Thermal vibration of single-walled carbon nanotubes with quantum effects

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The thermal vibration of a single-walled carbon nanotube (SWCNT) is investigated by using the models of Euler beam and Timoshenko beam with quantum effects taken into consideration when the law of energy equipartition is unreliable. The relation between temperature and the root of mean-squared (RMS) amplitude of thermal vibration at any cross section of the SWCNT is derived via the beam models in simply supported case and cantilevered case. The RMS amplitude of thermal vibration of SWCNT predicted by using Timoshenko beam is higher than that predicted by using Euler beam. The RMS amplitude of thermal vibration of an SWCNT predicted by the quantum theory is lower than that predicted by the law of energy equipartition. The quantum effect is more important for the thermal vibration of an SWCNT in the cases of higher-order modes, short length and low temperature.

1. Introduction

The effects of thermal fluctuations are very important to the mechanical properties of low dimensional systems. With the recently developed nanotechnology, people are trying to construct nanoscale devices working at molecular level and activated by thermal fluctuation. One example is the Brownian ratchet, which is a particle moving unidirectionally over a switchable anisotropic potential [1]. Previous studies have indicated that carbon nanotubes exhibit superior mechanical over any known materials [2]. Thus, carbon nanotube-based resonators present a unique opportunity to study the thermal vibration problems. Xu et al. [3] studied thermally...
driven large-amplitude fluctuations in carbon nanotube-based devices using molecular dynamics simulation. Treacy et al. [4] estimated the Young modulus of carbon nanotubes by measuring the amplitude of their intrinsic thermal vibrations in the transmission electron microscope. Krishnan et al. [5] conducted a detailed study on the relationship among Young’s modulus, size and the stand deviation of the tip vibration amplitude of a carbon nanotube at a specific temperature. Feng & Jones [6] computed the free thermal vibrations of cantilevered carbon nanotubes by using molecular dynamics and explained the resulting power spectral density of the tip displacement with statistical mechanics and beam theory. Later, they found that the quality factor of the cantilever carbon nanotube is independent from its length and that the intrinsic signal-to-noise ratio for a cantilever carbon nanotube improves with an increase in length of carbon nanotube [7]. Barnard et al. [8] simulated the behaviour of suspended carbon nanotube resonator over a broad range of temperature and found that thermal fluctuations induce strong coupling between resonance modes. Wang et al. [9] studied the thermal vibration of single-walled carbon nanotube (SWCNT) via the model of Timoshenko beam, together with the law of energy equipartition and molecular dynamic simulations. Very recently, Wang & Hu [10] studied the thermal vibration of a double-walled carbon nanotube by using a model of double Euler beams with van der Waals interaction between layers taken into consideration, and then validated the results by using the molecular dynamic simulations. Jiang et al. [11,12] developed a finite-temperature continuum model based on interatomic potentials by using the Helmholtz free energy as thermodynamic potential and adopting the quasi-harmonic and local harmonic approximations. They used the model to determine the thermo-mechanical properties of graphene sheets and SWCNTs. Guo et al. [13] investigated the thermo-mechanical properties of SWCNTs and graphene sheets at finite temperature by using the quasi-continuum model based on the temperature-related higher-order Cauchy–Born rule. Later, Wang & Guo [14] used the model to study the finite deformation of SWCNTs.

On the other hand, Hone et al. [15] observed the quantum effects on the nanotube phonon spectrum in their experiment. Li & Chou [16] proposed a model of quantized molecular structure mechanics for studying heated SWCNTs. They quantized the vibrational modes of the nanotube according to the quantum mechanics. Zimmermann et al. [17] developed a phenomenological force-constant model for the description of lattice dynamics of carbon nanotubes and graphene sheets. They paid particular attention to the exact dispersion law of the acoustic modes, which determine the low-frequency thermal properties and reveal the quantum effects in carbon nanotubes. These studies have shown that the quantum effects should be considered when the thermal vibration of carbon nanotubes, in particular, for the cases of lower temperature and higher frequency, is of concern.

