

## Mechanics of fullerenes oscillating in carbon nanotube bundles

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2007 J. Phys. A: Math. Theor. 40 13197

(<http://iopscience.iop.org/1751-8121/40/44/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.146

The article was downloaded on 03/06/2010 at 06:23

Please note that [terms and conditions apply](#).

# Mechanics of fullerenes oscillating in carbon nanotube bundles

Barry J Cox, Ngamta Thamwattana and James M Hill

Nanomechanics Group, School of Mathematics and Applied Statistics, University of Wollongong, Wollongong, NSW 2522, Australia

E-mail: [barryc@uow.edu.au](mailto:barryc@uow.edu.au)

Received 1 August 2007, in final form 28 September 2007

Published 16 October 2007

Online at [stacks.iop.org/JPhysA/40/13197](http://stacks.iop.org/JPhysA/40/13197)

## Abstract

In this paper, we examine the mechanics of a nano-scaled gigahertz oscillator comprising a fullerene that is moving within the center of a bundle of carbon nanotubes. Although numerical results specifically for a  $C_{60}$  fullerene are presented, the method is equally valid for any fullerene which can be modeled as a spherical molecule. A general definition of a nanotube bundle is employed which can comprise any number of parallel carbon nanotubes encircling the oscillating fullerene. Results are presented which prescribe the dimension of the bundle for any nanotube radius and the optimal configurations which give rise to the maximum suction energy for the fullerene. Prior results for fullerene single-walled nanotube oscillators are employed, and new results are also derived. These include a calculation of optimum nanotube bundle size to be employed for a  $C_{60}$ -nanotube bundle oscillator, as well as new analytical expressions for the force and energy for a semi-infinite nanotube and a fullerene not located on the axis of the cylinder.

PACS numbers: 46.70.-p, 61.46.-w

## 1. Introduction

Research into carbon nanostructures has progressed at a rapid rate since the discovery of the  $C_{60}$  fullerene in the 1980s. Fullerenes and related carbon nanotube structures have been investigated for many applications due to their outstanding mechanical properties such as high strength and low weight, as well as their electrical properties which can be selected based on the particular nanotube structure. However, the theoretical understanding of their structures, their properties and the mechanisms which lead to their material characteristics require a more complete understanding, as well as more reliable models to predict their behavior when these structures interact with other carbon nanotubes and their environment.

We use the term ‘nano-oscillator’ to describe a device comprising an oscillating body moving backward and forward in or around a nanostructure. Such a device generates motion from the van der Waals force acting between the oscillating body and the interacting structure. Cumings and Zettl [1] observe that the sliding resistance force in multi-walled carbon nanotubes is very low and propose that this can be exploited in nano-electromechanical systems. Furthermore, they observe that an extracted inner shell of a multi-walled carbon nanotube will quickly and completely retract into the nanotube due to the excess van der Waals interaction energy. This phenomenon gives rise to the possibility of using a multi-walled carbon nanotube as a nano-oscillator. The scale of the system relative to the magnitude of the restoring force, combined with the low-friction environment, means that the frequency of such oscillators can reach the gigahertz range, which presents new opportunities for devices such as resonators, nano-antennae and high-speed filters. Zheng and Jiang [2] investigate a multi-walled carbon nanotube oscillator, where one nanotube oscillates within another, and they note that the shorter the inner tube, the higher the frequency of oscillation. This motivates the use of a  $C_{60}$  fullerene as the oscillating core as this represents the ultimate limit of the shortest possible carbon nanostructure, and Liu *et al* [3] use a similar approach for a  $C_{60}$  fullerene oscillating inside a carbon nanotube.

Classical applied mathematical studies have also been undertaken, especially those of Baowan and Hill [4] and Baowan *et al* [5], who study double-walled carbon nanotube oscillators, and Hilder and Hill [6, 7] who study carbon nanotori oscillators and orbiters. The prior work of the authors [8–10] investigate the mechanics of nano-oscillators comprising a fullerene molecule oscillating inside a single-walled carbon nanotube which has open ends. There the notions of acceptance condition and suction energy for these systems are formulated which can be used to calculate the oscillatory frequency of such systems and good agreement is obtained with molecular dynamics simulations but with a much greatly reduced computational effort.

