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# A molecular motor constructed from a double-walled carbon nanotube driven by temperature variation

**Z C Tu**[1,2] **and Z C Ou-Yang**[1,3]

[1] Institute of Theoretical Physics, The Chinese Academy of Sciences, PO Box 2735, Beijing 100080, People's Republic of China
[2] Graduate School, The Chinese Academy of Sciences, Beijing, People's Republic of China
[3] Centre for Advanced Study, Tsinghua University, Beijing 100084, People's Republic of China

E-mail: tzc@itp.ac.cn and oy@itp.ac.cn

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**Abstract**
A new molecular motor is theoretically constructed from a double-walled carbon nanotube whose inner tube is a long (8, 4) single-walled carbon nanotube (SWNT) and whose outer tube a short (14, 8) SWNT. The interaction between the inner and outer tubes is derived by summing the Lennard-Jones potentials between atoms in the inner and outer tubes. It is proved that the molecular motor in a thermal bath exhibits a directional motion with the temperature variation of the bath.

It is well known that pollen in water exhibits Brownian motion. The forces on the pollen stem from two components [1]: a fluctuating force that averages to zero over time; and a viscous force that slows the motion. These two kinds of forces are related by temperature, so the fluctuation is often called thermal noise. The second law of thermodynamics suggests that biased Brownian motion requires two conditions [2]: (1) breaking of thermal equilibrium and (2) breaking of spatial inversion symmetry. In order to illustrate that the second law of thermodynamics cannot be violated, Feynman devised an imaginary ratchet system with a pawl in his famous lectures [3].

To explain matter transport in biological systems, the concept of a molecular motor is introduced [4, 5]. From the statistical viewpoint, many models [2] of molecular motor have been put forward, such as on–off ratchets [6, 7], fluctuating potential ratchets [1, 8], fluctuating force ratchets [9, 10], and temperature ratchets [11–13]. All these models satisfy the two conditions required by the second law of thermodynamics.

With the development of nanotechnology, especially the discovery of carbon nanotubes [14], people are putting their dreams of manufacturing nanodevices [15] into practice. Here a natural question arises: can we construct molecular motors from carbon nanotubes? In this paper, we will prove that it is possible to construct a molecular motor from

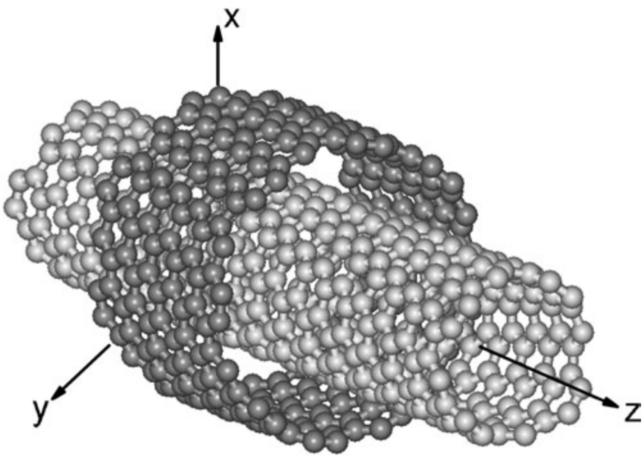


**Figure 1.** A double-walled carbon nanotube with the inner tube's index being (8, 4) and the outer tube's index being (14, 8). The $z$-axis is the tube axis, the $x$-axis perpendicular to $z$ passes through one of the carbon atoms in the inner tube and the $y$-axis is perpendicular to the $xz$-plane. There is obviously no relative motion along the radial direction between the inner and the outer tubes at low temperature. If we forbid motion of the outer tube in the direction of the $z$-axis, only rotation of the outer tube around the inner tube is permitted.

a double-walled carbon nanotube (DWNT). The molecular motor in a thermal bath exhibits a directional motion with the temperature variation of the bath.

A DWNT consists of two single-walled carbon nanotubes (SWNTs) with a common axis. The layer separation between the two tubes is about 3.4 Å [16, 17]. A SWNT without two end caps can be constructed by wrapping up a single sheet of graphite such that two equivalent sites of the hexagonal lattice coincide [18]. In our previous paper [19], we presented a simple formula for coordinates of carbon atoms in the SWNT and described how to construct the SWNT.

