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## Carbon molecules oscillating in carbon nanotube bundles

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### Abstract

Fullerenes  $C_{60}$  and carbon nanotubes are of considerable interest to researchers from many scientific areas due to their unique electronic and mechanical properties. One application of these carbon nanostructures that has recently attracted much attention is the creation of an oscillator that operates in the gigahertz range frequency. A number of studies have found that the sliding of the inner-shell inside the outershell of a multi-walled carbon nanotube can generate gigahertz oscillatory frequencies. In this paper, we investigate the mechanics of a gigahertz oscillator comprising a carbon nanotube oscillating within the centre of a uniform concentric ring or bundle of carbon nanotubes. Since much higher frequencies can be generated from a  $C_{60}$  fullerene oscillating inside a nanotube, we also consider the case of a  $C_{60}$  fullerene oscillating within a bundle of carbon nanotubes. Using the Lennard-Jones potential and the continuum approach, we obtain a relation between the bundle radius and the radii of the nanotubes forming the bundle, as well as the optimum bundle size which gives rise to the maximum oscillatory frequency for both the  $C_{60}$  and the nanotube bundle oscillators. While previous studies in this area have been undertaken through molecular dynamics simulations, this paper emphasizes the use of applied mathematical modelling techniques which provides considerable insight into the underlying mechanisms. The paper presents a synopsis of the major results derived in detail by the present authors in [1, 2].

### Keywords

component; carbon nanotubes; fullerenes; nanotube bundles; gigahertz oscillators; Lennard-Jones potential

### Disciplines

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# Carbon Molecules Oscillating in Carbon Nanotube Bundles

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**Abstract**—Fullerenes  $C_{60}$  and carbon nanotubes are of considerable interest to researchers from many scientific areas due to their unique electronic and mechanical properties. One application of these carbon nanostructures that has recently attracted much attention is the creation of an oscillator that operates in the gigahertz range frequency. A number of studies have found that the sliding of the inner-shell inside the outer-shell of a multi-walled carbon nanotube can generate gigahertz oscillatory frequencies. In this paper, we investigate the mechanics of a gigahertz oscillator comprising a carbon nanotube oscillating within the centre of a uniform concentric ring or bundle of carbon nanotubes. Since much higher frequencies can be generated from a  $C_{60}$  fullerene oscillating inside a nanotube, we also consider the case of a  $C_{60}$  fullerene oscillating within a bundle of carbon nanotubes. Using the Lennard-Jones potential and the continuum approach, we obtain a relation between the bundle radius and the radii of the nanotubes forming the bundle, as well as the optimum bundle size which gives rise to the maximum oscillatory frequency for both the  $C_{60}$  and the nanotube bundle oscillators. While previous studies in this area have been undertaken through molecular dynamics simulations, this paper emphasizes the use of applied mathematical modelling techniques which provides considerable insight into the underlying mechanisms. The paper presents a synopsis of the major results derived in detail by the present authors in [1, 2].

**Keywords**—component; carbon nanotubes; fullerenes; nanotube bundles; gigahertz oscillators; Lennard-Jones potential

## I. INTRODUCTION

Based on the experimental outcomes of Cumings and Zettl [3] and Yu et al. [4], Zheng and Jiang [5] and Zheng et al. [6] find that the sliding of the inner-shell inside the outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies up to several gigahertz. The results of Zheng et al. [6] also lead to the study of a  $C_{60}$  molecule oscillating inside a single-walled carbon nanotube, and the resultant frequencies are found to be much higher than those of the multi-walled carbon nanotube oscillators (Liu et al. [7]). Further, molecular dynamics simulations of Qian et al. [8] indicate that the acceptance of a  $C_{60}$  fullerene, which is initially at rest near the tube open end, only occurs for carbon nanotubes with radii greater than a certain critical value. After being accepted into the tube, these simulations clearly show the oscillation of the  $C_{60}$  molecule between the tube open ends. In Cox et al. [9, 10],

