

2008

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Chan, Y.; Cox, G. M.; and Hill, James M.: A carbon atom orbiting around the outside of a carbon nanotube 2008.

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Abstract

In this paper, we examine a carbon atom orbiting around the outside of a (6,6) carbon nanotube, where the orbiting phenomena is assumed to arise only from the van der Waals interactions between the carbon atom and the atoms on the surface of the carbon nanotube. We model the van der Waals forces utilizing the Lennard-Jones potential and assume that the carbon atoms are uniformly distributed over the surface of the carbon nanotube, so that a discrete sum of the atomic potential energy between the carbon atom and the molecule can be approximated by a line integral. The circular orbiting frequency of the system can be estimated by investigating the minimum energy configuration of the effective potential energy. An instability calculation is performed to ensure that the circular orbit remains stable, and the classification of the atom's possible loci is determined numerically. We find that the circular orbiting frequency of the proposed system reaches the gigahertz regime, which suggests that such a system has potential to be utilized as an ideal device in future technological development. We also briefly show that the results obtained from the above system can be extended to a fullerene orbiting around the outside of a carbon nanotube without conceptual difficulties, but with increased mathematical complexity.

Keywords

Carbon atom; carbon nanotube; van der Waals; Lennard-Jones potential; nano-orbiting system; gigahertz

Disciplines

Physical Sciences and Mathematics

Publication Details

This conference paper was originally published as Chan, Y, Cox, GM & Hill, JM, A Carbon Atom Orbiting Around the Outside of a Carbon Nanotube, International Conference on Nanoscience and Nanotechnology, ICONN 2008, Melbourne, 25-29 February 2008, 152-155. Copyright Institute of Electrical and Electronics Engineers 2008. Original conference paper available [here](#)

A carbon atom orbiting around the outside of a carbon nanotube

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Abstract—In this paper, we examine a carbon atom orbiting around the outside of a (6,6) carbon nanotube, where the orbiting phenomena is assumed to arise only from the van der Waals interactions between the carbon atom and the atoms on the surface of the carbon nanotube. We model the van der Waals forces utilizing the Lennard-Jones potential and assume that the carbon atoms are uniformly distributed over the surface of the carbon nanotube, so that a discrete sum of the atomic potential energy between the carbon atom and the molecule can be approximated by a line integral. The circular orbiting frequency of the system can be estimated by investigating the minimum energy configuration of the effective potential energy. An instability calculation is performed to ensure that the circular orbit remains stable, and the classification of the atom's possible loci is determined numerically. We find that the circular orbiting frequency of the proposed system reaches the gigahertz regime, which suggests that such a system has potential to be utilized as an ideal device in future technological development. We also briefly show that the results obtained from the above system can be extended to a fullerene orbiting around the outside of a carbon nanotube without conceptual difficulties, but with increased mathematical complexity.

Keywords—Carbon atom; carbon nanotube; van der Waals; Lennard-Jones potential; nano-orbiting system; gigahertz

I. INTRODUCTION

Carbon nanotubes and fullerenes have had a tremendous impact on the development of nanodevices, due to their small size and unique mechanical and chemical properties. Previously, as has been proposed by Cumings & Zettl [1] and Zheng & Jiang [2], carbon nanotubes and fullerenes have been utilized to create gigahertz oscillators, where a C_{60} oscillates spontaneously inside the nanotube. This behavior has been confirmed by Qian [3, 4], and Liu [5] utilizing molecular dynamical simulations. Here, in this paper, we investigate a related dynamical system that has potential to produce an orbiting motion with a gigahertz frequency. In particular, we examine a carbon atom orbiting around the outside of a (6,6) carbon nanotube, where the circular orbiting frequency is found to be in the gigahertz range, which is comparable to the oscillating frequencies of gigahertz oscillators. The van der Waals force is modeled by the Lennard-Jones potential, which is assumed to be the only interaction between the carbon atom and the atoms of the molecule. We note that this approach has

been successfully adopted by Cox et al. [6] to investigate the potential profile of a fullerene oscillating spontaneously inside a carbon nanotube.

The orbiting carbon atom and the molecule move relative to each other under the influence of their mutual central force arising from the Lennard-Jones potential. However, we have been unable to analytically integrate the atom's loci in terms of any well-known special functions. Therefore, we employ Euler's numerical method to determine the atom's loci. Finally, the atom's circular radius is estimated by seeking the minimum energy configuration of the effective potential energy. For such a system, we find that the circular orbiting frequency reaches the gigahertz range, which suggests the possibility of utilizing such a system in nano-scale devices. All results obtained in this paper are based on the assumption that there are no thermal fluctuations arising from the environment. Since the binding energy of the proposed orbiting system is very small, any thermal fluctuations would tend to raise the total energy of the carbon atom, and no orbiting phenomenon would be observed.

