Variational Calculus and its applications in Control Theory and Nanomechanics
Professor Sarthok Sircar

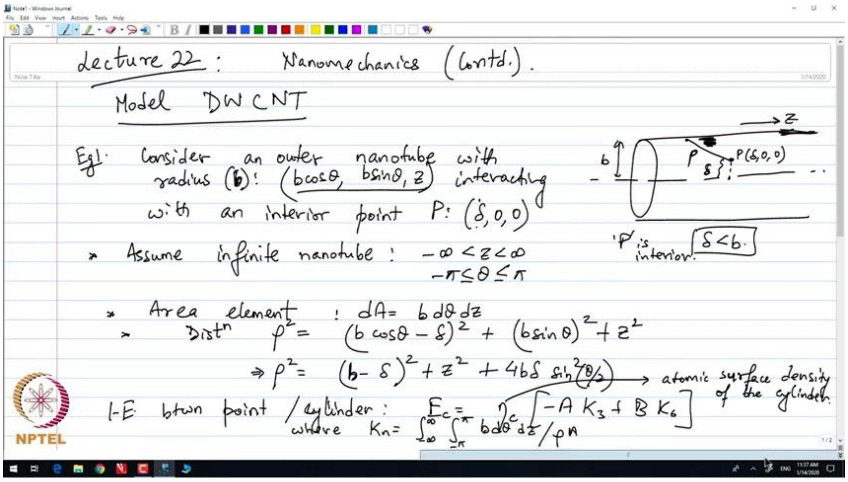
Department of Mathematics

Indraprastha Institute Of Information Technology

Lecture 64 Introduction to Nanomechanics Part 4

So, good afternoon everyone. So, in today's lecture which is the last lecture of our lecture series, we are going to continue our discussion on the modelling of nano rod oscillators.

(Refer Slide Time: 0:29)



So, let me just continue our discussion from our previous lecture. So, in my first example I am going to model a double walled carbon nanotube. So our goal is, to model an oscillatory double walled carbon nanotubes. So the first example that I have today is, we are going to look at the interaction of a carbon nanotube, let me draw the figure so we have a carbon nanotube it has a radius b, so it is a cylindrical shell and suppose I am given a point P which is (δ, 0, 0) and P is at a distance of δ from the axis of the cylinder and further, I assume that δ is less than B. So I want to model the interaction of this point, let say a carbon atom with the outer cylinder. So, the setup is as following, so consider an outer nanotube with radius b given by (b $\cos\theta$, b $\sin\theta, z$. So, consider an outer nanotube with this coordinates, we are only looking at a tube which is the shell, so it is a cylindrical shell so b is fixed interacting with an interior point, P which is (δ, 0, 0). Further assume that, we have an infinite nanotube, which means that my z axis is from minus infinity to infinity and my angular co-ordinate θ will be from minus π to plus π including the end points. Then let me just write down my area element for the interaction. Any area element on the cylinder is $dA = bd\theta dz$. So to evaluate the interaction energy we use the Lennard-Jones interaction energy and for Lennard-Jones we have to find the distance of this point P to any point on the cylinder, so let me denote this by ρ. So the distance row is given by

