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# Oscillation of carbon molecules inside carbon nanotube bundles

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## Abstract

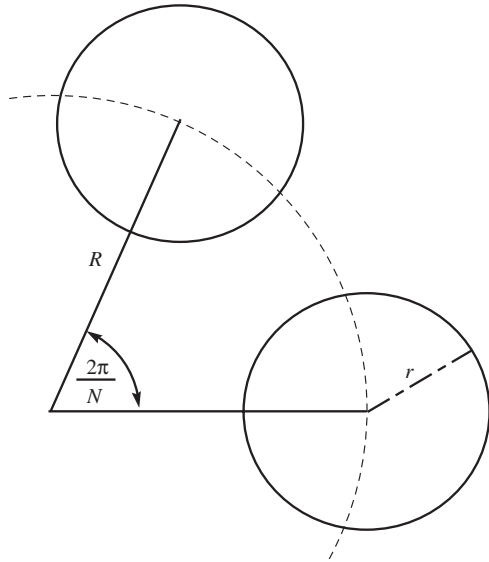
In this paper, we investigate the mechanics of a nanoscaled gigahertz oscillator comprising a carbon molecule oscillating within the centre of a uniform concentric ring or bundle of carbon nanotubes. Two kinds of oscillating molecules are considered, which are a carbon nanotube and a C<sub>60</sub> fullerene. 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 nanotube–bundle and the C<sub>60</sub>–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 of the nanoscaled oscillators. The paper presents a synopsis of the major results derived in detail by the present authors (Cox *et al* 2007 *Proc. R. Soc. A* **464** 691–710 and Cox *et al* 2007 *J. Phys. A: Math. Theor.* **40** 13197–208).

## 1. Introduction

The development of carbon nanotube based oscillators originates from experiments of Cumings and Zettl [3], who remove the cap from one end of the outer shell of a multi-walled carbon nanotube and attach a moveable nanomanipulator to the core in a high-resolution transmission electron microscope. By pulling the inner core out and releasing it back into the outer shell, they report an ultra-low sliding frictional force, and they also observe that the extruded core quickly and fully retracts inside the outer shell due to the restoring force resulting from the van der Waals interaction acting on the extruded core. These results lead Zheng and Jiang [4] and Zheng *et al* [5] to investigate the sliding of the inner shell inside the outer shell of a multi-walled carbon nanotube with both cap removed using molecular dynamics studies. They find that the inner core oscillates between both ends of the outer shell and the resultant oscillatory frequency is up to several gigahertz. Further, their results also support the experimental findings of Cumings and Zettl [3] that the frictional effect of the intershell sliding is very small. This phenomenon is also confirmed by a number of other molecular dynamics simulations, such as Legoas *et al* [6] and Rivera *et al* [7, 8]. From an applied mathematical modelling perspective, Baowan and Hill [9] use the continuum approach for the

Lennard-Jones potential and Newton's second law to study the force distribution for double-walled carbon nanotubes and the oscillation of the inner tube inside the outer tube, assuming that the frictional force can be neglected. They obtain an exact analytical expression for the interaction energy between the inner and outer tubes and the van der Waals interaction force. This model also predicts gigahertz oscillatory frequencies as expected for the double-walled carbon nanotube oscillators.

To create an oscillator with even higher frequency, instead of using a nanotube Liu *et al* [10] employ a C<sub>60</sub> fullerene as an inner oscillating molecule. This idea is based on the suggestion of Zheng *et al* [5] that the shorter the inner tube, the higher the frequency. We note that the interaction between a C<sub>60</sub> fullerene and a single-walled carbon nanotube has previously been studied by Qian *et al* [11]. While Liu *et al* [10] focus on the oscillation frequency, the study of Qian *et al* [11] is concerned with the suction (or repulsion) of a C<sub>60</sub> fullerene at the vicinity of the carbon nanotube open end and the velocity of the fullerene upon entering the nanotube. Further, issues from both of Lui *et al* [10] and Qian *et al* [11] are studied by Cox *et al* [12, 13] using elementary mechanical principles together with the continuum approach to provide a classical applied mathematical model for C<sub>60</sub>–carbon nanotube oscillators. In particular, Cox *et al* [12] determine an analytical expression for the suction energy of a C<sub>60</sub> molecule upon entering a carbon



**Figure 1.** Part of the bundle of  $N$  nanotubes, showing the angle between two adjacent tubes, bundle radius  $R$  and constituent tube radius  $r$ .

nanotube. This energy is imparted onto the  $C_{60}$  molecule in terms of kinetic energy and thus induces the oscillating motion. They also determine analytically the condition on the radius of the carbon nanotube that will accept the  $C_{60}$  molecule from rest in the vicinity of an open end of the tube. In Cox *et al* [13], a mathematical model for the oscillation of the  $C_{60}$ -carbon nanotube oscillators is provided where the axial van der Waals restoring force of the  $C_{60}$  molecule is approximated by two equal and opposite Dirac delta functions operating at both ends of the nanotube.