II. EQUATIONS OF MOTION

In this section, the equations of motion of a two body problem are presented. For a system of two objects that are connected by a potential energy $V(r)$, where the potential energy only depends upon the distance between their centers of mass r , the total energy E can be written as [7]

$$E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + V(r) = \frac{1}{2}m\dot{r}^2 + V_{eff}(r), \quad (1)$$

where m , θ and $V_{eff}(r) = \frac{h^2}{2mr^2} + V(r)$ denote the reduced mass of the system, the polar angle and the effective potential energy of the system, which comprises of both the angular kinetic energy and the molecular potential energy. Hence, the value of the circular orbiting radius R can be computed by minimizing $V_{eff}(r)$ with respect to r . In addition, assuming no external torque is acting on the system, then the conservation of angular momentum of the system h is given by

$$h = mr^2\dot{\theta}. \quad (2)$$

Readers are advised that equations (1) and (2) are extensively utilized in later sections.

III. A CARBON ATOM ORBITING OUTSIDE A CARBON NANOTUBE

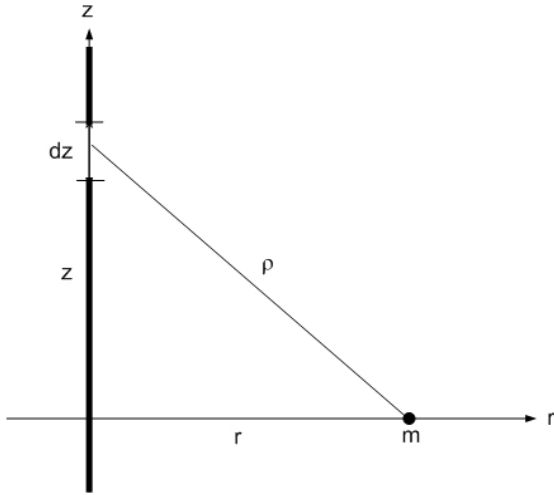


Fig.1 A carbon atom orbiting around the outside of a (6,6) carbon nanotube

In this section, we examine a single carbon atom orbiting around the outside of a (6,6) carbon nanotube under the influence of the van der Waals force, where the carbon nanotube is approximated by a thin infinite line. In particular, the van der Waals potential is modeled by the Lennard-Jones potential

$$V(\rho) = \frac{-A}{\rho^6} + \frac{B}{\rho^{12}}, \quad (3)$$

where ρ , A and B denote the distance between any two atoms, the attractive constant and the repulsive constant respectively. A schematics of the orbiting system and its relevant symbols are shown in Fig. 1. By symmetry, the atom will eventually move to the center of the carbon nanotube and start orbiting around the outside of the nanotube in a plane perpendicular to the nanotube. The total molecular potential energy of this system can be calculated by the line integral

$$V(r) = n_g \int_{-\infty}^{\infty} \left(\frac{-A}{\rho^6} + \frac{B}{\rho^{12}} \right) dz, \quad (4)$$

where $r=r(\rho)$ and n_g denote the distance between the nanotube's center of mass and the carbon atom and the mean surface density of the (6,6) carbon nanotube respectively. The value of these constants, and other relevant data, are given in Table I. Upon performing the integration, the total molecular potential energy of this system becomes

$$V(r) = -\frac{A'}{r^5} + \frac{B'}{r^{11}}, \quad (5)$$

where $A' = 3\pi n_g A/8$ and $B' = 63\pi n_g B/256$ denote the modified attractive and repulsive constants. According to equation (1), the effective energy of such a system is now given by

Radius of a (6,6) carbon nanotube	$c = 4.07 \text{ \AA}$
Radius of C_{60}	$b = 3.55 \text{ \AA}$
Mean surface density of a (6,6) carbon nanotube	$n_g = 0.38 \text{ \AA}^{-2}$
Mean surface density of C_{60}	$n_f = 0.38 \text{ \AA}^{-2}$
Mass of a single carbon atom	$m_a = 1.99 \times 10^{-26} \text{ kg}$
Mass of a single C_{60} fullerene	$m_f = 1.20 \times 10^{-24} \text{ kg}$
Attractive constant	$A = 17.4 \text{ eV \AA}^6$
Repulsive constant	$B = 29 \times 10^3 \text{ eV \AA}^{12}$