the issues relating to the oscillations of a  $C_{60}$  fullerene inside a single-walled carbon nanotube are investigated from an applied mathematical perspective. In particular, Cox et al. [9, 10] provide mathematical models which address the three issues regarding the determination of the critical radius of a nanotube that will accept or reject a  $C_{60}$  fullerene at the tube open end, the preferred position of the fullerene inside the tube, and the mechanics of the oscillatory motion of the fullerene. In this paper, we adopt similar techniques to those in [9, 10] for a new oscillator, the so-called bundle oscillators, for which the inner oscillating molecules are either a  $C_{60}$  fullerene or a single-walled carbon nanotube. We note that the nanotube-bundle oscillators have previously been studied by Kang et al. [11] using molecular dynamics simulations. However, here and in [1, 2] a more general definition of a bundle is adopted than that of Kang et al. [11]. Here we consider a bundle to comprise an integral number  $N$  of carbon nanotubes aligned parallel to and equidistant from a common axis, which is termed the bundle axis. The perpendicular distance from the bundle axis to the axis of each constituent nanotube is termed the bundle radius  $R$ . We assume that the constituent nanotubes are all of equal length  $2L$  and of radius  $r$ , and they are evenly distributed around the bundle axis, so that the angle subtended at the bundle axis of two adjacent nanotubes is  $2\pi/N$ .

## II. LENNARD-JONES POTENTIAL FOR NANOTUBE BUNDLE

Here, we adopt the classical Lennard-Jones potential function,  $\Phi(\rho) = -A\rho^{-6} + B\rho^{-12}$ , where  $\rho$  is the distance between two interacting atoms, and  $A$  and  $B$  denote the attractive and repulsive constants, respectively. Assuming a continuum approach where a molecule is modeled as a surface with a uniform atomic distribution, the total interaction energy for the two molecules is given by

$$E = \eta_1 \eta_2 \iint_{S_1} \iint_{S_2} \Phi(\rho) dS_1 dS_2, \quad (1)$$

where  $\eta_1$  and  $\eta_2$  are the mean atomic densities for each molecule,  $S_1$  and  $S_2$  represent the two surfaces and  $\rho$  is the distance between two typical surface elements  $dS_1$  and  $dS_2$  on each surface. Assuming the geometry of the bundle is as described above, we can prescribe a surface of the  $i$ th tube in the nanotube bundle in the Cartesian coordinates  $(x, y, z)$  by

$$\left( R \cos\left(\frac{2\pi(i-1)}{N}\right) + r \cos\theta_i, R \sin\left(\frac{2\pi(i-1)}{N}\right) + r \sin\theta_i, z_i \right),$$

where  $i \in \{1, \dots, N\}$ ,  $0 \leq \theta_i \leq 2\pi$  and  $-L \leq z_i \leq L$ . However, in certain sections of this paper, it is convenient to assume  $0 \leq z_i < \infty$  or assume  $-\infty < z_i < \infty$ . As derived in [1], the analytical expression  $E_{it}$  for the interaction potential per unit length of two parallel carbon nanotubes is given in terms of the Appell hypergeometric functions of two variables, thus

$$E_{it} = \frac{3}{2} \eta^2 r_1 r_2 \pi^3 \alpha^{-5} \left[ -A F_2\left(\frac{5}{2}, -\frac{3}{2}, \frac{1}{2}, 1, 1; -\frac{r_1^2}{\alpha^2}, -\frac{4r_2 \delta}{\alpha^2}\right) + \frac{21}{32} B \alpha^{-6} F_2\left(\frac{11}{2}, -\frac{9}{2}, \frac{1}{2}, 1, 1; -\frac{r_1^2}{\alpha^2}, -\frac{4r_2 \delta}{\alpha^2}\right) \right], \quad (2)$$

where  $\eta$  is the mean atomic density of a carbon nanotube,  $\delta$  denotes the distance between the axes,  $r_1$  and  $r_2$  are radii of the tubes,  $\alpha^2 = (\delta - r_2)^2 - r_1^2$  and  $F_2(a, b, b', c, c'; x, y)$  is an Appell hypergeometric function of two variables of the second kind as defined by Erdelyi et al. [12]. Knowing  $E_{it}(\delta)$  from (2), we can determine the total interaction energy  $E_B$  of a bundle comprising  $N$  tubes each of which has radius  $r$  by summing over all of the constituent interactions, namely

$$E_B = \frac{N}{2} \sum_{k=1}^{N-1} E_{it} \left( 2R \sin\left(\frac{k\pi}{N}\right) \right). \quad (3)$$