To the best knowledge of the author, however, neither experiments nor numerical simulations have been available for studying the quantum effects on the thermal vibration of any carbon nanotubes. The primary objective of this paper is to study the quantum effects on the thermal vibration of an SWCNT. For this purpose, the RMS amplitude of thermal vibration is derived in §2 by using the models of both Euler beam and Timoshenko beam with quantum effects taken into account. Then, a comparison is made in §3 for the thermal vibrations of SWCNTs described by using the quantum mechanics and the classical law of energy equipartition. Finally, some concluding remarks are made in §4.

2. Thermal vibration of a single-walled carbon nanotube predicted via beam models

(a) Model of Euler beam

As shown in previous publications, the SWCNT can be modelled as a slender beam when its transverse vibration is studied. This section starts with the dynamic equation of an Euler beam with uniform cross section placed along the $x$-direction in the frame of coordinates $(x, y, z)$, with
\( w(x, t) \) being the displacement of section \( x \) of the beam in the \( y \)-direction at the moment \( t \). In the case of small amplitudes, the free vibration of the Euler beam yields the following dynamic equation \[18\]
\[
\rho A \frac{\partial^2 w(x, t)}{\partial t^2} + EI \frac{\partial^4 w(x, t)}{\partial x^4} = 0, \tag{2.1}
\]
where \( E \) is Young’s modulus, \( I \) is the moment of inertia of the cross section, \( A \) is the area of the cross section and \( \rho \) is the mass density. The boundary conditions for a simply supported Euler beam are
\[
w(0, t) = 0, \quad \frac{\partial^2 w(0, t)}{\partial x^2} = 0, \quad w(L, t) = 0 \quad \text{and} \quad \frac{\partial^2 w(L, t)}{\partial x^2} = 0, \tag{2.2}
\]
where \( L \) is the length of the beam. The natural vibration of the \( n \)th order for such a beam is \[18\]
\[
w_n(x, t) = \hat{w}_n(x)e^{i\omega_nt} = D_n \sin \frac{n\pi x}{L} e^{i\omega_nt}, \tag{2.3}
\]
where \( j \equiv \sqrt{-1}, \omega_n \equiv (n\pi)^2 \sqrt{EI/\rho AL^4}, \ n = 1, 2, \ldots \) and \( D_n \) is to be determined from initial conditions.

The total energy \( E_n \) contained in the natural vibration of the \( n \)th order can be determined by calculating the following elastic energy
\[
E_n^{\text{elastic}} = \frac{EI}{2} \int_0^L \left( \frac{\partial^2 \hat{w}_n}{\partial x^4} \right)^2 \, dx = \frac{n^4\pi^4 EI D_n^2}{4L^3}, \tag{2.4}
\]
at the instant of maximal deflection when the beam is momentarily stationary, that is, \( e^{i\omega_nt} = 1 \).

The natural vibration of the Euler beam with one end clamped and the other end free is given in appendix A \[5,18\].

Now, the quantum effect on the thermal vibration of a carbon nanotube is analysed as follows. Each natural vibration of the beam can be considered as a harmonic oscillator with natural frequency \( \nu = \omega/2\pi \) at temperature \( T \). Here, \( \omega \) is the angular frequency. The statistical mechanics of the beam can be performed in the canonical \[19\] such that the partition function \( Z \) is
\[
Z = \sum_l e^{-\gamma E_l}, \tag{2.5}
\]
where \( \gamma = 1/k_B T, \ k_B = 1.38 \times 10^{-23} \text{ JK}^{-1} \) denotes the Boltzmann constant, and \( E_l = h\nu(l + 1/2) \) \((l = 0, 1, 2 \ldots)\). Here, \( h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s} \) is the Planck’s constant. If the energy scale is shifted and all energies are reckoned from the zero energy point of the oscillator, then the partition function can be modified as
\[
Z = \sum_l e^{-\gamma hvl} = \frac{1}{1 - e^{-\gamma hv}}. \tag{2.6}
\]
The expression for the mean energy becomes
\[
E = -\frac{\partial \ln Z}{\partial \beta} = \frac{hv}{e^{hv/k_B T} - 1}. \tag{2.7}
\]
From equation (2.4) and equation (2.7), it is easy to derive
\[
D_n^2 = \frac{4hvL^3}{n^4\pi^4 EI(e^{hv/k_B T} - 1)}. \tag{2.8}
\]
Then, the RMS amplitude of thermal vibration of the \( n \)th mode for the beam at \( x \) reads
\[
\hat{w}_n(x) = \frac{\sqrt{2}}{2} D_n f_n(x). \tag{2.9}
\]
As the natural modes are independent to each other, their contributions can be added incoherently. To average coherently over all the modes, the variances \( \hat{w}_n^2(x) \) can be added to obtain
the other Gaussian distribution with the standard deviation given by