TABLE I Constants utilized in this model

$$V_{eff}(r) = \frac{h^2}{2mr^2} - \frac{A'}{r^5} + \frac{B'}{r^{11}}, \quad (6)$$

where m denotes the reduced mass of the nano-orbiting system. From classical mechanics, the minimum energy configuration of equation (6) corresponds to the circular orbit that is obtained upon solving $dV_{eff}/dr = 0$, which results in the circular angular frequency ω being given by

$$\omega^2 = \frac{5A'}{mR^7} - \frac{11B'}{mR^{13}}, \quad (7)$$

where R is the circular orbiting radius of the atom. Utilizing an instability argument, we can show that R is approximately equal to

$$R = \left(\frac{3B'}{A'} \right)^{1/6} \approx 3.8 \text{ \AA}. \quad (8)$$

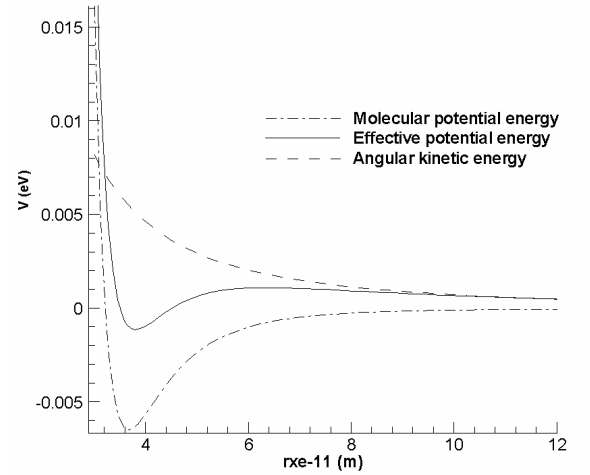


Fig. 2 The molecular potential energy, the angular kinetic energy and the effective potential energy of a carbon atom orbiting around the outside of a (6,6) carbon nanotube.

Given the circular orbiting radius R , the angular frequency of the system f can be estimated to be 29 GHz, which is in the gigahertz range. Furthermore, the angular kinetic energy can be easily calculated as $0.074/r^2$ eV. The angular kinetic energy, the total molecular potential energy, and the effective potential energy are plotted together in Fig. 2.

IV. NUMERICAL RESULTS

Utilizing the angular kinetic energy calculated in Section III, the total energy E of this system can be expressed as

$$E = \frac{1}{2}m\dot{r}^2 + \left(\frac{0.074}{r^2} - \frac{A'}{r^5} + \frac{B'}{r^{11}} \right). \quad (9)$$

After changing the coordinate system from t to θ by utilizing equation (2), we find that θ cannot be obtained by analytical integration in terms of any well-known special functions. Therefore, a numerical method is employed to compute the loci of such a system. Upon substituting $r = 1/u$ and dividing each complete revolution into N grid points, then the numerical scheme becomes

$$u_{i+1} = u_i \pm \varepsilon \frac{\sqrt{E - B'u_i^{11} + A'u_i^5 - 0.074u_i^2}}{\sqrt{0.074}}, \quad (10)$$

where $i = 1 \dots N$ and $\varepsilon = 2\pi/N$. The numerical results indicate that there are three distinct types of loci, namely that of circular, non-circular bounded and non-circular unbounded orbits. The numerical results strongly correlate with the characteristics of the effective potential energy curve in Fig. 2. Hence, from the features of such effective potential energy, we examine five energy levels, namely $E = -1.14$, -0.6 , 0 , 0.5 , and 1.1 meV, where -1.14 meV is the minimum energy of the effective potential energy, -0.6 meV is the mid-energy between zero and the minimum, 0.5 meV is the mid-energy between the peak and 0 eV and 1.1 meV is among the peak. Numerical results indicate that for $E = -1.14$ meV, only an initial radial position of $r_0 = 3.8$ Å is possible for a stable circular orbit, as illustrated in Fig. 3. For $E = -0.6$ meV, r_0 lies between 3.58 and 4.19 Å and hence the carbon atom is orbiting around the outside of the carbon nanotube in a non-circular bounded orbit, as illustrated in Fig. 4. For $E = 0$ meV, r_0 lies between 3.5 and 4.5 Å but this orbit is unbounded due to the fact that a point at infinity is also an accessible initial starting point, and the locus corresponds to a non-circular unbounded orbit, as illustrated in Fig. 5. For $E = 0.5$ meV, we have to consider two different scenarios. If r_0 lies somewhere between 3.46 and 4.86 Å, then the atom is orbiting around the outside of the carbon nanotube in a non-circular bounded orbit, while if r_0 lies beyond 10 Å, then the atom escapes from its initial location to infinity very quickly. Finally, it is straightforward to show that the carbon atom will swirl out to infinity for all accessible r_0 when $E = 1.1$ meV, as illustrated in Fig. 6.

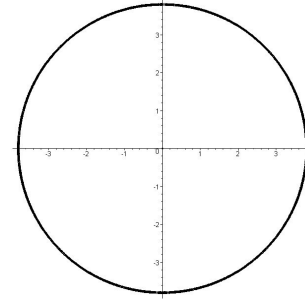


Fig. 3 A locus for $E = -1.14$ meV with an initial position of 3.8 Å. The atom is orbiting in a stable circular orbit.

