Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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Lecture 16

Last lecture

- Completed the calculation of interaction energy per unit length for two nanotubes
- Looked at a nanotube@nanotube oscillator
- Derived expressions for the interaction energy and force

Nanotube@nanotube oscillator - recap

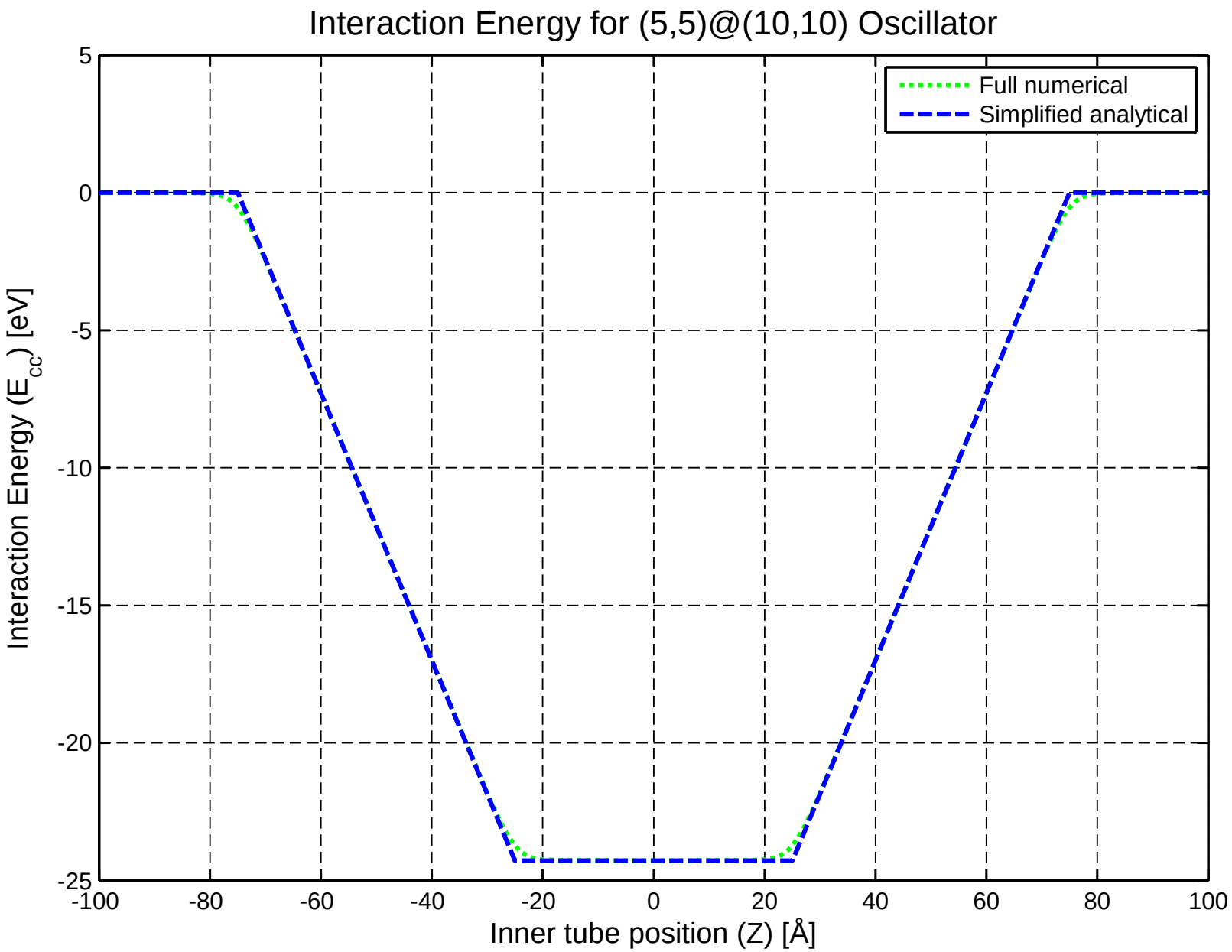
Interaction Energy

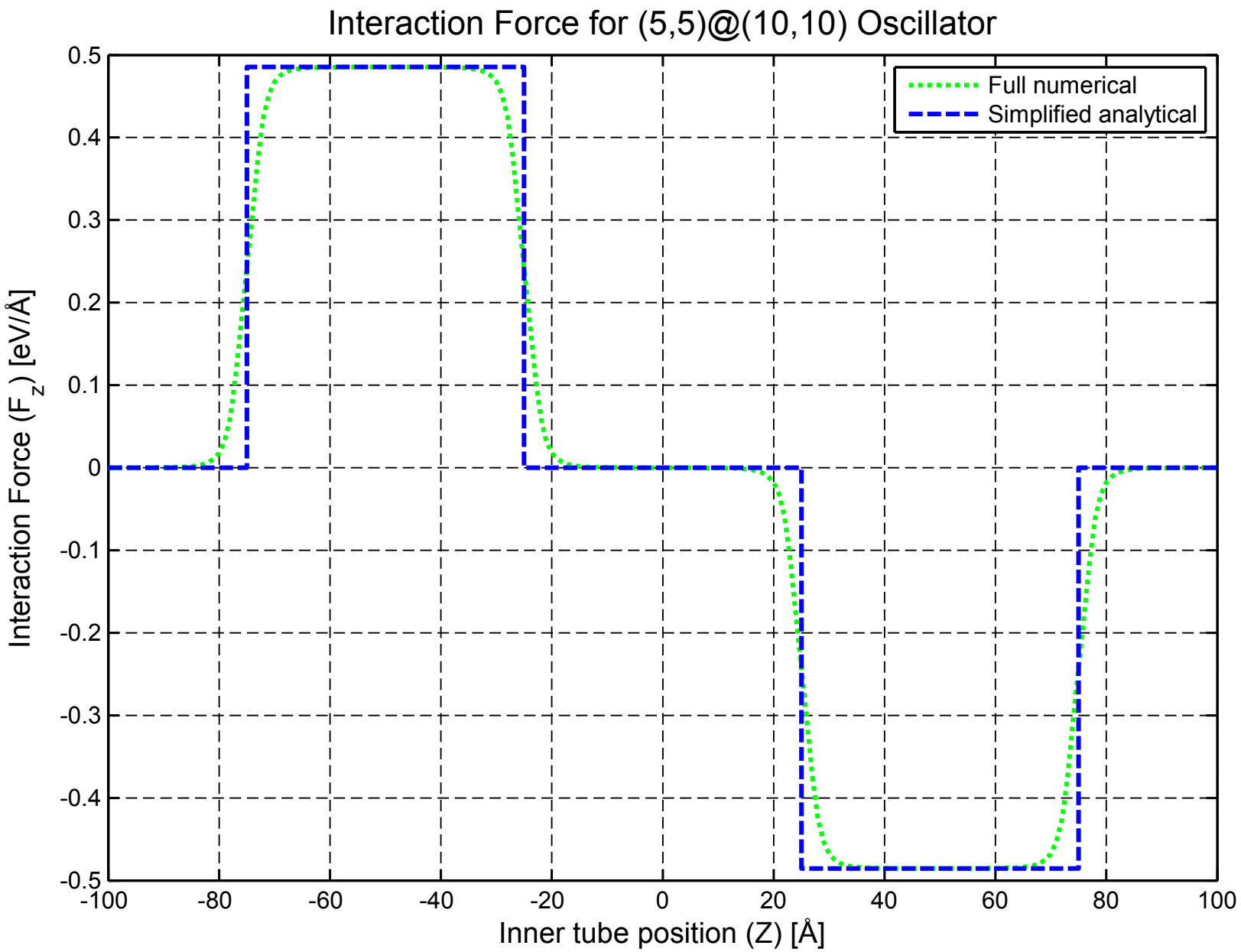
$$E_{cc} = E_{cc}^{\star}\left[(Z+L_+)H(Z+L_+) - (Z+L_-)H(Z+L_-)\right.$$
$$\left. -(Z-L_-)H(Z-L_-) + (Z-L_+)H(Z-L_+)\right],$$

where $L_+ = L_2 + L_1$ and $L_- = L_2 - L_1$. Also recall that $E_{cc}^{\star}$ is the interaction energy per unit length for the two nanotubes.