A novel development in this area has been the proposal to use a carbon nanotube bundle as the structure within which a body may oscillate. Kang *et al* [11] investigate such a system comprising a single-walled carbon nanotube oscillating in a nanotube bundle. In a recent paper, the authors [12] also investigate a nano-oscillator system comprising a single-walled carbon nanotube moving in the vacancy in a bundle of single-walled carbon nanotubes, and produce results which are in reasonable agreement with the molecular dynamics study. In this paper, we extend this idea to nano-oscillators comprising a spherical fullerene  $C_{60}$  oscillating inside the vacancy in a carbon nanotube bundle. Current studies concentrate on extracting a single or a number of nanotubes from a bundle comprising a triangular lattice of similar nanotubes. Here we propose a more general definition of a bundle which applies to the triangle lattice but it may also find future applicability to devices specifically constructed with a particular geometry which is designed to maximize the oscillatory frequency subject to some set of constraints.

In the following section, we outline the geometry of the nanotube bundle, the Lennard–Jones potential function and we combine these two to give the bundle energy which is used to determine equilibrium configurations of nanotube bundles. In section 3, the energy between a spherical fullerene and a doubly infinite nanotube is employed to calculate optimum configurations of  $C_{60}$ -nanotube bundle oscillators and the suction energies  $W$  is calculated for these optimal oscillators. Following this, in section 4, we use new expressions which are derived in appendices A and B to detail the nature of the suction of a  $C_{60}$  fullerene into the open end of a nanotube bundle, in terms of the force and energy profile, and after confirming that impulse-like forces are in operation at the bundle extremities, we go on to calculate

**Table 1.** Constants used in this model.

LJ attraction (graphene–graphene)	$A$	15.2	$\text{eV } \text{\AA}^6$
LJ repulsion (graphene–graphene)	$B$	$24.1 \times 10^3$	$\text{eV } \text{\AA}^{12}$
LJ attraction (graphene– $\text{C}_{60}$ )	$A$	17.4	$\text{eV } \text{\AA}^6$
LJ repulsion (graphene– $\text{C}_{60}$ )	$B$	$29 \times 10^3$	$\text{eV } \text{\AA}^{12}$
Atomic surface density (graphene)	$\eta_t$	0.3812	$\text{atom } \text{\AA}^{-2}$
Atomic surface density ( $\text{C}_{60}$ )	$\eta_f$	0.3789	$\text{atom } \text{\AA}^{-2}$
Radius of $\text{C}_{60}$ fullerene	$r_0$	3.55	$\text{\AA}$
Mass of $\text{C}_{60}$ fullerene	$m_f$	$1.196 \times 10^{-24}$	kg

the oscillatory frequency for the optimal configurations. Finally, in section 5 we provide a discussion and some conclusions.

## 2. Lennard–Jones potential for a nanotube bundle

### 2.1. Nanotube bundle geometry

In this paper, we adopt the same definition for a nanotube bundle as that used in the prior work [12] on a nanotube oscillating in a nanotube bundle. That is, a nanotube bundle is assumed to comprise an integral number  $N$  of carbon nanotubes aligned parallel to and equidistant from a common axis, which we term the bundle axis. The perpendicular distance from the bundle axis to the axis of each constituent nanotube is termed the bundle radius  $R$ . Furthermore, we assume 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 by two adjacent nanotubes is  $2\pi/N$ . We take the bundle axis to be collinear with the  $z$ -axis and therefore the  $i$ th tube in the nanotube bundle has a surface in rectangular Cartesian coordinates  $(x, y, z)$  which is given by

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

where  $i \in \{1, \dots, N\}$ ,  $0 \leq \theta_i \leq 2\pi$  and  $-L \leq z_i \leq L$ . However, it is convenient for some of the analysis in the present paper to assume a semi-infinite tube, with  $0 \leq z_i < \infty$ , or a completely infinite tube, with  $-\infty < z_i < \infty$ . The numerical values of the various constants used in this model are shown in table 1, where the Lennard–Jones constants are taken from Girifalco *et al* [13] and the surface densities are calculated from uniformly distributing the known number of atoms across the idealized surface.

### 2.2. Lennard–Jones potential

To calculate the van der Waals interaction energy we employ the six-twelve Lennard–Jones potential which gives the potential energy as a function of the form

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

where  $\rho$  is the distance between atoms and  $A$  and  $B$  are the Lennard–Jones attractive and repulsive constants, respectively. One method to calculate the total interaction energy between two molecules is to perform a discrete summation of all the pair-wise interactions for all atoms making up both molecules. However, the approach adopted here is to model the interaction using a continuum approximation together with the mean atomic surface densities,  $\eta_1$  and  $\eta_2$ ,

used to scale the interaction energy, which is then modeled by surface integrals over the two interacting molecules. Thus, the total energy  $E$  is given by

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

where  $S_1$  and  $S_2$  denote the surfaces of the two interacting molecules and  $\rho$  denotes the distance between typical surface elements on each surface.