\[ \hat{w}(x) = \left( \sum_{n=0}^{\infty} \hat{\omega}_n^2(x) \right)^{1/2}. \tag{2.10} \]

Hence, the RMS amplitude of thermal vibration of a simply supported SWCNT at \( x \) can be obtained via the model of Euler beam.

**Model of Timoshenko beam**

The governing equations of a Timoshenko beam with uniform cross section placed along \( x \)-direction in the frame of coordinates \((x, y, z)\) are [18]

\[
\rho \frac{\partial^2 w}{\partial t^2} + \beta G \left( \frac{\partial \phi}{\partial x} - \frac{\partial^2 w}{\partial x^2} \right) = 0 \tag{2.11a}
\]

and

\[
\rho L \frac{\partial^2 \phi}{\partial t^2} + \beta AG \left( \phi - \frac{\partial w}{\partial x} \right) - EI \left( \frac{\partial^2 \phi}{\partial x^2} \right) = 0, \tag{2.11b}
\]

where \( w(x, t) \) is the displacement of section \( x \) of the beam in the \( y \)-direction at the moment \( t \), \( E, I, \rho \) and \( A \) are all the same as those in §2a, \( G \) is the shear modulus, \( \phi \) is the slope of the deflection curve when the shearing force is neglected, \( \beta \) is the form factor of shear depending on the shape of the cross section and \( \beta = 0.5 \) holds for the circular tube of the thin wall [20]. The boundary conditions of simply supported beam are

\[ w(0, t) = 0, \quad \frac{\partial \phi(0, t)}{\partial x} = 0, \quad w(L, t) = 0 \quad \text{and} \quad \frac{\partial \phi(L, t)}{\partial x} = 0. \tag{2.12} \]

To study the vibration of a Timoshenko beam, let the dynamic deflection and slope be given by

\[ w = \hat{w}e^{j\omega t} \quad \text{and} \quad \phi = \hat{\phi}e^{j\omega t}, \tag{2.13} \]

where \( \hat{w} \) represents the amplitude of deflection of the beam, and \( \hat{\phi} \) is the amplitude of the slope of the beam owing to bending deformation alone. Let

\[ \xi = \frac{x}{L}. \tag{2.14} \]

Substituting equation (2.13) into equation (2.11) gives

\[
\frac{\partial^2 \hat{w}}{\partial \xi^2} - \frac{L}{b^2} \frac{\partial \hat{\phi}}{\partial \xi} + b^2 s^2 \hat{w} = 0 \tag{2.15a}
\]

and

\[
s^2 \frac{\partial^2 \hat{\phi}}{\partial \xi^2} + \frac{1}{b^2} \frac{\partial \hat{w}}{\partial \xi} - (1 - b^2 r^2 s^2) \hat{\phi} = 0, \tag{2.15b}
\]

where

\[ b^2 = \frac{\rho AL^4 \omega^2}{EI}, \quad r^2 = \frac{I}{AL^2} \quad \text{and} \quad s^2 = \frac{EI}{\beta AG L^2}. \tag{2.16} \]