We note that the interactions between tubes in a bundle are generally dominated by the nearest neighbour interactions, and as such equation (3) can be approximated as

$$E_B \approx N E_{it} (2R \sin(\pi/N)). \quad (4)$$

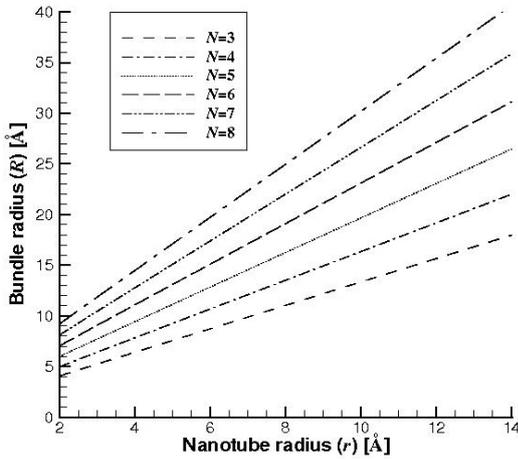


Figure 1. Bundle radius  $R$  versus nanotube radius  $r$  for bundles with  $N = 3, 4, \dots, 8$  at minimum energy configurations [1].

Now, if we assume that a nanotube bundle adopts the lowest energy configuration, then we can determine the bundle radius  $R$  from (4). In Fig. 1, we show the relation between the bundle radius  $R$  and the tube radius  $r$  which minimizes the energy  $E_B$  of the system. If we let  $\lambda$  be the equilibrium

interspacing between two tubes when the interaction energy is minimized, then as shown in Cox et al. [1], we can predict that the bundle radius  $R$  is given by  $R \approx (2r + \lambda)/[2\sin(\pi/N)]$ . We also find that  $\lambda$  varies slightly as a function of the nanotube radius  $r$ , but generally lies in the range 3.10–3.16 Å.

### III. INTERACTION OF CARBON NANOTUBE WITH NANOTUBE BUNDLE

Here, we consider the interaction between a single-walled carbon nanotube of radius  $r_0$  and a nanotube bundle formed from  $N$  nanotubes each of which has radius  $r$ .

#### A. Suction of nanotubes into bundles

From Fig. 2, we determine the condition that a carbon nanotube will be accepted into the vacancy located at the centre of the bundle.

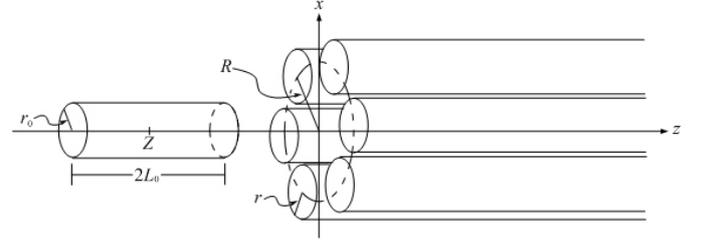


Figure 2. Geometry for a single nanotube entering a nanotube bundle.

If we define  $E$  as the interaction energy between the centre tube and a tube in the bundle, then the total interaction energy of a system with  $N$  tubes in the bundle is given by  $E_{tot} = NE$ . Using (1), we find the energy  $E$  to be given by

$$E = r r_0 \eta^2 \int_0^{2\pi} \int_0^{2\pi} \left[ \int_0^\infty \int_{-L_0}^{L_0} \left( -\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dz_0 dz_1 \right] d\theta_0 d\theta_1, \quad (5)$$

where  $\rho$  is given by

$$\rho^2 = (r \cos\theta_1 + R - r_0 \cos\theta_0)^2 + (r \sin\theta_1 - r_0 \sin\theta_0)^2 + (z_1 - z_0 - Z)^2.$$