The continuum approach has been employed for many different molecules and configurations, particularly in the work of Girifalco [14], Henrard *et al* [15] and Girifalco *et al* [13]. The present authors also employ this approach to study various fullerenes oscillating in a single-walled carbon nanotube [8–10] and a single-walled carbon nanotube oscillating in a nanotube bundle [12].

### 2.3. Nanotube bundle energy

As derived in [12], the potential energy per unit length for two identical, parallel carbon nanotubes of radius  $r$  and with axes separated by a distance  $\delta$  is given by

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

where the constants  $A$  and  $B$  are those from table 1 for graphene–graphene systems,  $\alpha^2 = \delta(\delta - 2r)$  and  $F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y)$  is an Appell hypergeometric function of two variables as described by Erdélyi *et al* ([16], section 5.7).

Following [12] to calculate the total bundle energy  $E_B$  we sum the individual interactions of each tube in the bundle with every other tube. This leads to the following expression

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

where  $E_{tt}(\delta)$  is given by (2), and (3) gives the tube–tube energy for two nanotubes of radius  $r$  at a distance  $\delta$ . A graph of the bundle energy  $E_B$  versus radius  $R$  is shown in figure 1 for carbon nanotubes of various radii.

In the design of a carbon nanotube bundle, the key question is that of determining the minimum energy configuration. This issue arises when considering the bundle radius that a collection of nanotubes adopt if free to move, or in the case of when the nanotubes are not free to move, the amount of strain in a nanostructure caused by the van der Waals interactions. In this paper, we assume that the bundle adopts its minimum energy position, and therefore the bundle radius  $R$  is determined from the number of nanotubes in the bundle  $N$  and the radii of the constituent nanotubes  $r$ . In figure 2, we show the relationship between the bundle radius  $R$  and the tube radius  $r$  leading to a minimized bundle energy for various values of  $N$ .

### 3. Interaction of spherical fullerene with nanotube bundle

Here we calculate the interaction potential between a fullerene of radius  $r_0$  located at a position  $(\epsilon \cos \phi, \epsilon \sin \phi, 0)$  relative to the center of a nanotube bundle, as illustrated in figure 3. To calculate the suction energy  $W$  as defined by [8, 9] we assume for the moment that the

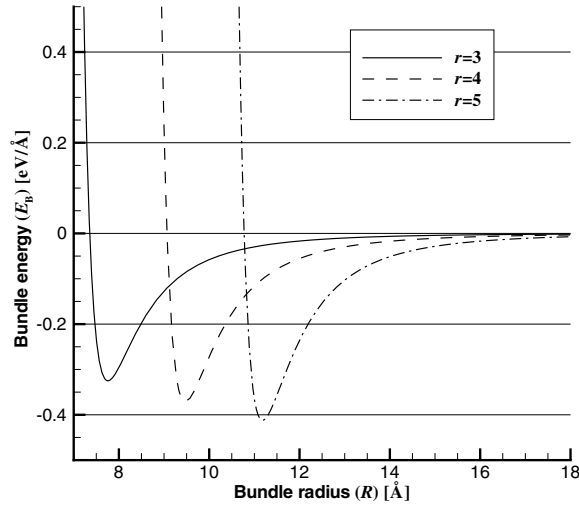


Figure 1. Bundle energy versus radius for three different radii of carbon nanotubes, with  $N = 5$ .

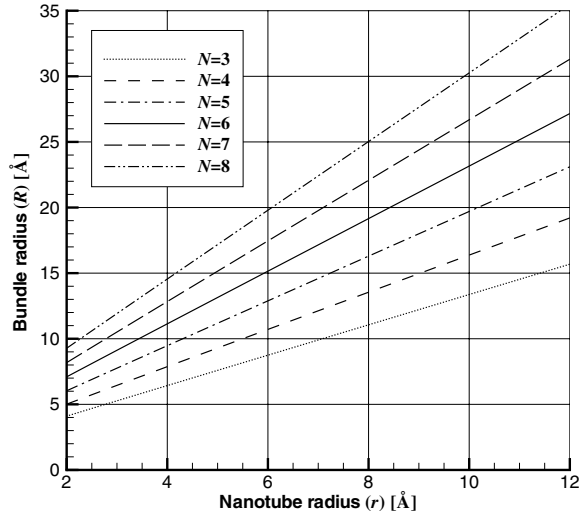
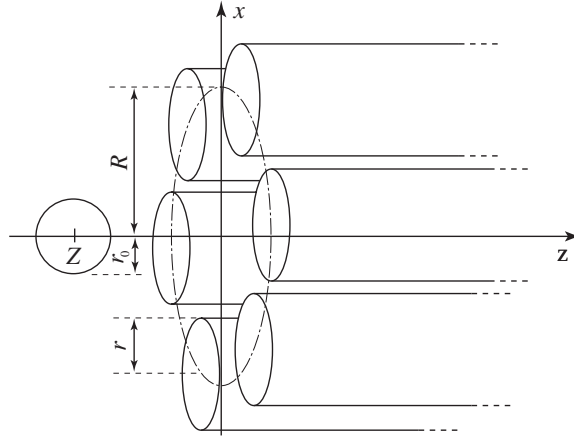