When \( (r^2 - s^2)^2 + 4/b^2 \) holds, the solutions of equation (2.15a, b) can be found as [21]

\[
\hat{w} = C_1 \cosh b\omega_1 \xi + C_2 \sinh b\omega_1 \xi + C_3 \cos b\alpha_2 \xi + C_4 \sin b\alpha_2 \xi \tag{2.17a}
\]

and

\[
\hat{\phi} = C'_1 \sinh b\omega_1 \xi + C'_2 \cosh b\omega_1 \xi + C'_3 \sin b\alpha_2 \xi + C'_4 \cos b\alpha_2 \xi, \tag{2.17b}
\]

where

\[
\frac{\alpha_1}{\alpha_2} = \sqrt{2} \left\{ \frac{\omega_1}{(r^2 + s^2) + \left[ (r^2 - s^2) + \frac{4}{b^2} \right]^{1/2}} \right\}^{1/2}. \tag{2.18}
\]
When \((r^2 - s^2)^2 + 4/b^2\) holds, equation (2.17a,b) can be replaced by [21]

\[
\hat{w} = C_1 \cos b \alpha'_1 \xi + jC_2 \sin b \alpha'_1 \xi + C_3 \cos b \alpha_2 \xi + C_4 \sin b \alpha_2 \xi \quad (2.19a)
\]

and

\[
\hat{\phi} = jC'_1 \sin b \alpha'_1 \xi + C'_2 \cos b \alpha'_1 \xi + C'_3 \sin b \alpha_2 \xi + C'_4 \cos b \alpha_2 \xi, \quad (2.19b)
\]

where

\[
\alpha'_1 = \frac{1}{\sqrt{2}} \left\{ (r^2 + s^2) - \left[ (r^2 - s^2) + \frac{4}{b^2} \right]^{1/2} \right\}^{1/2}. \quad (2.20)
\]

Solutions of equation (2.17a,b) or (2.19a,b) are naturally the solutions of the original coupled equations (2.15).

It should be noted that only a half of constants in equations (2.17a,b) or (2.19a,b) are independent. They are related by the equations (2.15) as follows [21]

\[
C'_1 = \frac{b}{L} \frac{\alpha^2_1 + s^2}{\alpha_1} C_1, \quad (2.21a)
\]

\[
C'_2 = \frac{b}{L} \frac{\alpha^2_1 + s^2}{\alpha_1} C_2, \quad (2.21b)
\]

\[
C'_3 = -\frac{b}{L} \frac{\alpha^2_2 - s^2}{\alpha_2} C_3 \quad (2.21c)
\]

and

\[
C'_4 = \frac{b}{L} \frac{\alpha^2_2 - s^2}{\alpha_2} C_4. \quad (2.21d)
\]

For both cases \([(r^2 - s^2)^2 + 4/b^2]^{1/2} \geq (r^2 + s^2)\) and \([(r^2 - s^2)^2 + 4/b^2]^{1/2} \leq (r^2 + s^2)\), the natural frequency of the simply supported beam yields [21]

\[
\sin b \alpha_2 = 0. \quad (2.22)
\]

The natural frequency \(\omega_n\) of the \(n\)th order for the Timoshenko beam can be obtained from equation (2.22). The natural mode \((\hat{w}_n, \hat{\phi}_n)\) of the \(n\)th order for the simply supported beam yields [21]

\[
\hat{w}_n = D_n f_{\hat{w}_n}(\xi) = D_n \sin b_n \alpha_{n2} \xi \quad (2.23a)
\]

and

\[
\hat{\phi}_n = D_n f_{\hat{\phi}_n}(\xi) = H_n \cos b_n \alpha_{n2} \xi, \quad (2.23b)
\]

where

\[
H_n = \frac{b_n}{L} \frac{\alpha^2_{n2} - s^2}{\alpha_{n2}} D_n. \quad (2.24)
\]

Here, \(\alpha_{n2} = (1/\sqrt{2}) \left\{ (r^2 + s^2) + \left[ (r^2 - s^2) + 4/b^2 \right]^{1/2} \right\}^{1/2}.

The natural vibration of Timoshenko beam with one end clamped and the other end free can be seen from appendix B [9,21].