Force

$$F_z = -E_{cc}^{\star}\left[H(Z+L_+) - H(Z+L_-)\right.$$
$$\left. -H(Z-L_-) + H(Z-L_+)\right].$$


Interaction Energy for (5,5)@(10,10) Oscillator
Full numerical
Simplified analytical
Interaction Energy (E_{cc}) [eV]
Inner tube position (Z) [Å]
5
0
-5
-10
-15
-20
-25
-100
-80
-60
-40
-20
0
20
40
60
80
100

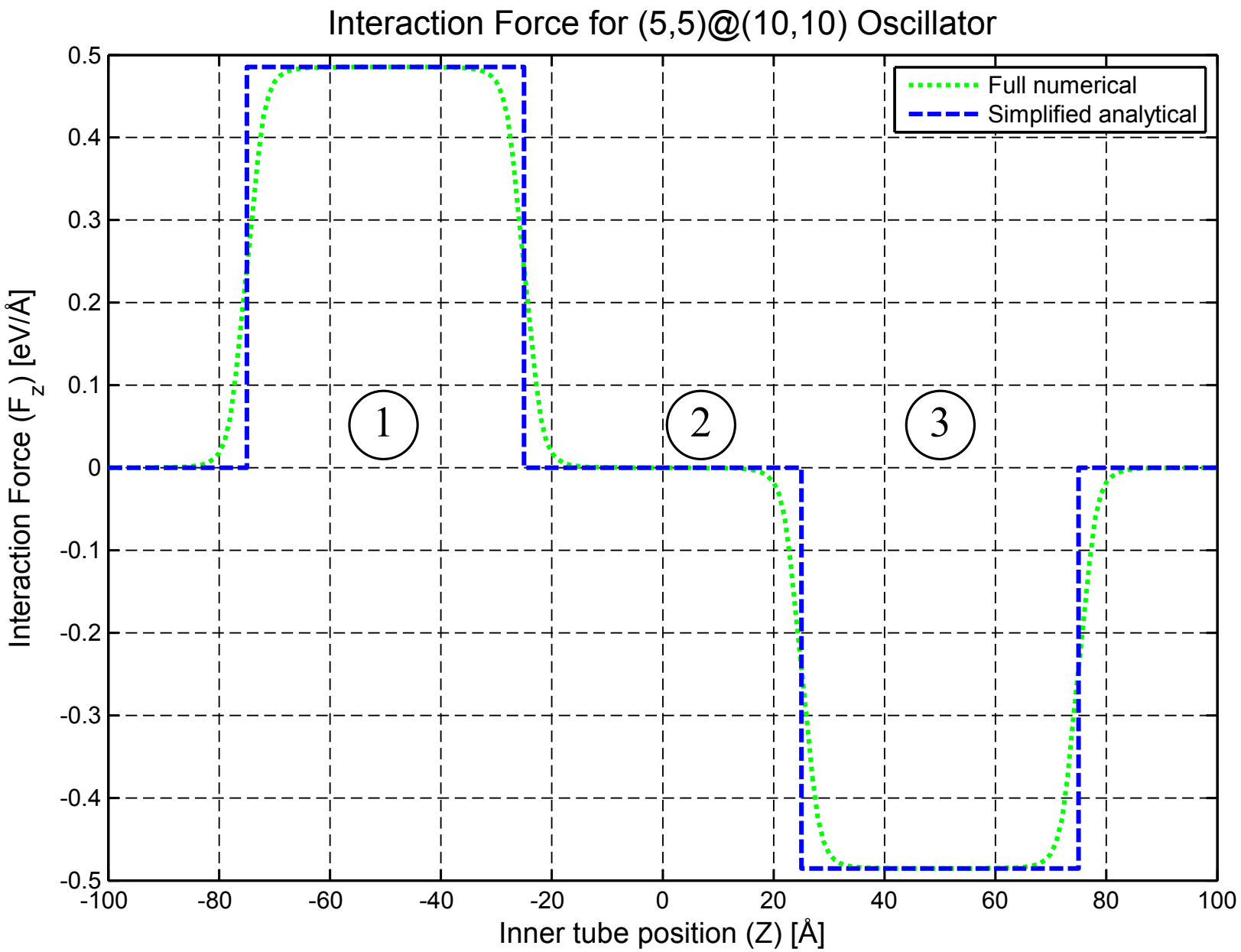

Interaction Force for (5,5)@(10,10) Oscillator
Full numerical
Simplified analytical
Interaction Force (F_z) [eV/Å]
Inner tube position (Z) [Å]
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-100
-80
-60
-40
-20
0
20
40
60
80
100

Oscillatory Behaviour

Newton's second law is also adopted here to describe the behaviour of a double-walled nanotube oscillator. We are interested in the case of a fixed outer nanotube and the inner nanotube is initially pulled out a distance d and then released.