Recently, Kang *et al* [14] propose a new type of nanoscaled oscillator based on a single-walled carbon nanotube oscillating within a bundle of six similar carbon nanotubes. Using molecular dynamics simulations, Kang *et al* [14] find that the nanotube-bundle oscillator also generates frequencies in the gigahertz range. In Cox *et al* [1, 2], we extend the analysis presented in Baowan and Hill [9] and Cox *et al* [12, 13] to study nanotube-bundle oscillators and also the special case of a  $C_{60}$  fullerene oscillating within the bundle. We comment that a more general definition of a bundle than that of Kang *et al* [14] is adopted in Cox *et al* [1, 2], which is a bundle that is assumed to comprise an integral number of  $N$  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  $R$ . It is also assumed that the constituent nanotubes are all of equal length  $2L$  and radius  $r$  and that they are evenly distributed around the bundle axis, so that the angle subtended at the bundle axis of two adjacent nanotubes is  $2\pi/N$  (see figure 1). Noting that when  $N = 6$ , the results for nanotube-bundle oscillators are consistent with those shown in Kang *et al* [14].

In this paper, we summarize the recent work of Cox *et al* [1, 2] on modelling the mechanics of nanoscaled oscillators, which are created from a carbon molecule (carbon nanotube or

**Table 1.** Values of constants used in this paper.

LJ attraction (CNT-CNT)	$A = 15.2 \text{ eV } \text{\AA}^6$
LJ repulsion (CNT-CNT)	$B = 24.1 \times 10^3 \text{ eV } \text{\AA}^{12}$
LJ attraction ( $C_{60}$ -CNT)	$A = 17.4 \text{ eV } \text{\AA}^6$
LJ repulsion ( $C_{60}$ -CNT)	$B = 29 \times 10^3 \text{ eV } \text{\AA}^{12}$
Radius of (5, 5) nanotube	$r_0 = 3.392 \text{ \AA}$
Radius of (8, 8) nanotube	$r_0 = 5.428 \text{ \AA}$
Radius of (10, 10) nanotube	$r_0 = 6.784 \text{ \AA}$
Radius of $C_{60}$	$r_0 = 3.55 \text{ \AA}$
Atomic surface density of $C_{60}$	$\eta_f = 0.3789 \text{ \AA}^{-2}$
Atomic surface density of CNT	$\eta_t = 0.3812 \text{ \AA}^{-2}$
Mass of a single carbon atom	$m_0 = 19.92 \times 10^{-27} \text{ kg}$

$C_{60}$ ) oscillating in carbon nanotube bundles. In the following section, we present the interaction energy between tubes in the bundle and the total suction energies for nanotube-bundle and  $C_{60}$ -bundle oscillators. In section 3, we consider the oscillatory behaviour for both oscillators, and finally in section 4, a summary of the paper is presented.

## 2. Interaction energy

Using the continuum approach which assumes that carbon atoms are uniformly distributed over the surface of the molecule, the total interaction energy between the two molecules can be obtained which is given by

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

where  $\eta_1$  and  $\eta_2$  are the atomic densities of atoms on each molecule,  $S_1$  and  $S_2$  denote the two surfaces,  $\rho$  is the distance between the typical surface elements  $dS_1$  and  $dS_2$  on each surface and  $\Phi$  represents a potential function. Here we adopt the six-twelve Lennard-Jones potential which has the form