The total energy \(E_n\) contained in the natural vibration of the \(n\)th order can be determined by calculating the following elastic energy

\[
E_n^{\text{elastic}} = \int_0^L \left( \frac{EI}{2} \left( \frac{\partial^2 \psi_n}{\partial x^2} \right)^2 + \frac{\beta AG}{2} \left( \phi_n - \frac{\partial \psi_n}{\partial x} \right)^2 \right) dx \quad (2.25)
\]

\[
= D_n \int_0^L \left( \frac{EI}{2} \left( \frac{\partial^2 \phi_n}{\partial x^2} \right)^2 + \frac{\beta AG}{2} \left( \phi_n - \frac{\partial \phi_n}{\partial x} \right)^2 \right) dx,
\]

at the instant of maximal deflection when the beam is momentarily stationary, that is, \(e^{j \omega_n t} = 1\).
From equation (2.25) with equation (2.7) considered, it is easy to obtain

\[
D_n^2 = \frac{\rho_{\text{elastic}}}{\int_0^L \left[ \left( \frac{EI}{2} \left( \frac{\partial^2 \phi_n}{\partial x^2} \right)^2 + \left( \beta AG/2 \right) \left( f_{\psi n} - \frac{\partial f_{\psi n}}{\partial x} \right)^2 \right] dx}
= \frac{\hbar \nu_n}{\left( e^{\hbar \nu_n / k_B T} - 1 \right)} \int_0^L \left[ \left( \frac{EI}{2} \left( \frac{\partial^2 \phi_n}{\partial x^2} \right)^2 + \left( \beta AG/2 \right) \left( f_{\psi n} - \frac{\partial f_{\psi n}}{\partial x} \right)^2 \right] dx,
\]

(2.26)

where \( \nu_n = \omega_n / 2\pi \). Then, the RMS amplitude of thermal vibration of the \( n \)th mode for the beam at \( x \) reads

\[
\hat{w}_n(x) = \frac{\sqrt{2}}{2} D_n f_{\psi n}(x).
\]

(2.27)

As the natural modes are mutually independent, the vibration profile for the combined natural modes also yields a Gaussian distribution, with standard deviation given by the summation of the variances. The RMS amplitude of thermal vibration of SWCNT at \( x \) can be obtained by using equation (2.10). Hence, the RMS amplitude of thermal vibration of an SWCNT at any point can be obtained via the model of Timoshenko beam.

### 3. Comparisons between classical theory and quantum results

This section presents the predictions to the RMS amplitude of thermal vibration of an SWCNT according to the analysis in §2. Figure 1 shows the RMS amplitudes of thermal vibration of the first four modes of an armchair (10, 10) SWCNT 9.8 nm long with both ends simply supported at room temperature 300 K. Here, the symbol EBQ represents the RMS amplitude of thermal vibration of the SWCNT predicted via the Euler beam with quantum effects taken into consideration. The symbol EBC represents that predicted via the Euler beam with the law of energy equipartition. The symbols TBQ and TBC represent those predicted from the Timoshenko beam with quantum effects taken into consideration and with the law of energy equipartition, respectively. The Young modulus of the SWCNT is \( E = 1 \) TPa when the thickness is chosen as \( h = 0.34 \) nm, and Poisson’s ratio is \( \nu = 0.20 \). There follows the shear modulus \( G = E / (2(1 + \nu)) \). The mass density is \( \rho = 2237 \) kg m\(^{-3}\). In figure 1a, only a very little difference can be identified among the results of Euler beam with the quantum theory, Euler beam with the law of energy equipartition, Timoshenko beam with the quantum theory and Timoshenko beam with the law of energy equipartition. The differences among the results of these four models become more and more obvious with an increase of the mode order. The RMS amplitude of thermal vibration predicted by the law of energy equipartition is larger than that predicted by the quantum theory. The RMS amplitude of thermal vibration predicted by Euler beam with quantum effects is smaller than that predicted by Timoshenko beam with quantum effects.

Figure 2 shows the RMS amplitude of thermal vibration of the first four modes of an armchair (10, 10) SWCNT 9.8 nm long with one end clamped, and the other end free at room temperature 300 K predicted by a cantilever Euler beam or Timoshenko beam with quantum effects taken into consideration compared with that together with the law of energy equipartition. Similar conclusion can be drawn as the simply supported case in figure 1.