Figure 2. Bundle radius versus nanotube radius for bundles with  $N \in \{3, 4, \dots, 8\}$ .

nanotubes are infinite in length. The distance from the center of the fullerene to the axis of the  $k$ th tube in the bundle  $d_k$  is given by

$$\begin{aligned} d_k^2 &= \left( R \cos\left(\frac{2k\pi}{N}\right) - \epsilon \cos\phi \right)^2 + \left( R \sin\left(\frac{2k\pi}{N}\right) - \epsilon \sin\phi \right)^2 \\ &= (R - \epsilon)^2 + 4R\epsilon \sin^2\left(\frac{k\pi}{N} - \frac{\phi}{2}\right), \end{aligned}$$

and we require that  $d_k > r_0 + r$ , for all  $k \in \{1, 2, 3, \dots, N\}$ .



**Figure 3.** C<sub>60</sub> near the open end of a nanotube bundle.

We denote the interaction energy between the fullerene and a single tube which is a distance  $d_k$  away by  $E_{ft}(d_k)$  so that the total suction energy of the fullerene  $W$  is given by

$$W = - \sum_{k=1}^N E_{ft} \left( \left[ (R - \epsilon)^2 + 4R\epsilon \sin^2 \left( \frac{k\pi}{N} - \frac{\phi}{2} \right) \right]^{1/2} \right).$$

For infinite nanotubes, an expression for the function  $E_{ft}$  already appears in Cox *et al* [9] as<sup>1</sup> given by

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

where the constants  $A$  and  $B$  are those from table 1 for graphene-C<sub>60</sub> systems and the integrals  $J_n$  are defined by

$$J_n = \int_{-\pi}^{\pi} \frac{d\theta}{(r^2 + d_k^2 - r_0^2 - 2rd_k \cos \theta)^{n+1/2}},$$

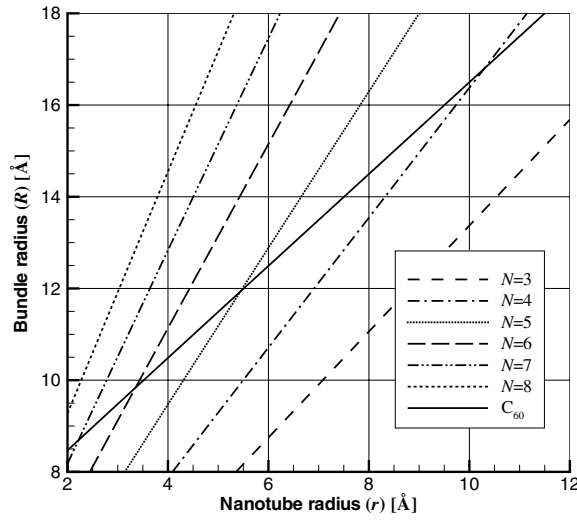
which can be expressed analytically in terms of hypergeometric functions as

$$J_n = \frac{2\pi}{[(r - d_k)^2 - r_0^2]^{n+1/2}} F \left( \frac{1}{2}, n + \frac{1}{2}; 1; -\frac{4rd_k}{(r - d_k)^2 - r_0^2} \right), \quad (5)$$

where  $F(a, b; c; z)$  is the usual hypergeometric function. The reader is referred to ([9], appendix A) for the full details of the derivations of equations (4) and (5).

Assuming that the equilibrium position for the C<sub>60</sub> fullerene is located at the center of the nanotube bundle, the total energy  $W$  can be simplified to  $W = -NE_{ft}(R)$ , and the minimum for any value of  $N$  is given by the minimum of the  $E_{ft}$  function, which is the equilibrium position for the fullerene on the outside of a single tube. By calling this distance, the bundle radius  $R$  which optimizes the suction energy for a particular tube radius  $r$ , we can thereby determine a relationship between these two radii which would lead to an optimized oscillator

<sup>1</sup> The fraction 315/256 was incorrectly reported as 105/128 in [9].