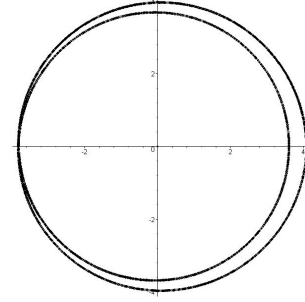


Fig. 4 A locus for $E = -0.6$ meV with an initial position of 3.6 Å. The orbiting atom is bounded between 3.58 Å and 4.19 Å.

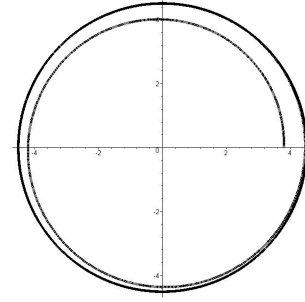


Fig. 5 A locus for $E = 0$ meV with an initial position of 3.8 Å. The orbiting atom is swirling away from its bounded locus gradually.

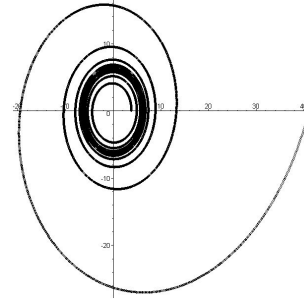


Fig. 6 A locus for $E = 1.1$ meV with an initial position of 3.8 Å. The orbiting atom escapes from its initial position to infinity very quickly.

V. ANOTHER POSSIBLE NANO-ORBITING SYSTEM

In this section, we briefly discuss another possible nano-orbiting system, namely a C_{60} fullerene orbiting around the outside of a (6,6) carbon nanotube. The same mathematical and numerical methods, which have been employed in the earlier case of an atom orbiting around the outside of a carbon nanotube, can be applied for this nano-orbiting system without any conceptual difficulties. However, the mathematical derivation of the more complicated system is lengthier, where arises from the fact that the total molecular energy of the system involves a discrete sum of the atomic potential energy between two molecules. We approximate this discrete sum by the double surface integral

$$V = n_g n_f \iint \left(-\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) d\Sigma_g d\Sigma_f, \quad (11)$$

where n_g , n_f , ρ , $d\Sigma_f$ and $d\Sigma_g$ denote the mean surface density of the (6,6) carbon nanotube, the mean surface density of the C_{60} , the distance between carbon atoms on the surface of two molecules and the elements of the surface area of the fullerene and the carbon nanotube respectively. The total molecular potential energy for the system can be obtained analytically, and the shape of the effective potential energy and the classification of loci are very similar to the case of the carbon atom orbiting around the outside of the carbon nanotube. Once again, the circular orbiting frequency of such a system can be shown to lie in the gigahertz range, i.e., 4 GHz.

VI. DISCUSSION AND ANALYSIS

In this study we have ignored any thermal fluctuations, arising from the environment. It is easy to show that if the thermal energy for the case of the carbon atom orbiting around the outside of the carbon nanotube is greater than 2.2 meV, which is the difference between the global minimum and the local maximum of the effective potential energy curve in Fig. 2, then the orbiting behavior might not be observed. Further, assuming that all the thermal energy is taken up into the atom's translational kinetic energy, we may eventually obtain its escape velocity as 133 ms^{-1} , which indicates that no orbiting behavior of such an atom can be observed at room temperature. In addition, since we investigate a two body problem at the nano-scale, any further Coulomb's objects will disturb the atom's orbiting behaviors in varying degrees, and therefore the assumption of a vacuum environment is also a prerequisite in this paper.

VII. CONCLUSION

In this paper, a classical two body problem is examined at the nano-scale. In particular, a carbon atom orbiting around the outside of a (6,6) carbon nanotube is examined. The classification of the atom's loci can not be determined by analytical integration in terms of any well-known functions, and therefore a numerical method is employed to find the loci for these systems. Three types of loci are predicted, namely circular, non-circular bounded and non-circular unbounded orbits. Criteria for the occurrence of the various types of loci

are determined by examining the atom's initial total energies and positions. The circular orbiting frequency reaches the gigahertz range, which suggests that the proposed nano-scale system can be utilized in possible future nano-devices. In addition, another possible nano-orbiting system, namely a C_{60} fullerene orbiting around the outside of a (6,6) carbon nanotube, is briefly mentioned. Finally, restrictions for the existence of such a system are discussed in Section VI.

ACKNOWLEDGMENT

We gratefully acknowledge the financial support from the Discovery Project Scheme of the Australian Research Council and the University of Wollongong.

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