We approximate the van der Waals force experienced by the oscillating tube using the Heaviside unit step function and we assume that the inner nanotube travels through three regions.

1. Region of fixed positive force (Constant acceleration)
2. Region of zero net force (Zero acceleration)
3. Region of fixed negative force (Constant deceleration)


Interaction Force for (5,5)@(10,10) Oscillator
Full numerical
Simplified analytical
1
2
3
Interaction Force (F_Z) [eV/Å]
Inner tube position (Z) [Å]
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-100
-80
-60
-40
-20
0
20
40
60
80
100

1. Constant Acceleration

Here we have from Newton's second law

$$M\frac{\mathrm{d}^2 Z}{\mathrm{d}t^2} = -E^{\star}_{cc} = \frac{W}{d},$$

where M denotes the mass of the oscillating nanotube.

We assume the inner nanotube is initially at rest at $Z = L_1 - L_2 - d$, where d is an extrusion distance. We may derive a velocity for this region as given by

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = \frac{W}{Md}t,$$

and therefore the position is given by

$$Z = L_1 - L_2 - d + \frac{W}{2Md}t^2.$$

Solving for the boundary between the first and second region $Z = L_1 - L_2$ we find the tube spends

$$t_1 = d\sqrt{\frac{2M}{W}},$$

time in region one, at the end of which time it is travelling at a velocity of

$$\left.\frac{\mathrm{d}Z}{\mathrm{d}t}\right|_{t=t_1} = \sqrt{\frac{2W}{M}}.$$

2. Zero Acceleration

In region two the oscillating nanotube experiences no net force and therefore it travels between $Z = L_1 - L_2$ and $Z = L_2 - L_1$ at the terminal speed from region one.

The total distance travelled is $2L_2 - 2L_1$ and therefore the total time spend in this region is

$$t_2 = 2(L_2 - L_1)\sqrt{\frac{M}{2W}}.$$

3. Constant Deceleration

In the third region the nanotube will be slowed down at the same rate as it was accelerated in region one. Therefore the time taken for it to slow to a stop will be the same as t_1 from the region one calculation. At this point in time the nanotube will now be at the location $Z = L_2 - L_1 + d$ and by symmetry the whole process will repeat for the return journey.

Therefore the total period of oscillation T is given by

$$\begin{aligned} T &= 4t_1 + 2t_2 = 4d\sqrt{\frac{2M}{W}} + 4(L_2 - L_1)\sqrt{\frac{M}{2W}} \\ &= 4(L_2 - L_1 + 2d)\sqrt{\frac{M}{2W}}. \end{aligned}$$