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

**Table 2.** Parameters for optimized  $C_{60}$  fullerene/nanotube bundle oscillators.

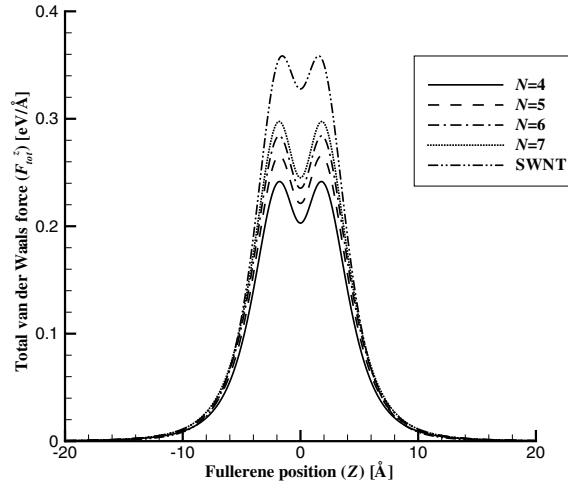
Number $N$	Tube radius $r$ (Å)	Bundle radius $R$ (Å)	Suction energy $W$ (eV)
4	10.294	16.792	2.314
5	5.439	11.930	2.551
6	3.355	9.838	2.731
7	2.219	8.692	2.850

for any value of  $N$ . In figure 4, we graph the relationship between the nanotube radius  $r$  and the bundle radius  $R$  which optimizes the suction energy for the  $C_{60}$  fullerene. On the same figure, we also show the nanotube radii versus bundle radii data from figure 2. The points where the lines intersect prescribe the specific values of  $r$  and  $R$  which lead to optimized oscillators for specific values of  $N$ . As can be seen from the figure, limiting the tube radius  $r$  to the range 2–12 Å means that oscillators can only be constructed for  $N \in \{4, 5, 6, 7\}$ . More precise parameters for these ideal oscillators are given in table 2, including the suction energy for each configuration. We note that the suction energy  $W$  increases with the number of tubes  $N$  forming the bundle, so that one way to optimize a bundle oscillator is to design the bundle to have as many tubes as is practical. However, we also observe that the maximum value of suction energy  $W = 2.85$  eV is still less than the maximum suction energy that may be obtained for a single-walled carbon nanotube–fullerene oscillator, since Cox *et al* [8] find the maximum value to be  $W_{\max} = 3.242$  eV.

#### 4. Suction of a fullerene into a nanotube bundle

In this section, we use the expressions given in appendix A for the van der Waals force between a fullerene and semi-infinite tube to describe the suction of a  $C_{60}$  fullerene into a nanotube

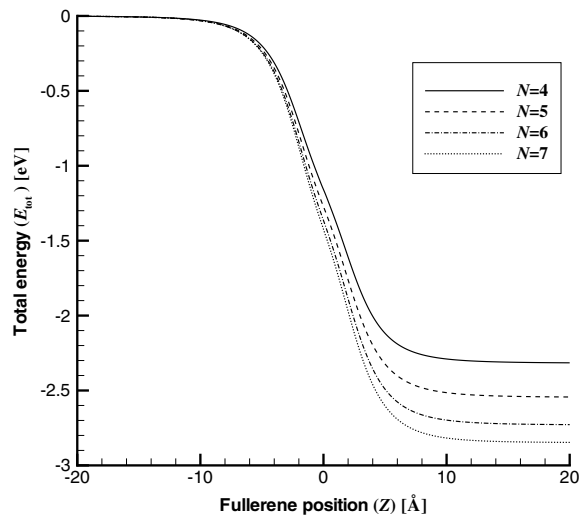




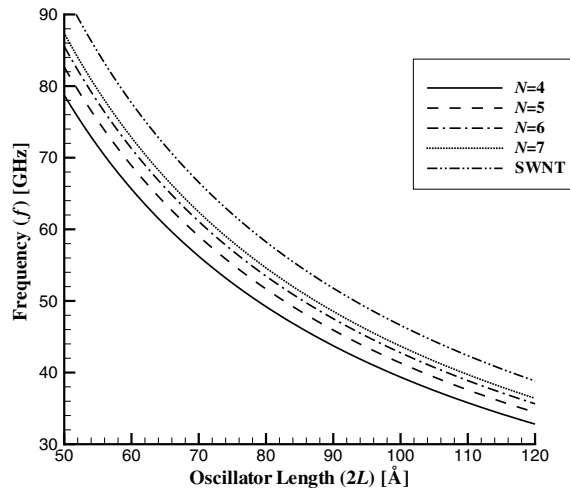
**Figure 5.** Total van der Waals force for a fullerene entering a nanotube bundle for various configurations of ideal oscillators.