Figure 3 gives the RMS amplitude of thermal vibration of (10,10) SWCNTs of different lengths and with both ends simply supported. Here, the symbols EBQ, EBC, TBQ and TBC represent the same meaning as those in figure 1. From these figures, little difference between the quantum theory and the classical theory can be observed for an SWCNT 19.6 nm long from the comparison between the Euler beam and the Timoshenko beam. Clear difference can be identified for an SWCNT 4.9 nm long modelled by both Euler beam and Timoshenko beam. More obvious difference can be seen when the length of an SWCNT decreased to 2.45 nm. The RMS amplitude of thermal vibration predicted via the law of energy equipartition is larger than that predicted by using the quantum theory. The RMS amplitude of thermal vibration predicted from...
Figure 1. RMS amplitude of thermal vibration of the first four modes of an armchair (10, 10) SWCNT 9.8 nm long with simply supported boundary conditions at 300 K. (Online version in colour.)

Figure 2. RMS amplitude of thermal vibration of the first four modes of an armchair (10, 10) SWCNT 9.8 nm long with one end clamped and the other end free at 300 K. (Online version in colour.)
Figure 3. RMS amplitude of thermal vibration of (10,10) SWCNTs of different lengths with simply supported boundary conditions. (Online version in colour.)

Figure 4. RMS amplitude of thermal vibration of (10,10) SWCNTs of different lengths with one end clamped and the other end free. (Online version in colour.)
Figure 5. RMS amplitude of thermal vibration of an armchair (10,10) SWCNT 9.8 nm long predicted by a simply supported Timoshenko beam at different temperatures. (Online version in colour.)

Figure 4 shows the RMS amplitude of thermal vibration of a cantilever armchair (10, 10) SWCNTs of different lengths at 300 K predicted by a cantilever Euler beam or Timoshenko beam with quantum effects taken into consideration or together with the law of energy equipartition. Similar conclusion can be obtained as those in figure 3.

Figure 5 illustrates the RMS amplitude of thermal vibration of an armchair (10, 10) SWCNT 9.8 nm long with both ends simply supported at different temperatures, (a) 300, (b) 100, (c) 30, (d) 10, (e) 3 and (f) 1 K. Here, the symbols TBQ and TBC keep the same meaning as before. The parameters of the Timoshenko beam are also the same as before. It can be seen that both Timoshenko beams with either quantum effect or the law of energy equipartition can roughly predict the thermal vibration of the SWCNT at 300 K from figure 5. Their difference can be seen clearly, when the temperature of the SWCNT is decreased to 100 K. The difference of RMS amplitude of thermal vibration of SWCNT predicted by the law of energy equipartition and
Figure 6. RMS amplitude of thermal vibration of an armchair (10,10) SWCNT 9.8 nm long predicted by a cantilever Timoshenko beam at different temperatures. (Online version in colour.)

The quantum theory keep increasing with a decrease of temperature. When the temperature is decreased to 1 K, the RMS amplitude of thermal vibration of SWCNT predicted by the quantum theory is less than 6% of that predicted by the law of energy equipartition. That is, the thermal vibration of the SWCNT is frozen.

Figure 6 illustrates the RMS amplitude of thermal vibration of an armchair (10,10) SWCNT 9.8 nm long with one end clamped and the other end free at different temperatures predicted by a cantilever Timoshenko beam with quantum effects taken into consideration or together with the law of energy equipartition. Similar conclusions can also be drawn as those in figure 5.

4. Concluding remarks

The paper presented a detailed study on the thermal vibration of the SWCNTs via the models of Euler beam and Timoshenko beam for both simply supported case and cantilevered case with the help of the quantum theory and the law of energy equipartition. The study indicates that quantum effects are not obvious for the RMS amplitude of thermal vibration of the first-order mode...
for not very short SWCNT, say 9.8 nm long, at room temperature. The Timoshenko beam with quantum effects taken into consideration predicts the lower RMS amplitude of thermal vibration of SWCNTs than that via the law of energy equipartition, especially for the cases of lower temperature, higher-order of natural modes or shorter length SWCNTs. When the temperature is extremely low, say only 1 K, the thermal vibration of an SWCNT is frozen.

Acknowledgements. The invaluable help of Professor Quanshui Zheng is greatly appreciated.

Funding statement. This work was supported in part by the National Natural Science Foundation of China under grant no. 11072108, FANEDD of China under grant no. 201028, Programme for New Century Excellent Talents in University under grant no. NCET-11-0832 and in part by the Fundamental Research Funds for the Central Universities of China.