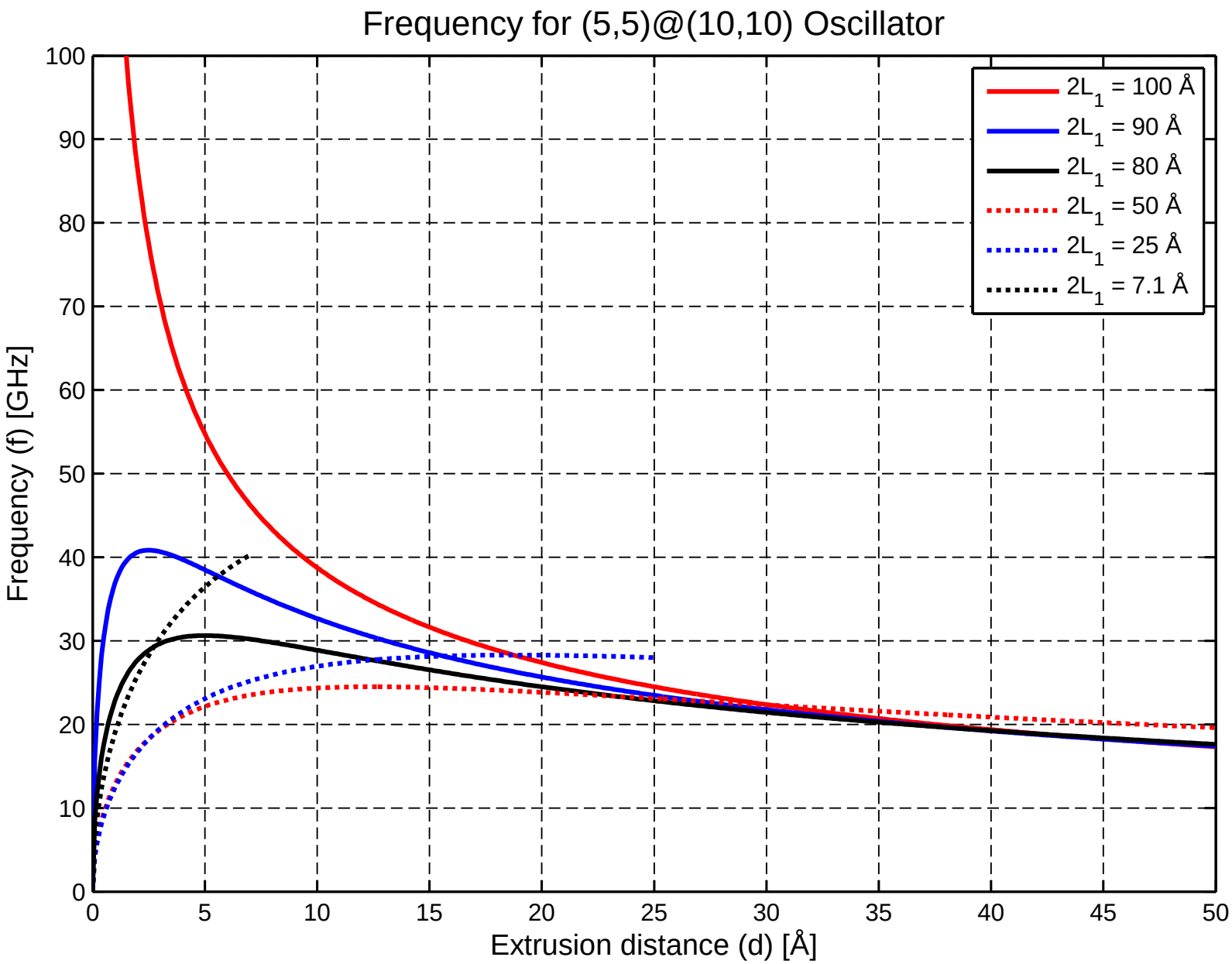
Oscillatory Frequency

The frequency f is nothing more than the reciprocal of the period T and therefore the frequency of the oscillation is given by

$$f = \frac{1}{4(L_2 - L_1 + 2d)}\sqrt{\frac{2W}{M}},$$

where we should remember that W also depends on d via the relationship $W = -E^{\star}_{cc}d$.

On the next slide we graph f for (5,5)@(10,10) oscillators with $2L_2 = 100$ Å and various length of the oscillating nanotube $2L_1$, and for a range of extrusion distance d.


Frequency for (5,5)@(10,10) Oscillator
Frequency (f) [GHz]
Extrusion distance (d) [Å]
0
10
20
30
40
50
60
70
80
90
100
0
5
10
15
20
25
30
35
40
45
50
2L1 = 100 Å
2L1 = 90 Å
2L1 = 80 Å
2L1 = 50 Å
2L1 = 25 Å
2L1 = 7.1 Å

As can be seen on the previous graph, the frequency in singular when $L_1 = L_2$ and the extrusion distance $d \to 0$. This is due to the oscillator making faster and faster, low amplitude oscillations and in the limit of the amplitude approaching zero the frequency approaches infinity. This is not a physically relevant result since we are using a step function approximation for the force profile which is in reality smooth. Furthermore small amplitude oscillations occur in practice anyway but they are too fast and small to reliably measure and therefore of no practical interest.

Also note that for the short oscillating nanotubes we cut off at the maximum extrusion distance of $d_{max} = 2L_1$. This is because a larger extrusion distance would completely dislocate the inner tube and lead to failure of the oscillator.