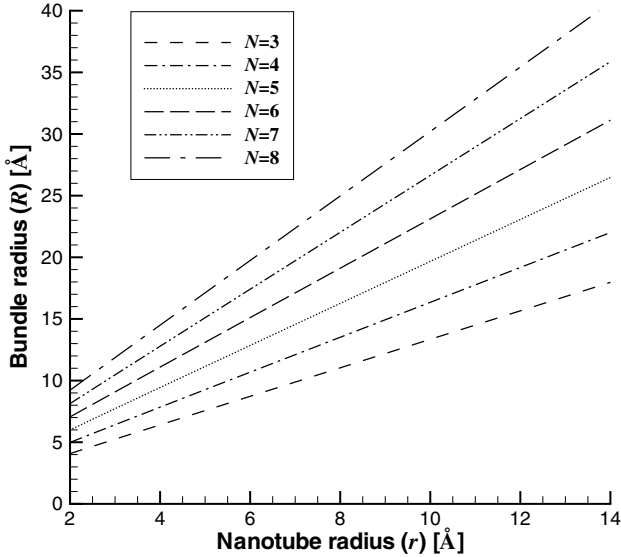
$$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}}, \quad (2)$$

where  $A$  and  $B$  are the attractive and the repulsive constants, respectively. The values of constants used throughout this paper are presented in table 1. We note that the values of the attractive and repulsive constants, namely  $A$  and  $B$ , are taken from Girifalco *et al* [15].

In order to obtain the potential energy of a nanotube bundle, we first need the energy of two parallel nanotubes. Upon using (1) and (2), Cox *et al* [1] derive the analytical expression for the interaction potential per unit length  $E_{tt}$  of two parallel nanotubes of radii  $r_1$  and  $r_2$ , which is given in terms of the Appell hypergeometric functions of two variables as

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

where  $\alpha^2 = (\delta - r_2)^2 - r_1^2$ ,  $\delta$  is the distance between the central axes of the nanotubes and  $F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y)$  is an Appell



**Figure 2.** Bundle radius  $R$  versus nanotube radius  $r$  for  $N \in \{3, 4, \dots, 8\}$  [1].

hypergeometric function of two variables of the second kind as defined in Erdélyi *et al* [16]. Next, assuming that the bundle is formed from  $N$  nanotubes each of which has radius  $r$ , we can determine the total interaction energy  $E_B$  of a bundle by summing all of the constituent interactions, namely

$$E_B = \frac{N}{2} \sum_{k=1}^{N-1} E_{tt} \left( 2R \sin \left( \frac{k\pi}{N} \right) \right). \quad (4)$$

We comment that van der Waals force is a short range force, and therefore the interactions between tubes in the bundle are dominated by only the nearest neighbour interactions. As a result, the total energy for a bundle as shown in (4) can be approximated as

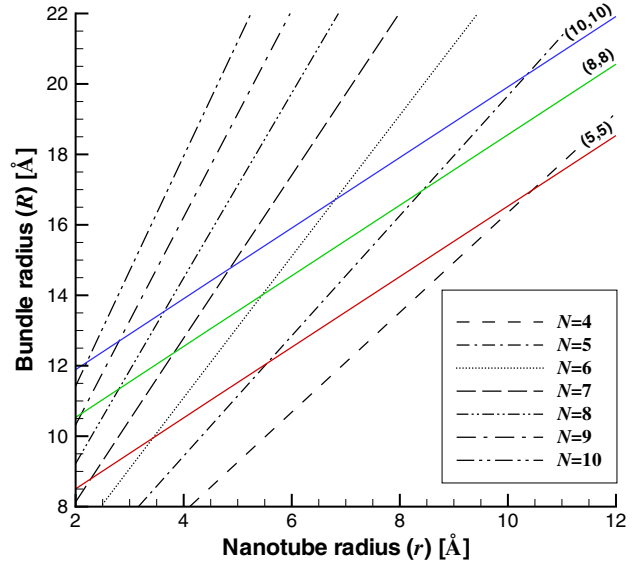
$$E_B \approx N E_{tt} \left( 2R \sin \left( \frac{\pi}{N} \right) \right). \quad (5)$$

Next, if we assume that the carbon nanotubes in a bundle arrange themselves such that the bundle configuration is at equilibrium (i.e. the energy is minimum), then we can determine the bundle radius  $R$  from (5). In figure 2, we show the relation between the radius  $r$  of the tubes forming the bundle and the bundle radius  $R$  which minimizes the energy  $E_B$  of the system. As shown in Cox *et al* [1], we can estimate the bundle radius  $R$  by the expression

$$R \approx \frac{2r + \lambda}{2 \sin(\pi/N)}, \quad (6)$$

where  $\lambda$ , which is the inter-tube equilibrium spacing, varies slightly as a function of the nanotube radius, but generally lies in the range 3.10–3.16 Å.