bundle end. Due to the short range nature of the van der Waals interaction, when the fullerene is more than 1 nm from the bundle end, either inside or outside of the bundle, then for all practical purposes the force is negligible. Using this observation, we can use the expressions given in appendix A to characterize the force at both ends of a finite tube, provided that the tube half-length  $L$  is greater than 1 nm. For the optimized bundles given in the previous section, the equilibrium position for the fullerene is on the bundle axis and therefore the total van der Waals force is given by  $F_{\text{tot}}^z = N F_{\text{vdW}}^z$  where the latter is given by equations (A.1) and (A.2). In figure 5, we show the force profiles for the four optimal oscillator configurations given in the previous section and, for comparison, the profile for a  $C_{60}$  single-walled nanotube from Cox *et al* [8] with a nanotube radius of 6.783 Å. We note that the force is always positive and therefore the  $C_{60}$  fullerene is sucked into the bundle. We also note that as also found in [8] the force is essentially an impulse acting at the end of the nanotube only and therefore provided the bundle length is sufficiently large, the van der Waals force can be modeled as a Dirac delta function. However, it can be seen from this figure that the force for bundle oscillators is substantially less than that generated by the optimal single-walled carbon nanotube oscillator. The reason that the single-walled nanotube generates substantially more force is that for this configuration the curvature of the nanotube wall matches the curvature of the oscillating fullerene and therefore a greater van der Waals interaction can be generated in the optimum region at the base of the potential well. Another interesting feature in figure 5 is the local minimum which occurs when the fullerene is positioned at the nanotube opening,  $Z = 0$ . The reason for this is that the wall of the fullerene which is closest to the nanotube, is closer than the van der Waals equilibrium distance, and therefore causes a small reduction in the force just as the fullerene crosses into the nanotube bundle. We comment that the same feature is present in the case of the optimal single-walled nanotube oscillator. Likewise, the total interaction energy  $E_{\text{tot}} = N E$  where  $E$  is given by equations (B.1) and (B.2). In figure 6, we plot this force and observe that the energy profile is similar to that found in [8].

Given the similarities between the force and energy profiles that we find here and those in [8, 9], we adopt exactly the same model and we use the equation for frequency of  $f = (2W/m_f)^{1/2}/4L$ , where  $m_f$  is the mass of the fullerene. In figure 7, we plot the



**Figure 6.** Total interaction energy for a fullerene entering a nanotube bundle for various configurations of ideal oscillators.



**Figure 7.** Frequency for a fullerene nanotube bundle oscillator for various configurations of ideal oscillators varying the bundle length ( $2L$ ).

oscillation frequency for the various ideal oscillators, varying the bundle length  $2L$ . As anticipated by the suction energy results in table 2, the configuration with  $N = 7$  provides the highest frequency. However, as anticipated by the results for the force, the single-walled nanotube oscillator provides a higher frequency, for the same oscillator length, than all the bundle geometries studied here.

## 5. Conclusions

In this paper, we consider nano-oscillators comprising a spherical fullerene oscillating in a nanotube bundle. The Lennard–Jones potential is used to calculate the interaction energy

between the nanotubes forming the bundle and this is employed to determine the optimum bundle size for various oscillators comprising an oscillating spherical  $C_{60}$  fullerenes. This latter result is used to predict the oscillator bundle configuration which optimizes the suction energy and therefore leads to a maximum oscillation frequency. New analytical results are derived for the interaction force and energy between a spherical fullerene and a semi-infinite carbon nanotube for the case when the fullerene is located at an arbitrary offset distance from the nanotube axis. The van der Waals interaction force is a simple rational function while the energy is given in terms of a finite sum of Appell hypergeometric functions of the first kind. These relationships are employed to confirm that the nature of the suction into the carbon nanotube is similar to that already described for the  $C_{60}$ -nanotube oscillator and the frequency for bundle oscillators is calculated using the same model for the motion with the van der Waals forces operating at the ends of the bundle being modeled as Dirac delta functions.

The primary contribution of this work is that it provides a general framework which enables optimum dimensions for nano-oscillators to be determined from classical geometrical and mechanical principles. While the model is an idealization, it provides guidance in the design by indicating fundamental relationships between the bundle geometry and the nanotube radius, which optimizes the van der Waals suction energy and therefore the oscillation frequency. Although temperature effects, friction and energy losses in other modes of vibration will qualitatively affect the performance of bundle oscillators, such effects will be comparable between oscillators and therefore the qualitative predictions made from figure 4 will still be valid. The other important finding from this work is that from the perspective of purely maximizing the suction energy, the optimal single-walled nanotube oscillator performs better than that of the optimal bundle configurations, leading to a higher frequency as shown in figures 5 and 7.