We refer to Cox et al. [1] for a detailed analytical evaluation of (5). For a (5,5) carbon nanotube of length 30 Å entering a sixfold symmetry bundle of (5,5) nanotubes and of semi-infinite length, using (5) we plot the total energy  $E_{tot}$  versus the position  $Z$  of the central tube, for different sizes of bundle radius  $R$ , as shown in Fig. 3. From this figure, we can see that the acceptance of a nanotube into a bundle depends on the bundle radius  $R$ . For  $R = 9.47$  Å, the high energy barrier prevents the tube from being accepted inside the bundle. By increasing  $R$  to 9.48 Å, there is an energy well that attracts the tube to be inside; however as the other end of the nanotube approaches into the bundle, the tube encounters an energy barrier which prevents the tube from being completely sucked into the bundle. For  $R = 9.49$  Å, it is clear that the nanotube is accepted into the bundle, although it experiences a small repulsion as the far end of the tube crosses over into the bundle. Further, we find that as the bundle radius  $R$  becomes greater

than 9.49 Å, the (5,5) carbon nanotube is accepted into the bundle without any repulsion effect.

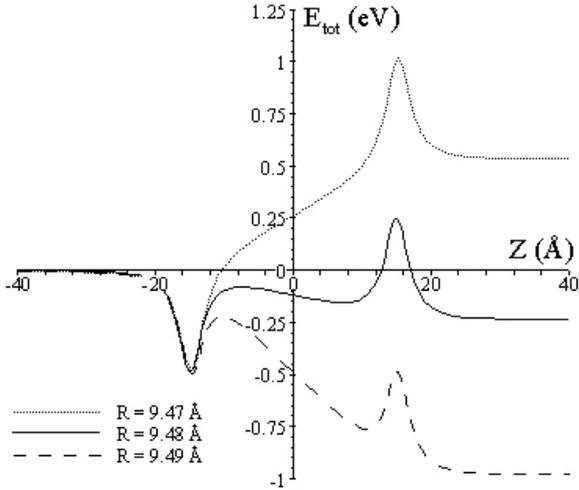


Figure 3. Total energy of (5,5) nanotube of length  $2L_0 = 30$  Å entering into the middle of the sixfold symmetry bundle of (5,5) nanotubes of semi-infinite length (Dotted line,  $R = 9.47$ ; solid line,  $R = 9.48$ ; dashed line,  $R = 9.49$ ) [1].

### B. Oscillating nanotubes in bundles

Here, we consider the situation after the nanotube of length  $2L_0$  is accepted into the bundle. The nanotube oscillates in the middle of the bundle of  $N$ -fold symmetry for which each tube comprising the bundle is assumed to be of length  $2L$ . We assume that the centre of the oscillating tube remains on the  $z$ -axis throughout its motion. As for equation (5), the interaction energy between the central tube and a typical tube in the bundle is given by

$$E = rr_0 n^2 \int_0^{2\pi} \int_0^{2\pi} \left[ \int_{-L}^L \int_{-L_0}^{L_0} \left( -\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dz_0 dz_1 \right] d\theta_0 d\theta_1,$$

so that the total interaction energy is obtained from  $E_{tot} = NE$ .

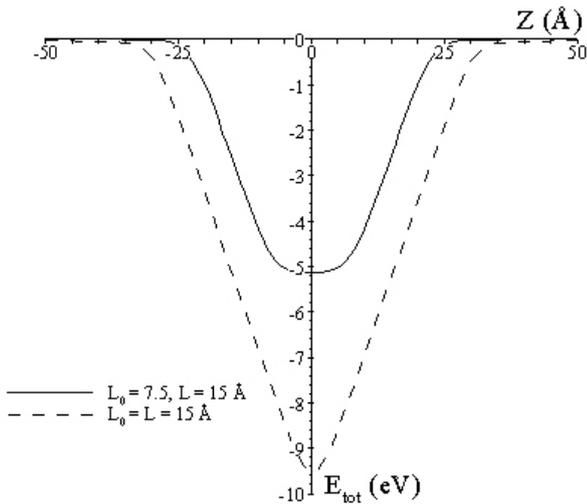


Figure 4. Potential energy of (5,5) nanotube of length  $2L_0$  oscillating inside the middle of sixfold symmetry bundle of (5,5) nanotubes of length  $2L = 30$  Å (Dashed line,  $L_0 = 15$  Å; solid line,  $L_0 = 7.5$  Å) [1].