We construct the molecular motor from a double-walled carbon nanotube as shown in figure 1. The inner tube's index is (8, 4) with a length large enough to be regarded as infinite. The outer tube is set to be a (14, 8) tube with just a single unit cell[4]. Obviously, they are both chiral nanotubes and their layer separation is about 3.4 Å. If we prohibit motion of the outer tube in the direction of nanotube axis, it will be proved that this system in a thermal bath exhibits a directional rotation when the temperature of the system varies with time. Thus it could serve as a thermal ratchet.

To see this, we first select an orthogonal coordinate system, shown in figure 1, whose $z$-axis is the tube axis and whose $x$-axis passes through one of carbon atoms in the inner tube. We fix the inner tube and forbid $z$-directional motion of the outer tube. We denote the angle of rotation of the outer tube around the inner tube as $\theta$.

We take the interaction between atoms in the outer tube and the inner tube as the Lennard-Jones potential $u(r_{ij}) = 4\epsilon[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^6]$, where $r_{ij}$ is the distance between atom $i$ in the inner tube and atom $j$ in the outer tube, $\epsilon = 28$ K, and $\sigma = 3.4$ Å [20]. We calculate the potential $V(\theta)$ [19] when the outer tube rotates around the inner tube by angle $\theta$ and plot this in figure 2. We find that $V(\theta)$ is periodic (with period $\pi/2$) and violates spatial inversion symmetry. Thus the second condition for making a molecular motor is satisfied. Now we can explain why we select the (8, 4) tube and (14, 8) tube. The following three criteria were

[4] If we consider several unit cells, the final results of this paper are unchanged.

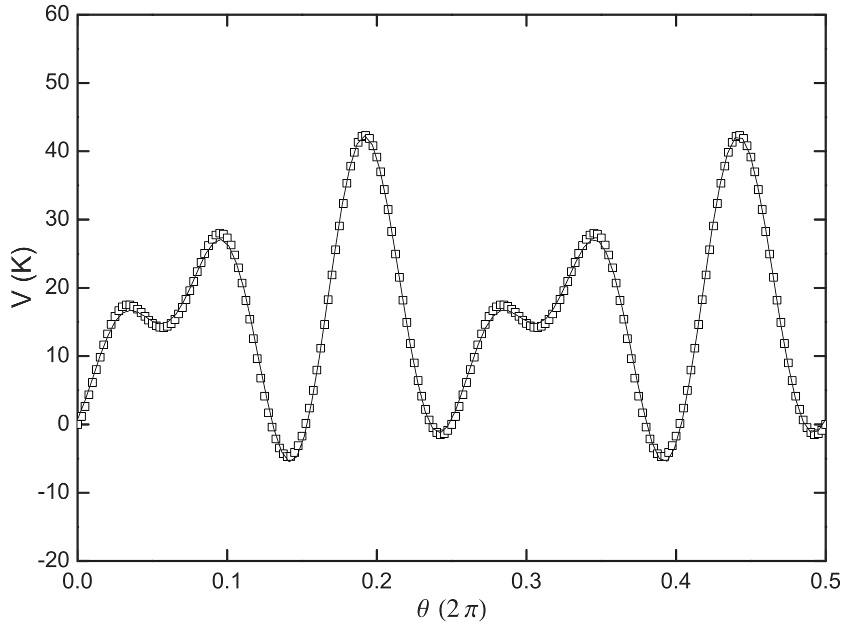


**Figure 2.** The potentials $V(\theta)$ between the outer and the inner tubes with the outer tube rotating around the inner tube. $\theta$ is the rotation angle. Here we have set $V(0) = 0$. The squares are the numerical results which can be well fitted by $V(\theta) = 15.7 - 0.6\cos 4\theta + -2.2\sin 4\theta - 12.7\cos 8\theta - 6\sin 8\theta - 1.7\cos 12\theta + 10.8\sin 12\theta$ (solid curve).

considered: (1) the layer separation is about 3.4 Å; (2) the shape of $V(\theta)$ is not too complicated; (3) the difference of the maximum and minimum of $V(\theta)$ is remarkable. We find that only (8, 4) and (14, 8) tubes satisfy these criteria for $0 < n_1, n_2 < 30$ in our calculation.

The easiest way to satisfy the first condition is to put our system into a thermal bath full of He gas whose temperature varies with time. We will show that the outer tube will exhibit a directional rotation.