### Acknowledgments

The authors are grateful to the Australian Research Council for their support through the Discovery Project Scheme and the provision of an Australian Postdoctoral Fellowship for NT and an Australian Professorial Fellowship for JMH. The authors also wish to acknowledge Professor Quanshui Zheng of Tsinghua University for motivating this work and for his many helpful comments and discussions.

### Appendix A. Van der Waals force for an offset fullerene

In Cox *et al* [9], the total energy for an offset fullerene and a doubly infinite nanotube was calculated. Here we take this analysis further to calculate the  $z$  component of the van der Waals force  $F_{\text{vdW}}^z$  for an offset fullerene and a semi-infinite nanotube. This is then extended in the following appendix to calculate the energy for the fullerene.

We begin with a sphere centered at  $(0, 0, Z)$  and radius  $r_0$  interacting with a cylinder with an axis parallel to the  $z$  axis and a perpendicular distance  $R$  from the  $z$  axis. The surface of the cylinder is given by (1) with  $i = 1$ , and  $0 \leq \theta_1 \leq 2\pi$  and  $0 \leq z_i < \infty$ . From ([9], equations (2.12) and (2.13)) and using  $F_{\text{vdW}}^z = -\partial E / \partial z$  gives

$$F_{\text{vdW}}^z(Z) = 4\pi r r_0^2 \eta_i \eta_i [A(J_3 + 2r_0^2 J_4) - (B/5)(5J_6 + 80r_0^2 J_7 + 336r_0^4 J_8 + 512r_0^6 J_9 + 256r_0^8 J_{10})], \quad (\text{A.1})$$

where the  $J_n$  are defined by the integral

$$J_n = \int_{-\pi}^{\pi} [(R - r)^2 - r_0^2 + Z^2 + 4rR \sin^2(\theta_1/2)]^{-n} d\theta_1.$$

By employing the substitution  $t = \sin^2(\theta_1/2)$  and, for algebraic convenience, the substitution  $\mu = (R - r)^2 - r_0^2 + Z^2$ , gives

$$J_n = 2\mu^{-n} \int_0^1 t^{-1/2}(1-t)^{-1/2}[1 + (4rR/\mu)t]^{-n} dt,$$

which is in fundamental integral form of the usual hypergeometric function, and therefore

$$J_n = 2\pi\mu^{-n} F(n, 1/2; 1; -4rR/\mu),$$

where  $F(a, b; c; z)$  is the usual hypergeometric function. By employing Erdélyi *et al* ([16, section 2.9, equation (18)]) we may transform this function into a degenerate series thus

$$J_n = 2\pi\mu^{-1/2}(\mu + 4rR)^{1/2-n} F(1-n, 1/2; 1; -4rR/\mu),$$

which can be written as the finite sum

$$J_n = 2\pi(\mu + 4rR)^{1/2-n} \sum_{m=0}^{n-1} \frac{(1-n)_m (1/2)_m}{(m!)^2} (-4rR)^m \mu^{-1/2-m}. \quad (\text{A.2})$$

So equation (A.1) combined with the solution for  $J_n$  (A.2) constitute an analytical solution to the problem of determining the  $z$ -component of the van der Waals force  $F_{\text{vdW}}^z$  for an offset fullerene and a semi-infinite carbon nanotube.

## Appendix B. Interaction energy for an offset fullerene

In the previous appendix, the van der Waals force for an offset fullerene is given. To calculate the total interaction energy we require to integrate this force from  $-\infty$  to  $Z$  such that  $E = -\int_{-\infty}^Z F_{\text{vdW}}^z(z) dz$ . Since the force  $F_{\text{vdW}}^z$  is an even function of  $z$ , we can say that for  $Z \leq 0$ ,  $E = -\int_{-Z}^{\infty} F_{\text{vdW}}^z(z) dz$  and for positive  $Z > 0$ ,  $E = 2E(0) - E(-Z)$ . Therefore from equations (A.1) and (A.2), we need to evaluate the following integral

$$K_{n,m} = \int_{-Z}^{\infty} (v + z^2)^{-1/2-m} (v + 4rR + z^2)^{1/2-n} dz,$$

where  $v = (R - r)^2 - r_0^2$  is substituted for algebraic convenience. We now employ the substitution  $u = (v + Z^2)/(v + z^2)$  which after some routine algebra gives

$$K_{n,m} = \frac{(v + Z^2)^{1/2-n-m}}{2} \int_0^1 u^{n+m-3/2} [1 + u4rR/(v + Z^2)]^{1/2-n} \\ \times [1 - uv/(v + Z^2)]^{-1/2} du,$$

which is in fundamental integral form of Euler's type for the Appell hypergeometric function of two variables and gives

$$K_{n,m} = \frac{(v + Z^2)^{1/2-n-m}}{2n + 2m - 1} F_1\left(n + m - \frac{1}{2}; n - \frac{1}{2}, \frac{1}{2}; n + m + \frac{1}{2}; -4rR/(v + Z^2), v/(v + Z^2)\right),$$

where  $F_1(\alpha; \beta; \beta'; \gamma; x, y)$  is an Appell hypergeometric function as defined in Erdélyi *et al* [16].