Variational approach

We could pose the problem as one of finding the position of the inner tube as a function of time $Z(t)$. The kinetic energy would be

$$K = \frac{1}{2} M \dot{Z}^2,$$

and the potential energy

$$\begin{aligned} V = E_{cc}^{\star} \left[(Z + L_+) H(Z + L_+) - (Z + L_-) H(Z + L_-) \right. \\ \left. -(Z - L_-) H(Z - L_-) + (Z - L_+) H(Z - L_+) \right], \end{aligned}$$

The Lagrangian would be $\mathcal{L} = K - V$. So the action would be given by

$$F\{Z(t)\} = \int (K - V)\, dt,$$

and by Hamilton's principle the path of the tube would be an extremal of the action.

As we saw earlier since K and V are independent of t we may write that

$$\begin{aligned} \dot{Z}\frac{\partial \mathcal{L}}{\partial \dot{Z}} - \mathcal{L} &= \text{const} \\ M\dot{Z}^2 - K + V &= \text{const} \\ K + V &= \text{const.} \end{aligned}$$

In other words, the sum of kinetic and potential energy is conserved.

So if we take the initial energy to be give by W (the work done to extrude the inner tube a distance d,

$$W = -dE^{\star}_{cc}.$$

and the kinetic energy is initially zero. So the constant above is $W + 2L_1 E^{\star}_{cc}$.

Then we can write an expression for the kinetic energy of the inner tube at any location Z as

$$\begin{aligned}
K &= W + 2L_1 E^\star_{cc} - V \\
&= (2L_1 - d)E^\star_{cc} - E^\star_{cc}\,[\,(Z+L_+)H(Z+L_+) - (Z+L_-)H(Z+L_- \\
&\quad -(Z-L_-)H(Z-L_-) + (Z-L_+)H(Z-L_+)] \\
&= -E^\star_{cc}\,[\,d - 2L_1 + (Z+L_+)H(Z+L_+) - (Z+L_-)H(Z+L_-) \\
&\quad -(Z-L_-)H(Z-L_-) + (Z-L_+)H(Z-L_+)] \\
&= k(Z).
\end{aligned}$$

And since $K = M\dot{Z}^2/2$, from this we can derive that

$$\dot{Z} = \sqrt{\frac{2k(Z)}{M}}.$$

Period of oscillation

We can't do too much with this formula for $\dot{Z}$ in terms of a general expression for Z as an explicit function of t but we can determine the period of oscillation since the time to travel from a starting position from the left to a stationary position on the right may be expressed as an integral in Z.

$$\begin{aligned}\frac{1}{2}T &= \int_{-L_- -d}^{L_- +d} \frac{ds}{v} = \int_{-L_- -d}^{L_- +d} \frac{dZ}{\dot{Z}} \\ &= \int_{-L_- -d}^{-L_-} \frac{dZ}{\dot{Z}} + \int_{-L_-}^{L_-} \frac{dZ}{\dot{Z}} + \int_{L_-}^{L_- +d} \frac{dZ}{\dot{Z}}.\end{aligned}$$

In each of these regions $\dot{Z}$ is a simple function of Z

In each of these regions k (and hence $\dot{Z}$) is a simple function of Z

$$k(Z) = \begin{cases} -E^{\star}_{cc}\left(d + L_{-} + Z\right), & -L_{-} - d \leqslant Z \leqslant -L_{-} \\ -E^{\star}_{cc} d, & -L_{-} \leqslant Z \leqslant L_{-} \\ -E^{\star}_{cc}\left(d + L_{-} - Z\right), & L_{-} \leqslant Z \leqslant L_{-} + d \end{cases}$$

So returning to our integrals we have

$$\frac{1}{2}T = \sqrt{-\frac{M}{2E^{\star}_{cc}}}\left\{\int_{-L_{-}-d}^{-L_{-}} \frac{dZ}{\sqrt{d + L_{-} + Z}} + \int_{-L_{-}}^{L_{-}} \frac{dZ}{\sqrt{d}} + \int_{L_{-}}^{L_{-}+d} \frac{dZ}{\sqrt{d + L_{-} - Z}}\right\}.$$

$$\frac{1}{2}T = \sqrt{-\frac{M}{2E^{\star}_{cc}}}\left\{\left[2\sqrt{d+L_-+Z}\right]_{-L_--d}^{-L_-} + \left[\frac{Z}{\sqrt{d}}\right]_{-L_-}^{L_-} + \left[-2\sqrt{d+L_--Z}\right]_{L_-}^{L_-+d}\right\}$$