We can write the Langevin equation [21] for the outer tube $m\rho^2\ddot{\theta} = -V'(\theta) - \eta\dot{\theta} + \xi(t)$, where $m$ and $\rho$ are respectively the mass and the radius of the outer tube, $\eta$ is the rotation viscosity coefficient, and the dot and prime indicate, respectively, differentiations with respect to time $t$ and angle $\theta$. $\xi(t)$ is thermal noise which satisfies $\langle\xi(t)\rangle = 0$ and the fluctuation-dissipation relation $\langle\xi(t)\xi(s)\rangle = 2\eta T(t)\delta(t-s)$ [22], where $T(t)$ is the temperature and the Boltzmann factor is set to 1. Let us consider the overdamped case where the inertial term $m\rho^2\ddot{\theta}$ is much less than the thermal fluctuations and can be neglected. We arrive at $\eta\dot{\theta} = -V'(\theta) + \xi(t)$ and the corresponding Fokker–Planck equation [2, 23]

$$\frac{\partial P(\theta,t)}{\partial t} = \frac{\partial}{\partial\theta}\left[\frac{V'(\theta)P(\theta,t)}{\eta}\right] + \frac{T(t)}{\eta}\frac{\partial^2 P(\theta,t)}{\partial\theta^2}, \tag{1}$$

where $P(\theta,t)$ represents the probability of finding the outer tube in angle $\theta$ at time $t$ which satisfies $P(\theta+\pi/2,t) = P(\theta,t)$. If the period of temperature variation is $\mathcal{T}$, we arrive at the average angular velocity in the long-time limit [2]

$$\langle\dot{\theta}\rangle = \lim_{t\to\infty}\frac{1}{\mathcal{T}}\int_t^{t+\mathcal{T}}\mathrm{d}t\int_0^{\pi/2}\mathrm{d}\theta\left[-\frac{V'(\theta)P(\theta,t)}{\eta}\right]. \tag{2}$$

For example, set $T(t) = \bar{T}[1 + A\sin(2\pi t/\mathcal{T})]$ with $\bar{T} = 50$ K and $|A| \ll 1$. Let $D = \eta/\bar{T}$, $t = D\tau$, $U(\theta) = V(\theta)/\bar{T}$, $\mathcal{T} = D\mathcal{J}$, and $\tilde{P}(\theta,\tau) = P(\theta, D\tau)$, We arrive at the dimensionless

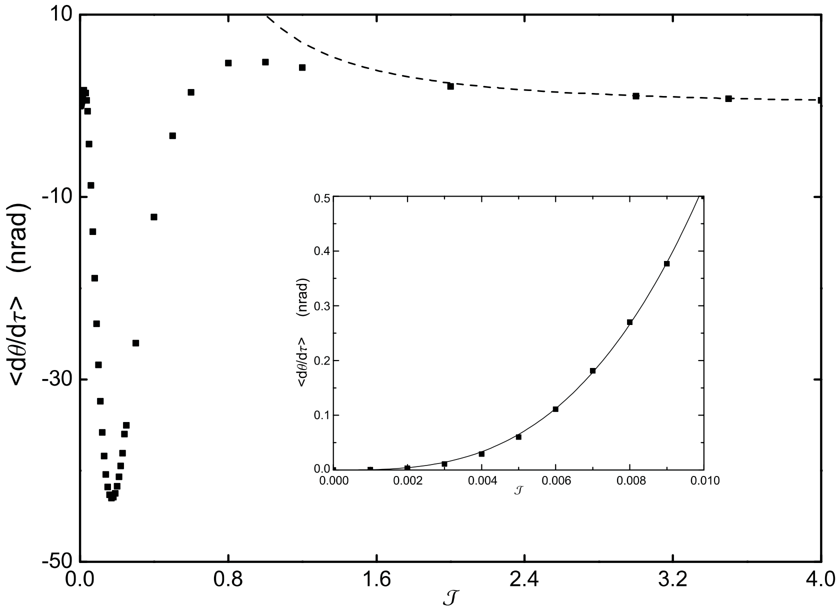

**Figure 3.** The average dimensionless angular velocity $\langle \mathrm{d}\theta/\mathrm{d}\tau \rangle$ of the outer tube rotating around the inner tube in a thermal bath whose temperature changes with the dimensionless period $\mathcal{J}$. The minus sign means that the rotation around the $z$-axis is left handed. Squares are the numerical results. The dashed curve corresponds to $\langle \mathrm{d}\theta/\mathrm{d}\tau \rangle = 10/\mathcal{J}^2$ and the solid curve (in the inset) corresponds to $\langle \mathrm{d}\theta/\mathrm{d}\tau \rangle = 5.2 \times 10^5 \mathcal{J}^3$.