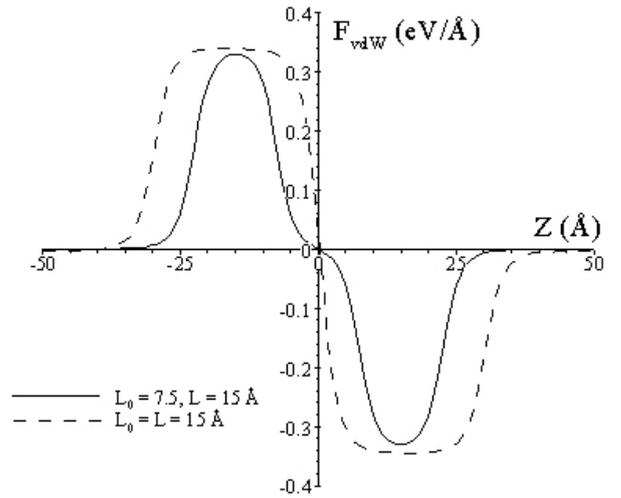


Figure 5. van der Waals force of (5,5) nanotube of length  $2L_0$  oscillating inside the middle of a sixfold symmetry bundle of (5,5) nanotubes of length  $2L = 30$  Å (Dashed line,  $L_0 = 15$  Å; solid line,  $L_0 = 7.5$  Å) [1].

In Figs. 4 and 5, we plot energy  $E_{tot}$  and the van der Waals force  $F_{vdW} = -dE_{tot}/dZ$ , for a (5,5) nanotube oscillating in a sixfold symmetry (5,5) carbon nanotube bundle. We assume that the length of the tubes in the bundle is  $2L = 30$  Å and we consider two lengths  $2L_0$  for the oscillating tube. We note that we adopt  $R = 9.941$  Å in this case, since it maximizes the suction energy  $W_t = -NE_t(R)$  [1], giving rise to a maximum velocity and oscillatory frequency. From the figures, the single nanotube has the minimum energy at  $Z = 0$  inside the nanotube bundle. By pulling the tube away from this point in either direction, the van der Waals force operates to propel the tube back into the minimum energy configuration, which results in an oscillatory motion of the tube inside the bundle. This behaviour is similar to that of the double-walled carbon nanotube oscillators studied by Baowan and Hill [13].

From Fig. 5 and as shown in Cox et al. [1] and Baowan and Hill [13], when  $L \geq L_0$  the van der Waals force  $F_{vdW}$  experienced by the oscillating tube can be approximated by

$$F_{vdW} = W_t \left[ H(Z + L + L_0) - H(Z + L - L_0) - H(Z - L + L_0) + H(Z - L - L_0) \right],$$

where  $H(z)$  is the Heaviside unit step function and  $W_t$  is the suction energy. As detailed in [1], assuming the nanotube is initially at rest and extruded by a distance  $d$  out of the bundle, the resulting oscillatory frequency  $f$  can be found from

$$f = \frac{1}{4} \sqrt{\frac{2W_t}{M}} \left( \frac{\sqrt{d}}{2d + (L - L_0)} \right),$$

for which the maximum frequency occurs when  $d = (L - L_0)/2$ . As such, the maximum frequency  $f_{max}$  is given by

$$f_{max} = \frac{1}{8} \sqrt{\frac{W_t}{M(L - L_0)}}, \quad (6)$$

noting that  $M$  is the mass of the oscillating tube which is given

by  $M = 4\pi r_0 L_0 \eta m_0$ , where  $m_0$  is the mass of a single carbon atom. From an analysis in [1], there are limitations on  $L$ ,  $L_0$  and the minimum extrusion distance  $d_{\min}$  which gives rise to  $f_{\max}$  (6), and these limitations can be written succinctly as  $L_0 + 2d_{\min} < L < 5L_0$ . Upon ignoring energy dissipations and thermal effects during the oscillation, we find that our model gives reasonable results as compared with the molecular dynamics studies of Kang et al. [11] (for more details see Cox et al. [1]).