$$= \sqrt{-\frac{M}{2E^{\star}_{cc}}}\left\{2\left[\sqrt{d}-0\right] + \frac{1}{\sqrt{d}}\left[L_- - (-L_-)\right] - 2\left[0-\sqrt{d}\right]\right\}$$

$$= 2\sqrt{-\frac{M}{2E^{\star}_{cc}d}}\left(2d+L_-\right).$$

And so the period of oscillation is (as before)

$$T = 4\sqrt{\frac{M}{2W}}\left(2d+L_2-L_1\right).$$

Extensions

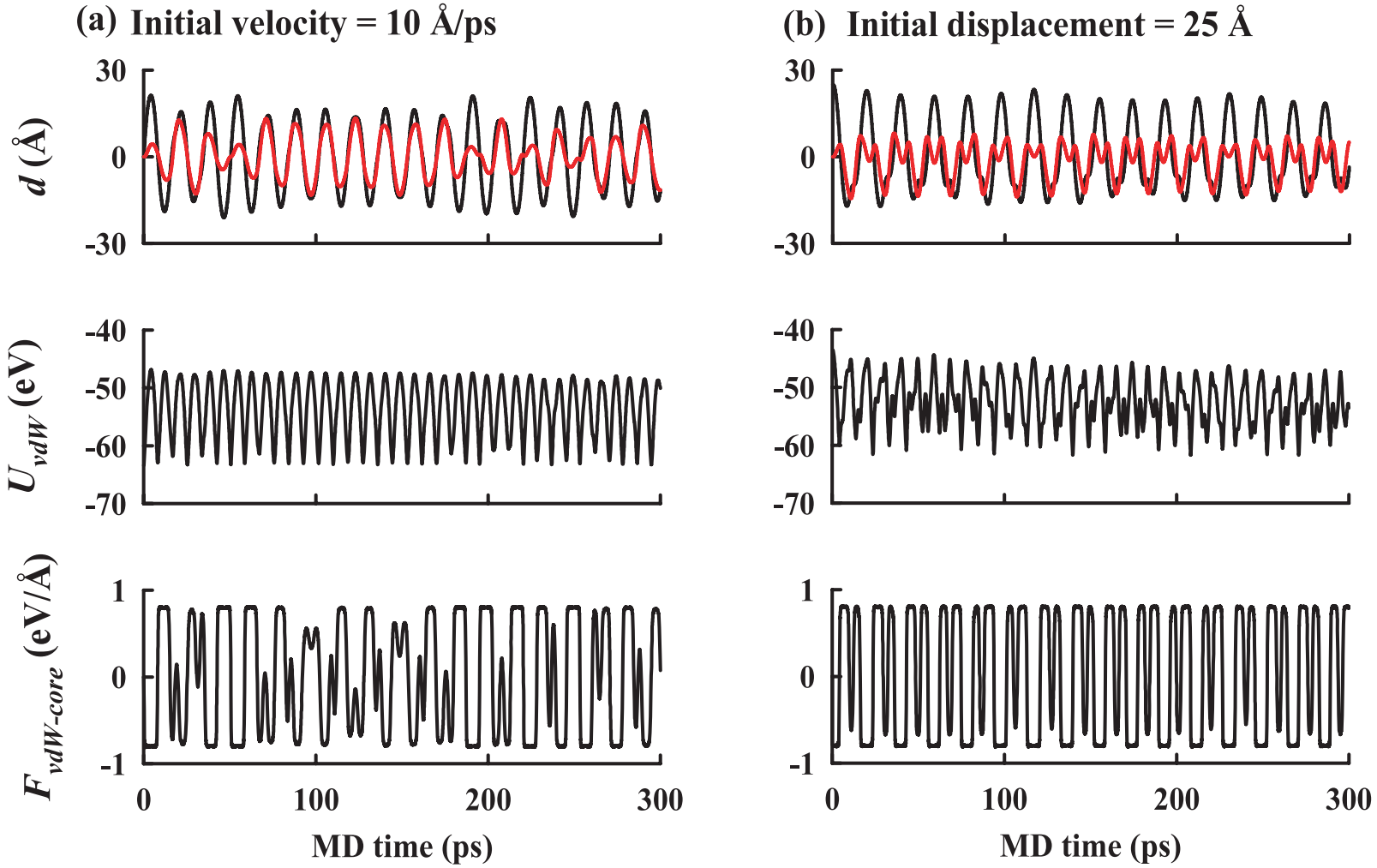
In the previous calculations we have assumed that the outer nanotube was fixed which reduced the problem to a single variable problem in 1D. We could have looked at the dynamics if both nanotubes were free to move.