This then allows us to give an analytic expression for the energy for the offset fullerene as

$$E(Z) = 8\pi^2 r r_0^2 \eta_i \eta_f \left[ -A(L_3 + 2r_0^2 L_4) \right. \\ \left. + (B/5)(5L_6 + 80r_0^2 L_7 + 336r_0^4 L_8 + 512r_0^6 L_9 + 256r_0^8 L_{10}) \right], \quad (\text{B.1})$$

where

$$L_n = \sum_{m=0}^{n-1} \frac{(1-n)_m (1/2)_m}{(m!)^2} (-4rR)^m \frac{(v+Z^2)^{1/2-n-m}}{2n+2m-1} \times F_1\left(n+m-\frac{1}{2}; n-\frac{1}{2}, \frac{1}{2}; n+m+\frac{1}{2}; -4rR/(v+Z^2), v/(v+Z^2)\right). \quad (\text{B.2})$$

We comment that this is a fully analytical solution to the problem which has not previously appeared in the literature.

## References

- [1] Cumings J and Zettl A 2000 Low-friction nanoscale linear bearing realized from multiwalled carbon nanotubes *Science* **289** 602–4
- [2] Zheng Q and Jiang Q 2002 Multiwalled carbon nanotubes as gigahertz oscillators *Phys. Rev. Lett.* **88** 045503
- [3] Liu P, Zhang Y W and Lu C 2005 Oscillatory behavior of C60-nanotube oscillators: a molecular-dynamics study *J. Appl. Phys.* **97** 094313
- [4] Baowan D and Hill J M 2007 Force distribution for double-walled carbon nanotubes and gigahertz oscillators *Z. Angew. Math. Phys.* at press (doi:101007/s00033-006-6098-z)
- [5] Baowan D, Thamwattana N and Hill J M 2007 Suction energy and offset configuration for double-walled carbon nanotubes *Commun. Nonlinear Sci. Numer. Simulat.* at press (doi:101016/j.cnsns200701002)
- [6] Hilder T A and Hill J M 2007 Orbiting atoms and C<sub>60</sub> fullerenes inside carbon nanotori *J. Appl. Phys.* **101** 064319
- [7] Hilder T A and Hill J M 2007 Oscillating carbon nanotori along carbon nanotubes *Phys. Rev. B* **75** 125415
- [8] Cox B J, Thamwattana N and Hill J M 2007 Mechanics of atoms and fullerenes in single-walled carbon nanotubes: I. Acceptance and suction energies *Proc. R. Soc. A* **463** 461–76
- [9] Cox B J, Thamwattana N and Hill J M 2007 Mechanics of atoms and fullerenes in single-walled carbon nanotubes: II. Oscillatory behaviour *Proc. R. Soc. A* **463** 477–94
- [10] Cox B J, Thamwattana N and Hill J M 2007 Mechanics of spheroidal fullerenes and carbon nanotubes for drug and gene delivery *Q. J. Mech. Appl. Math.* **60** 231–53
- [11] Kang J W, Song K O, Hwang H J and Jiang Q 2006 Nanotube oscillator based on a short single-walled carbon nanotube bundle *Nanotechnology* **17** 2250–8
- [12] Cox B J, Thamwattana N and Hill J M 2007 Mechanics of nanotubes oscillating in carbon nanotube bundles *Proc. R. Soc. A* submitted
- [13] Girifalco L A, Hodak M and Lee R S 2000 Carbon nanotubes, buckyballs, ropes, and a universal graphitic potential *Phys. Rev. B* **62** 13104–13110
- [14] Girifalco L A 1992 Molecular properties of C<sub>60</sub> in the gas and solid phases *J. Phys. Chem.* **96** 858–61
- [15] Henrard L, Hernández E, Bernier P and Rubio A 1999 Van der Waals interaction in nanotube bundles: consequences on vibrational modes *Phys. Rev. B* **60** R8521–R8524
- [16] Erdélyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol I (New York: McGraw-Hill)