In the following two subsections we consider the cases when the bundle interacts with a single nanotube and a C<sub>60</sub> fullerene, respectively.



**Figure 3.** Bundle radius versus nanotube radius for (5, 5), (8, 8) and (10, 10) carbon nanotubes and nanotube bundles with  $N \in \{4, 5, \dots, 10\}$  [1].

(This figure is in colour only in the electronic version)

### 2.1. Tube–bundle

For a single carbon nanotube of radius  $r_0$  located with its axis along the bundle axis and centred at a nanotube bundle assumed infinite in length, we find that the suction energy or the total interaction potential energy per unit length of the single nanotube interacting with the bundle is given by

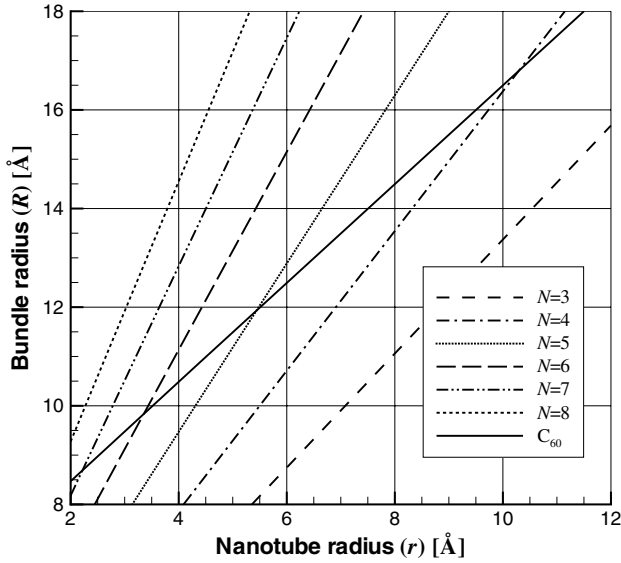
$$W_t = -N E_{tt}(R), \quad (7)$$

noting that  $N$  is the number of nanotubes forming the bundle and  $E_{tt}$  is given by (3). For a given value of  $r_0$ , we can determine from (7) the relationship between the radii of nanotubes forming the bundle  $r$  and the bundle radius  $R$ , for which the suction energy  $W_t$  is maximized. By showing this relationship against the data from figure 2, we can determine the equilibrium configurations for the interaction of the centred nanotube and the bundle. As shown in figure 3 for (5, 5), (8, 8) and (10, 10) nanotubes, the points of intersection with the optimal bundle configurations represent the specific values of  $r$  and  $R$  that lead to optimized energy  $W_t$  for the nanotube for each value of  $N$ .

Further, for the configuration of a bundle comprising nanotubes of radii  $r$  with a nanotube of radius  $r_0$  at the centre, the relationship between  $R$ ,  $r$  and  $r_0$  can be expressed as  $R \approx r_0 + r + \lambda$ , where  $\lambda$  is the inter-tube equilibrium spacing. Thus combining this with (6), we may find a formula for the radius of the constituent tubes in a bundle that maximizes the suction energy for an oscillating tube of radius  $r_0$  as

$$r \approx \frac{(r_0 + \lambda) \sin(\pi/N) - \lambda/2}{1 - \sin(\pi/N)}. \quad (8)$$

We note that when  $N = 6$ , we have  $r \approx r_0$  as expected.



**Figure 4.** Bundle radius versus nanotube radius for a  $C_{60}$  fullerene and nanotube bundles with  $N \in \{3, 4, \dots, 8\}$  [2].

## 2.2. $C_{60}$ -bundle

The total suction energy of a  $C_{60}$  fullerene of radius  $r_0$  located at the centre of the nanotube bundle of infinite in length is given by

$$W_f = -NE_{ft}(R), \quad (9)$$

where  $E_{ft}$  is the energy for an interaction between a  $C_{60}$  and a single nanotube in the bundle. Using Cox *et al* [13] we find that  $E_{ft}$  is given by

$$E_{ft}(R) = 4\pi^2 r_0^2 r \eta_f \eta_t \left[ \frac{B}{5} \left( \frac{315}{256} J_5 + \frac{1155}{64} r_0^2 J_6 + \frac{9009}{128} r_0^4 J_7 + \frac{6435}{64} r_0^6 J_8 + \frac{12155}{256} r_0^8 J_9 \right) - \frac{A}{8} (3J_2 + 5r_0^2 J_3) \right], \quad (10)$$

where  $J_n$  is given in terms of the usual hypergeometric functions  $F(a, b; c; z)$  as

$$J_n = \frac{2\pi}{[(r-R)^2 - r_0^2]^{n+1/2}} \times F\left(\frac{1}{2}, n + \frac{1}{2}; 1; -\frac{4rR}{(r-R)^2 - r_0^2}\right). \quad (11)$$

We refer the reader to Cox *et al* [2, 13] for detailed derivation of (10) and (11).