$$\rho^2 = (b\cos\theta - \delta)^2 + (b\sin\theta)^2 + z^2$$

$$\text{Thus,} \qquad \rho^2 = (b-\delta)^2 + z^2 + 4b\delta\sin^2(\theta/2)$$

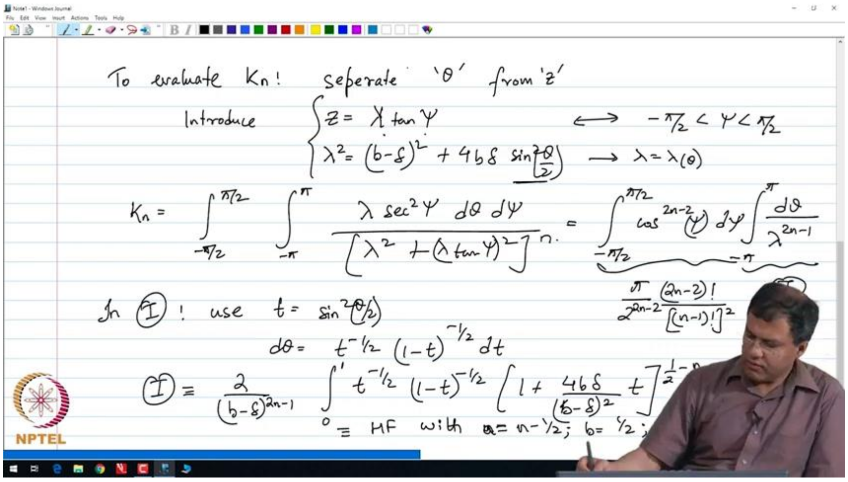
So then, so we are ready to write down our interaction energy. The interaction energy between the point and the cylinder is:

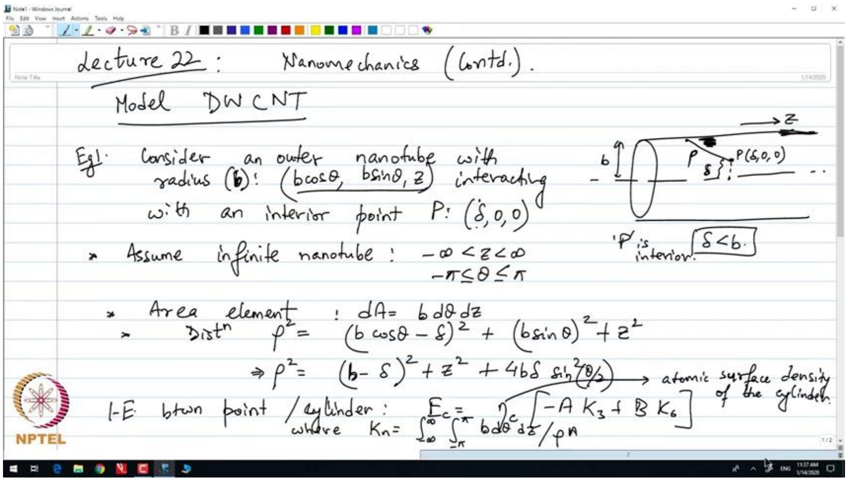
$$E_c = \eta_c[-AK_3 + BK_6]$$

$$\text{where,} \qquad K_n = \int_{-\infty}^{\infty}\int_{-\pi}^{\pi} bd\theta dz/\rho^n$$

So, I have to integrate and find this value of K_n, so let us do that quickly because that will be required later on and before I do that, I also need to mention that η_c is the atomic surface density of the cylinder or is the number of atoms per unit area.

(Refer Slide Time: 7:30)





So then let us separate two interactions, so I need to evaluate the integral K_n. To evaluate K_n, I see that I separate the θ from z in my integration. So to do that, let me introduce the following variables,

$$
\begin{aligned}
z &= \lambda \tan\psi, \qquad -\pi/2 < \psi < \pi/2 \\
\lambda^2 &= (b-\delta)^2 + 4b\delta \sin^2(\theta/2), \qquad \lambda = \lambda(\theta) \\
\text{Thus, } K_n &= \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} \frac{\lambda \sec^2 \psi d\theta d\psi}{[\lambda^2 + (\lambda \tan\psi)^2]^n} \\
&= \int_{-\pi/2}^{\pi/2} \cos^{2n-2}(\psi) d\psi \int_{-\pi}^{\pi} \frac{d\theta}{\lambda^{2n-1}}
\end{aligned}
$$