versions of equations (1) and (2):

$$\frac{\partial \tilde{P}}{\partial \tau} = \frac{\partial}{\partial \theta}[U'(\theta)\tilde{P}] + \left(1 + A \sin \frac{2\pi\tau}{\mathcal{J}}\right)\frac{\partial^2 \tilde{P}}{\partial \theta^2}, \tag{3}$$

$$\left\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \right\rangle = \lim_{\tau\to\infty} \frac{1}{\mathcal{J}} \int_{\tau}^{\tau+\mathcal{J}} \mathrm{d}\tau \int_0^{\pi/2} \mathrm{d}\theta \, [-U'(\theta)\tilde{P}]. \tag{4}$$

Let $A = 0.01$; we can numerically solve equation (3) and calculate equation (4) with different $\mathcal{J}$. The squares in figure 3 show the relation between the average dimensionless angular velocity $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle$ and the dimensionless period $\mathcal{J}$ of the temperature variation. We find that $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle \simeq 0$ for very small and large $\mathcal{J}$, and $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle \neq 0$ for intermediate $\mathcal{J}$, which implies that the outer tube has an evident directional rotation in this period range. Thus we have constructed a temperature ratchet.

For He gas at temperature $\bar{T} = 50$ K, we can calculate $\eta = 861$ K ns from its value at 273 K and $D = 17.2$ ns. It is necessary to note that the rotation viscosity coefficient $\eta$ is not the viscosity coefficient of gas $\eta_c$ in the common sense. Here their relationship is $\eta = 2\pi\rho^2 L\eta_c$ ($L$ is the length of the outer tube). Generally speaking, $\eta$ depends on the temperature [24], and here the temperature varies with time. Therefore $\eta$ depends on the time. But if the range of temperature variation is very small, we can still regard $\eta$ as a constant. On the basis of these data, we obtain $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle = -43$ nrad when $\mathcal{J} = 0.17$, i.e. $\langle \dot{\theta} \rangle = \frac{1}{D}\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle = -2.5$ nrad ns$^{-1}$ when $\mathcal{T} = 2.9$ ns. Here the minus sign of the average angular velocity means that the rotation of the outer tube around the $z$-axis is left handed. We note that $\langle \dot{\theta} \rangle = -2.5$ nrad ns$^{-1}$ is a remarkable value ($-2.5$ rad s$^{-1}$) which is easy to observe in experiment. If consider the inertial effect of the outer tube, this value may be changed. But we believe that it would still be an observable quantity.

Furthermore, from figure 3 we observe that the sign of $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle$ changes from '+' to '−' and back to '+' with $\mathcal{J}$ increasing, which suggests that the outer tube's rotation around the inner tube is right handed for small and large periods $\mathcal{J}$, and left handed for intermediate periods $\mathcal{J}$. Through data fitting, we find that $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle$ is proportional to $\mathcal{J}^3$ for very small period $\mathcal{J}$ (solid curve of figure 3) and proportional to $\mathcal{J}^{-2}$ for period $\mathcal{J}$ large enough (the dashed curve of figure 3), which agrees with the results of asymptotic analysis [2]. In terms of [2], $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle$ decreases proportionally to $\mathcal{J}^{-2}$ for large $\mathcal{J}$ in the case where $T(t)$ is symmetric under time inversion, and $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle = \tilde{B}\mathcal{J}^2 + \mathcal{O}(\mathcal{J}^3)$ for small $\mathcal{J}$. Here we obtain $\tilde{B} = 0$ in the case of $T(t) = \bar{T}[1 + A\sin(2\pi t/\mathcal{T})]$. Thus $\langle \frac{\mathrm{d}\theta}{\mathrm{d}\tau} \rangle \sim \mathcal{J}^3$ for small $\mathcal{J}$.

To summarize, we have theoretically constructed a temperature ratchet using a DWNT, but some practical difficulties remain. How does one synthesize the appropriate DWNT? How does one forbid axial translation of the outer tube? How does one control the temperature in the system? If these obstacles can be overcome, molecular motors constructed from DWNTs must be realizable. Otherwise, our results would require overdamped conditions, which could be realized by modulating the density of He; this is also a difficult matter.

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