From (9) we can find for any value of  $N$  the relation between the nanotube radius  $r$  and the bundle radius  $R$  which optimizes the suction energy  $W_f$  for the  $C_{60}$  fullerene ( $r_0 = 3.55 \text{ \AA}$ ), and this is shown graphically in figure 4. On the same figure, we also show the nanotube radii versus bundle radii data from figure 2. Again, the points where the lines intersect represent the specific values of  $r$  and  $R$  that lead to optimized energy for  $C_{60}$  fullerene for each value of  $N$ . Further, it can be seen from figure 4 that if we consider the tube radius  $r$  only in the range 2–12  $\text{\AA}$  then the  $C_{60}$ -bundle oscillators can only be constructed from  $N \in \{4, 5, 6, 7\}$ . In table 2, we present the parameters of the oscillators which optimize the suction

**Table 2.** Parameters for optimized  $C_{60}$ -nanotube bundle oscillators [2].

Number $N$	Tube radius $r$ ( $\text{\AA}$ )	Bundle radius $R$ ( $\text{\AA}$ )	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

energy  $W_f$ . We comment that as the suction energy is directly converted into kinetic energy, results shown in table 2 can be used as a guideline for constructing  $C_{60}$ -bundle oscillators that achieve the maximum velocity and frequency.

## 3. Oscillatory behaviours

In this section, we consider a molecule oscillating in the middle of a bundle of finite length carbon nanotubes of  $N$ -fold symmetry, and we assume that the centre of the oscillating molecule remains on the  $z$ -axis during its motion.

### 3.1. Nanotube-bundle oscillators

According to the geometry of a nanotube-bundle oscillator as shown in figure 5, the total interaction energy of the oscillating nanotube inside a bundle is given by  $E_{\text{tot}} = NE$ , where  $N$  is the number of tubes in the bundle and  $E$  is the energy of the interaction between the centred tube of coordinates  $(r_0 \cos \theta_0, r_0 \sin \theta_0, z_0 + Z)$  and a nanotube in the bundle which has coordinates  $(r \cos \theta_1 + R, r \sin \theta_1, z_1)$ . We note here that  $-L_0 \leq z_0 \leq L_0$ ,  $-L \leq z_1 \leq L$  and  $Z$  is the distance between the centre of the oscillating tube and the origin. Using the Lennard-Jones potential and the continuum approach we obtain the interaction energy  $E$  as

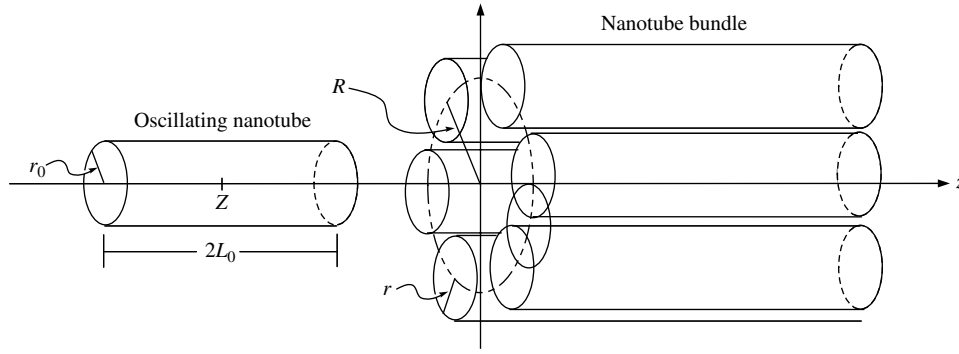
$$E = r r_0 \eta_t^2 \times \int_0^{2\pi} \int_0^{2\pi} \left\{ \int_{-L}^L \int_{-L_0}^{L_0} \left( -\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dz_0 dz_1 \right\} d\theta_0 d\theta_1, \quad (12)$$

where  $\eta_t$  is the mean density of atom on a nanotube and  $\rho$  denotes the distance between two typical surface elements on each nanotube. We refer to Cox *et al* [1] and Baowan and Hill [9] for a detailed analytical evaluation of (12).