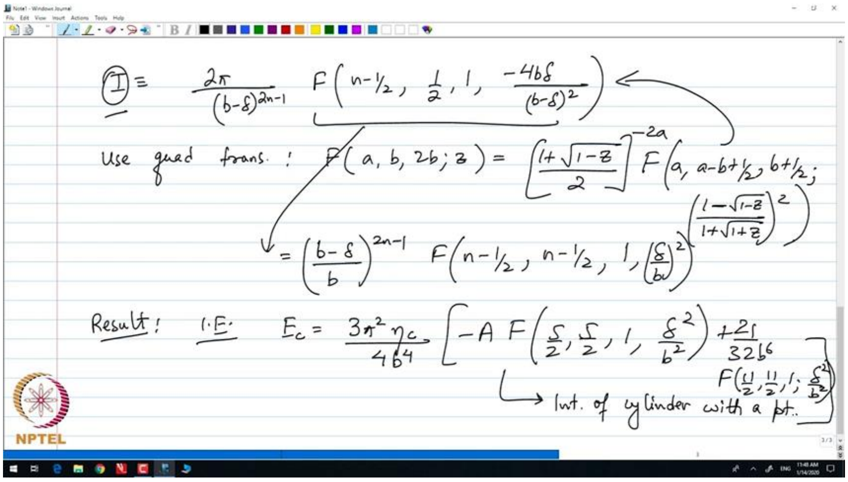
Note that, λ is a function of θ itself, so I have separated out ψ and θ. So the first integral is quite straight forward to evaluate and we see that the value is:

$$\frac{\pi}{2^{2n-2}} \frac{(2n-2)!}{[(n-1)!]^2}$$

Let me call this second integral by I, so all I have to do is to integrate this integral which is given by I. For this, we have to do another substitution, so use:

$$t = \sin^2(\theta/2)$$
$$d\theta = t^{-1/2}(1-t)^{-1/2}dt$$
$$\text{Thus,} \qquad I = \frac{2}{(b-\delta)^{2n-1}} \int_0^1 t^{-1/2}(1-t)^{-1/2}\left[1+\frac{4b\delta}{(b-\delta)^2}t\right]^{1/2-n}$$

(Refer Slide Time: 13:28)



$$I = \frac{2\pi}{(b-\delta)^{2n-1}} F\left(n-1/2, 1/2, 1, \frac{-4b\delta}{(b-\delta)^2}\right)$$

So notice that this form of hypergeometric function is slightly more complicated and I am going to use my quadratic transformation discussed in my previous lecture to simplify this further. Use our quadratic transformation which was

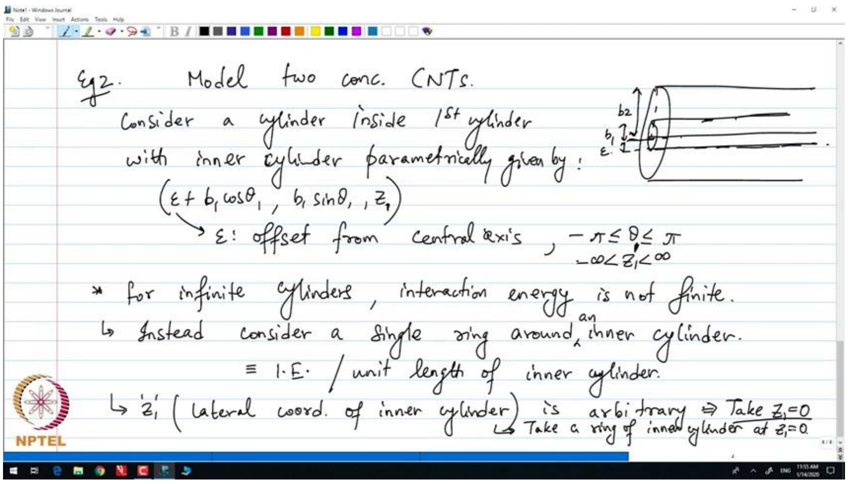
$$F(a,b,2b;z) = \left[\frac{1+\sqrt{1-z}}{2}\right]^{-2a} F\left(a, a-b+1/2, b+1/2; \left(\frac{1-\sqrt{1-z}}{1+\sqrt{1+z}}\right)^2\right)$$
$$= \left(\frac{b-\delta}{b}\right)^{2n-1} F\left(n-1/2, n-1/2, 1, (\delta/b)^2\right)$$