Appendix A. Root of mean-squared amplitude of thermal vibration of a cantilevered Euler beam

For an Euler beam described by equation (2.1) in §2a, the boundary conditions for the cantilever case are

\[ w(0,t) = 0, \quad \frac{\partial w(0, t)}{\partial x} = 0, \quad \frac{\partial^2 w(L, t)}{\partial x^2} = 0 \quad \text{and} \quad \frac{\partial^3 w(L, t)}{\partial x^3} = 0. \tag{A 1} \]

The solution for the natural vibration of the \( n \)th order reads [18]

\[ w_n(x, t) = \hat{w}_n(x)e^{j\omega_nt} = D_n f_n(x)e^{j\omega_nt}, \tag{A 2} \]

where \( j \equiv \sqrt{-1}, \quad \alpha_n^4 \equiv \frac{\rho A}{EI}\omega_n^2, \quad \alpha_n L = 1.8751, 4.6941, 7.8548, 10.9955, 14.1372, \ldots \), and \( D_n \) is to be determined from initial conditions.

The total energy \( E_n \) contained in the natural vibration of the \( n \)th order can be determined by calculating the following elastic energy

\[ E_n^{\text{elastic}} = \frac{EI}{2} \int_0^L \left( \frac{\partial^2 \hat{w}_n}{\partial x^2} \right)^2 \, dx = \frac{EILD_n^2 \alpha_n^4}{8}, \tag{A 3} \]

at the instant of maximal deflection when the cantilever beam is momentarily stationary, i.e. \( e^{j\omega_nt} = 1 \). From equation (2.7), it is easy to derive

\[ D_n^2 = \frac{8\hbar v}{EIL\alpha_n^4(e^{\hbar v/kBT} - 1)}. \tag{A 4} \]

Then, the RMS amplitude of thermal vibration of the \( n \)th mode for the beam at \( x \) yields equation (2.9). The RMS amplitude of thermal vibration of SWCNT can be obtained from equation (2.10).

Appendix B. Root of mean-squared amplitude of thermal vibration of a cantilevered Timoshenko beam

For a Timoshenko beam described by equation (11) in §2b, the boundary conditions for the cantilever case are

\[ w(0,t) = 0, \quad \psi(0,t) = 0, \quad \frac{\partial^2 w(L, t)}{\partial x^2} = 0 \quad \text{and} \quad \frac{\partial^2 \psi(L, t)}{\partial x^2} = 0. \tag{B 1} \]

Following the step of simply supported case in §2b, but different from equation (2.22) for the case when \([r^2 - s^2]^2 + 4/b^2]^{1/2} > (r^2 + s^2)\), the natural frequency of the cantilever beam yields [21]

\[ 2 + \left[ b^2(r^2 - s^2)^2 + 2 \right] \cosh b\alpha_1 \cos b\alpha_2 - \frac{b(r^2 + s^2)}{(1-b^2r^2s^2)^{1/2}} \sinh b\alpha_1 \sin b\alpha_2 = 0. \tag{B 2} \]
The natural frequency $\omega_n$ of the $n$th order of the Timoshenko beam can be obtained from equation (B2) in this case.

The natural mode ($\hat{w}_n, \hat{\phi}_n$) of the $n$th order for the cantilever beam satisfies [21]

$$\hat{w}_n = D_n \hat{w}_n(\xi) = D_n \left[ \cos b_n a_{n1}^\prime \xi - \lambda_n \zeta_n \delta_n \sin b_n a_{n2} \xi - \cos b_n a_{n1} \xi + \delta \sin b_n a_{n2} \xi \right]$$ (B3a)

and

$$\hat{\phi}_n = D_n \hat{\phi}_n(\xi) = H_n \left[ \cos b_n a_{n1}^\prime \xi + \frac{\theta_n}{\lambda_n \zeta_n} \sin b_n a_{n1} \xi - \cos b_n a_{n2} \xi + \theta_n \sin b_n a_{n2} \xi \right],$$ (B3b)

where

$$H_n = \frac{b_n}{L} \frac{a_{n1}^2 + s^2}{\alpha_n} D_n,$$ (B4a)

