hill [17]. However, to obtain an equation for the Lennard-Jones energy of the buckyball, only the leading order terms were included and as a result there is a distinction between the two models.

Figure 2. Lennard-Jones energy against buckyball position ϵ , for (10, 10) dashed and (16, 16) solid nanotori.

B. Orbital velocity

Since gravity is found to be negligible, Newton's second law can be shown to reduce to

$$\frac{\partial V_1}{\partial R} = mR\omega^2, \quad (5)$$

where V_1 is the Lennard-Jones energy given by (4), m is the buckyball mass, ω is the angular velocity and R is the distance from the centre of rotation to the centre of the rotating body ($R = c + \epsilon \cos \phi_1$ and $\phi_1 = 0$). We can rearrange to determine a relationship between the angular velocity and the buckyball position, ϵ . Figure 3 illustrates the angular velocity of a nanotorus created from closing a (10, 10) tube against the buckyball position, ϵ . The buckyball will automatically locate itself to its equilibrium position and as a result there is no angular velocity until we reach this position. To move the buckyball from the equilibrium position, away from the centre of the nanotorus, an angular velocity must be applied. As shown in Fig. 3, this velocity increases exponentially as the distance ϵ increases. This shift away from the center of rotation occurs for angular velocities in the gigahertz range, where the shift is greater as the angular velocity increases. For example, for the (10, 10) carbon nanotorus, a frequency of 34 GHz moves the buckyball $0.4 \text{ \AA}$ away from the equilibrium position, whereas a frequency of 150 GHz moves the buckyball $1 \text{ \AA}$ away. Cox, Thamwattana and Hill [17] find a frequency of 36.13 GHz for the C_{60} -nanotube oscillator comprised of a (10, 10) carbon nanotube.

Figure 3. Angular velocity of (10, 10) nanotorus against buckyball position

IV. CONCLUSIONS

As a first attempt to model this system we follow Cumings and Zettl [4] and ignore any frictional effects. We find that for a horizontally inclined nanotorus the effects of gravity are considerably less than those arising from the Lennard-Jones potential and the centrifugal effect.

The equilibrium position for the buckyball is found to depend on the nanotorus tube radius b , where the buckyball moves closer to the tube wall as the radius increases. A similar observation is made by Cox, Thamwattana and Hill [17]. Inclusion of the centrifugal force causes the buckyball to move further from the centre of the nanotorus (centre of rotation) and hence closer to the tube wall. The effect varies with nanotorus tube radius b , and is more prominent as the angular velocity increases. Taking the limit as c tends to infinity for Eq. (4) obtains overall agreement for the energy and predicted location given by Cox, Thamwattana and Hill [17].

Frequencies for the C_{60} -nanotorus oscillator are in the gigahertz range. The advantage over the C_{60} -nanotube oscillator is the ability to reach frequencies as high as 100 GHz by the controlled increase of the distance ϵ with no change in geometry necessary.

We finish by noting that the C_{60} -nanotorus oscillator is speculative in nature and presents exciting possibilities, however, there are still numerous practical challenges that need to be overcome before the C_{60} -nanotorus oscillator can be realized.

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