In this case if assume both tubes were initially at rest the would both move towards each other and the centre of mass of the whole system would be constant.

Another possibility would be to have a multi-walled nanotube with more than two shells. You could have one with three, four, etc, shells all oscillating in response to the interaction with one another.

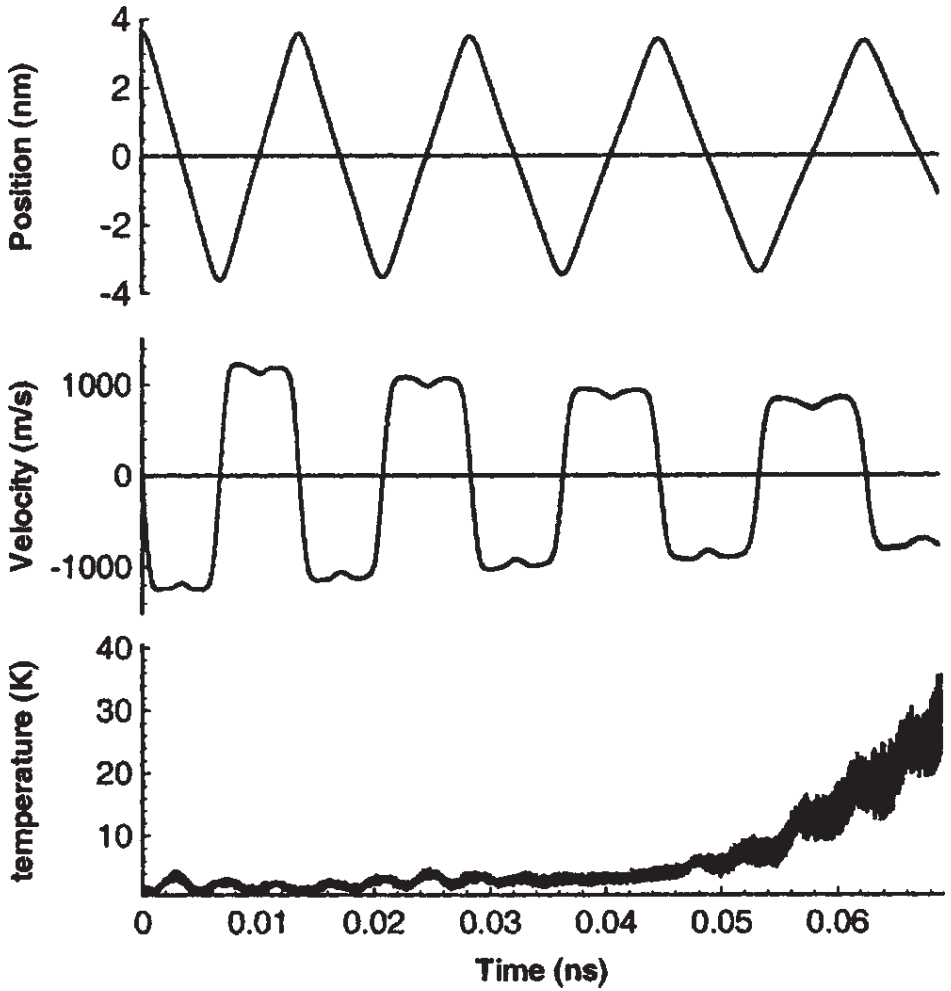
Lastly, would could consider a fullerene C_{60} as a very small nanotube and so how would a C_{60}@nanotube oscillator behave?

Triple-walled oscillator



From: Kang & Lee *Nanotechnology* **19** (2008) 285704

Fullerene@nanotube oscillator



From: Liu, Zhang & Lu *Journal of Applied Physics* **97** (2005) 094313