$$\delta_n = \frac{(1/\lambda_n) \sinh b_n a_{n1} + \sin b_n a_{n2}}{\lambda_n \cosh b_n a_{n1} + \cos b_n a_{n2}},$$ (B4b)

$$\theta_n = -\frac{\lambda_n \sin b_n a_{n1} + \sin b_n a_{n2}}{(1/\zeta_n) \cosh b_n a_{n1} + \cos b_n a_{n2}},$$ (B4c)

and

$$\frac{\alpha_{n1}}{\alpha_{n2}} = \frac{1}{\sqrt{2}} \left\{ \left[ r^2 + s^2 \right] + \left[ \left( r^2 - s^2 \right) + \frac{4}{b_n^2} \right]^{1/2} \right\}^{1/2}.$$ (B4d)

When $[(r^2 - s^2)^2 + 4/b_n^2]^{1/2} < (r^2 + s^2)$ holds, the natural frequency $\omega_n$ of the $n$th order for the Timoshenko beam can be obtained from [21]

$$2 + \left[ \frac{r^2}{s^2} \frac{b_n^2}{s^2} \frac{4}{b_n^2} \right] \cos b a_1^\prime \cos b a_2 - \frac{b^2 (r^2 + s^2)}{(b^2 r^2 s^2 - 1)^{1/2}} \sin b a_1^\prime \sin b a_2 = 0.$$ (B5)

The natural mode ($\hat{w}_n, \hat{\phi}_n$) of the $n$th order for the cantilever Timoshenko beam yields

$$\hat{w}_n = D_n \hat{w}_n(\xi) = D_n \left[ \cos b_n a_{n1}^\prime \xi + \lambda_n^\prime \zeta_n \eta_n \sin b_n a_{n1}^\prime \xi - \cos b_n a_{n2} \xi + \eta_n \sin b_n a_{n2} \xi \right]$$ (B6a)

and

$$\hat{\phi}_n = D_n \hat{\phi}_n(\xi) = H_n \left[ \cos b_n a_{n1}^\prime \xi - \frac{\mu_n}{\lambda_n \zeta_n} \sin b_n a_{n1}^\prime \xi - \cos b_n a_{n2} \xi + \mu_n \sin b_n a_{n2} \xi \right],$$ (B6b)

where

$$H_n = -\frac{b_n}{L} \frac{-a_{n1}^2 + s^2}{\alpha_n} D_n,$$ (B7a)

$$\eta_n = \frac{(1/\lambda_n') \sinh b_n a_{n1} - \sin b_n a_{n2}}{\lambda_n' \cosh b_n a_{n1} + \cos b_n a_{n2}},$$ (B7b)

$$\mu_n = \frac{\lambda_n' \sin b_n a_{n1} - \sin b_n a_{n2}}{(1/\zeta_n) \cosh b_n a_{n1} + \cos b_n a_{n2}},$$ (B7c)

and

$$a_{n1}' = \frac{1}{\sqrt{2}} \left\{ \left[ r^2 + s^2 \right] - \left[ \left( r^2 - s^2 \right) + \frac{4}{b_n^2} \right]^{1/2} \right\}^{1/2}.$$ (B7d)

In equations (B2)–(B7), the following expressions hold true

$$\zeta_n = \frac{a_{n1}^2 + r^2}{a_{n1}^2 + s^2} = \frac{a_{n1}^2 - s^2}{a_{n1}^2 - r^2} = \frac{a_{n2}^2 + r^2}{a_{n2}^2 - s^2} = \frac{a_{n2}^2 + s^2}{a_{n2}^2 - r^2},$$ (B8a)

and

$$\lambda_n = \frac{a_{n1}}{a_{n2}} = \frac{1}{\lambda_n'}. $$ (B8b)

Following the same step from equation (2.25) to equation (2.26), the RMS amplitude of thermal vibration of the $n$th mode for the beam at $x$ yields equation (2.27) in §2b. The RMS amplitude of thermal vibration of an SWCNT at $x$ can be obtained by using equation (2.10) of §2a.
References

4. Treacy MMJ, Ebbesen TW, Gibson JM. 1996 Exceptionally high Young’s modulus observed for individual. Nature 381, 678–680. (doi:10.1038/381678a0)