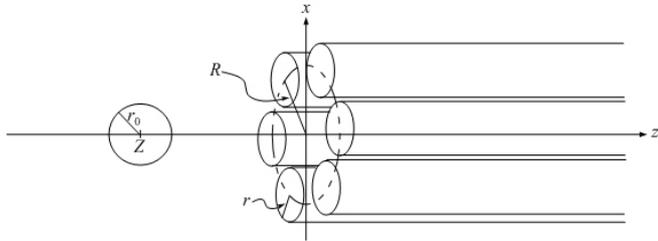


Figure 6. Geometry for a  $C_{60}$  fullerene entering a nanotube bundle.

#### IV. INTERACTION OF FULLERENE WITH NANOTUBE BUNDLE

The study of a fullerene oscillating inside a single-walled carbon nanotube [9, 10] and from the previous sections lead us to examine other possible gigahertz oscillators, which are created from a fullerene oscillating in the centre of a nanotube bundle, as shown in Fig. 6. In this section, we summarize the results derived in Cox et al. [2] for this newly introduced oscillator.

Assuming that a  $C_{60}$  fullerene is located at the centre of the nanotube bundle, we have the suction energy  $W_f$  given by  $W_f = -NE_{fi}$ , where  $N$  is the number of tubes forming the bundle and  $E_{fi}$  is the interaction energy between the fullerene and a single nanotube, which is equation (2.15) given in [10]. In Table I, we present the parameters of the oscillators which optimize the suction energy. As the suction energy is directly converted to the kinetic energy, results shown in Table I are particularly important as a guide to construct bundle oscillators to achieve the maximum velocity and frequency.

TABLE I. PARAMETERS FOR OPTIMIZED  $C_{60}$  FULLERENE-BUNDLE OSCILLATORS [2].

Number $N$	Tube radius $r$ (Å)	Bundle Radius $R$ (Å)	Suction energy $W_f$ (eV)
4	10.294	16.792	2.314
5	5.439	11.930	2.551
6	3.355	9.838	2.731
7	2.219	8.692	2.850

From [2] we find that the force and the energy profiles for  $C_{60}$ -bundle oscillators are similar to those of  $C_{60}$ -single-walled carbon nanotube oscillators [9, 10], and therefore here we adopt the same model as presented in [9, 10]. Using the equation for frequency  $f = (2W_f / m_f)^{1/2} / (4L)$  where  $m_f$  is the mass of the fullerene, we plot Fig. 7 showing the oscillatory

frequency for various bundle oscillators, varying the bundle length  $2L$ . As expected from Table I, the configuration with  $N = 7$  gives rise to the highest frequency. However, we find that the frequency obtained from a  $C_{60}$  oscillating in a single-walled nanotube is higher than that of the  $C_{60}$ -bundle oscillators studied here.

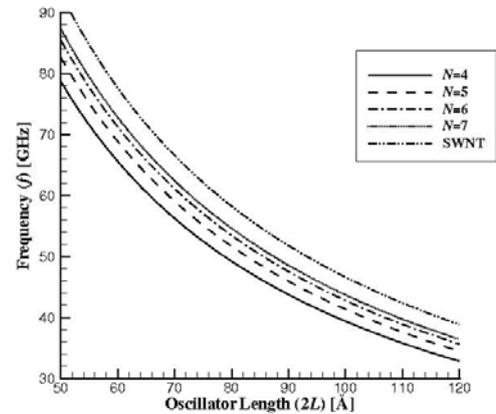


Figure 7. Frequency for a fullerene nanotube bundle oscillator for various configurations and for a fullerene oscillating in a single-walled carbon nanotube [2].

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