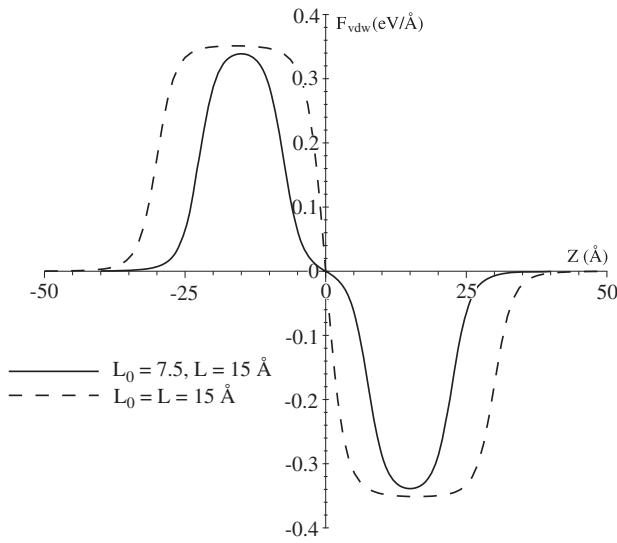
For the total van der Waals interaction force between the tube and the bundle we have  $F_{\text{vdW}} = -\partial E_{\text{tot}} / \partial Z = -N(\partial E / \partial Z)$ . Thus using (12) we plot figure 6 showing the van der Waals force  $F_{\text{vdW}}$  for a (5, 5) carbon nanotube oscillating in a six-fold symmetry (5, 5) carbon nanotubes bundle. From the figure, we see that the single carbon nanotube has minimum energy at  $Z = 0$  inside the bundle. By pulling the tube away from the equilibrium configuration in either direction, the van der Waals force tends to propel the tube back towards the centre of the bundle, and as a result, we have an oscillatory motion of the nanotube inside the bundle.

From figure 6, we see that when  $L \geq L_0$  the van der Waals force of the oscillating tube might be approximated in terms of





**Figure 5.** Geometry of a nanotube-bundle oscillator for  $N = 6$ .



**Figure 6.** Force distribution of a (5, 5) nanotube of length  $2L_0$  oscillating inside a 6-fold symmetry bundle comprising (5, 5) nanotubes of length  $2L$ .

step functions and formally given by

$$F_{vdw} = W_t [H(Z + L + L_0) - H(Z + L - L_0) - H(Z - L + L_0) + H(Z - L - L_0)], \quad (13)$$

where  $H(z)$  is the Heaviside unit step function and  $W_t$  is the suction energy per unit length as given by (7). Assuming that the nanotube is initially at rest and extruded by a distance  $d$  out of the nanotube bundle, following Baowan and Hill [9] the resulting oscillatory frequency  $f$  can be found to be given by

$$f = \frac{1}{4} \sqrt{\frac{2W_t}{M}} \left( \frac{\sqrt{d}}{2d + (L - L_0)} \right), \quad (14)$$

where  $M$  is the mass of the oscillating nanotube, which is given by  $M = 4\pi r_0 L_0 \eta_t m_0$ , where  $m_0$  is the mass of a single carbon atom. From (14) when the extrusion distance is such that  $d = (L - L_0)/2$  the maximum frequency is obtained which is given by

$$f_{\max} = \frac{1}{8} \sqrt{\frac{W_t}{M(L - L_0)}}. \quad (15)$$

We note that the case  $L = L_0$  gives rise to oscillations near a stable equilibrium point, where the oscillation period is very short and therefore the maximum frequency occurs. From a practical point of view we need  $d$  to be measurable (i.e.  $d_{\min} < d$ , where  $d_{\min}$  is a minimum extrusion distance). Further, we require that  $d$  must be less than the length of the oscillating nanotube  $2L_0$ . Thus, the extrusion length  $d = (L - L_0)/2$  must satisfy  $d_{\min} < d < 2L_0$ , which gives rise to the constraints  $L_0 + 2d_{\min} < L < 5L_0$  for the bundle length.

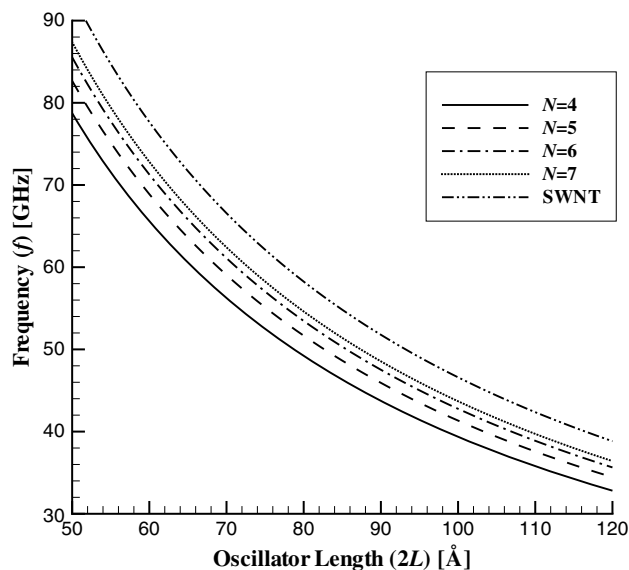
Next we compare our results with those of Kang *et al* [14] for the scenario of a (5, 5) nanotube oscillating in a six-fold nanotube bundle which also comprises (5, 5) nanotubes, and both the bundle and the oscillating nanotube having the same half-length  $L = L_0 = 15$  Å. As mentioned in Cox *et al* [1] upon ignoring energy dissipations and thermal effects during the oscillation, we find that our model with  $d = 6.3$  Å gives a frequency of approximately 80 GHz, which is in reasonable agreement with the frequency of 72 GHz obtained from the molecular dynamics studies of Kang *et al* [14] after the oscillation has stabilized.

### 3.2. $C_{60}$ -bundle oscillators

From figure 6, we may observe that in the limit  $L_0 \ll L$ , which is the case for a  $C_{60}$  oscillating inside the bundle, we obtain the peak-like forces at both ends of the bundle, which can be estimated using the Dirac delta function, namely  $F_{vdw} = W_f [\delta(Z + L) - \delta(Z - L)]$ . We note that this behaviour is similar to that of a  $C_{60}$  oscillating inside a single-walled carbon nanotube [13]. As such, the model presented in Cox *et al* [13], which involves approximating the impulse-like forces operating at both ends of the tube as Dirac delta functions, can also be used for  $C_{60}$ -bundle oscillators. Thus, from [13] we have the equation for frequency of the  $C_{60}$ -bundle oscillators, namely

$$f = (2W_f/m_f)^{1/2}/(4L), \quad (16)$$

where here  $W_f$  is given by (9) and  $m_f = 60m_0$  is the mass of the fullerene, noting that  $m_0$  is the mass of a single carbon atom. Using (16) with values of  $r$ ,  $R$  and  $W_f$  given in table 2 for each bundle type, we plot in figure 7 the oscillatory frequencies for various bundle oscillators, varying the bundle length  $2L$ . As expected from table 2, the configuration with  $N = 7$  gives rise to the highest frequency. However, we find



**Figure 7.** Frequency for a fullerene nanotube bundle oscillator for various configurations varying the bundle length  $2L$  [2].

that the frequency obtained from a  $C_{60}$  oscillating in a (10, 10) single-walled nanotube is higher than that of the  $C_{60}$ -bundle oscillators presented here. As described in Cox *et al* [2], the higher force from the  $C_{60}$ -nanotube oscillator is due to the fact that the curvature of the nanotube wall matches the curvature of the fullerene and thus a greater portion of the fullerene surface is located at the optimal distance for van der Waals interactions.

#### 4. Summary

In this paper we summarize some recent results on modelling the mechanisms of a new type of nanoscaled oscillator, which are known as carbon nanotube bundle oscillators. We investigate two scenarios for bundle oscillators: the first has a single-walled carbon nanotube oscillating inside the bundle; and the second has a  $C_{60}$  fullerene as the inner oscillating molecule. By using the Lennard-Jones potential together with the continuum approach, formal mathematical expressions for the van der Waals interaction energy and force are determined. The results obtained can be used to predict the oscillator bundle configuration which optimize the suction energy and therefore leads to a maximum frequency oscillator. We emphasize that the major contribution of the authors in this area is the use of elementary mechanics and classical applied mathematics to formulate explicit analytical solutions and ideal model

behaviour in a scientific context previously only elucidated through experiments and molecular dynamics studies.

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