So, then I club all my results together I found all the other values of the integral so my result is that the interaction energy after plugging in all the values of the integral is

$$E_c = \frac{3\pi^2\eta_c}{4b^4}\left[-AF\left(5/2, 5/2, 1, \delta^2/b^2\right) + 21/32b^6 F\left(11/2, 11/2, 1, \delta^2/b^2\right)\right]$$

So that is the interaction of a cylinder with a point. So then, next we are going to describe the interaction of two carbon nanotubes.

(Refer Slide Time: 17:16)

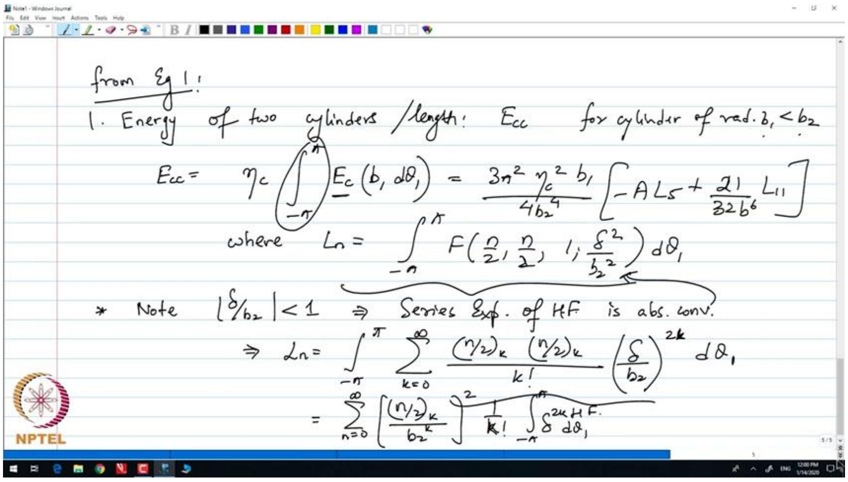


So now I am in a case where I have to model two concentric carbon nanotubes. Let us assume I have an outer nanotube or a cylindrical shell with a radius b_2 and then I have an inner shell of radius b_1. So I have an outer shell and an inner shell. So the setup of the problem is as follows we consider a cylinder inside the first cylinder and I also further assume my original axis is at an offset epsilon. So let me consider a cylinder inside the first cylinder with the inner cylinder parametrically given by $(\epsilon + b_1 \cos\theta_1, b_1 \sin\theta_1, z_1)$ where I assume that ϵ is my offset from the concentric axis which is the common axis of the non offsetted concentric cylinders. So ϵ is an offset, from I would say from the central axis which is a common to both the concentric cylinders. So then further I have that

$$-\pi \le \theta_1 \le \pi$$
$$-\infty < z_1 < \infty$$

So the solution is as follows, we need to look at the interaction of these two infinite cylinders. So well of course the first observation is that when we are modelling two infinite cylinders, we have to essentially do an infinite integration of the interaction terms which is finite, which we found out in the previous example for point with a cylinder, which means that the answer that we are going to get for the interaction between two infinite cylinder is infinity. So again which means that we have to look for interaction energy per unit area, and we are going to evaluate the interaction energy of per unit area of the inner cylinder. So again, let me just highlight what I just said the interaction energy for infinite cylinder is not finite. Instead we are going to consider a single ring of the inner cylinder interacting with an outer cylinder. So essentially we are saying that we are going to calculate the interaction energy per unit length of the inner cylinder. So then, since z_1 is the z coordinate of the of any point on the surface of the inner cylinder. So we are going to take without loss of generality that z_1 is 0. So in that case all I have to do is use our previous result for the point cylinder interaction case and integrate it over all points on this perimeter or this rim which will be $2\pi b(b\theta)$.

(Refer Slide Time: 24:18)



So what I just said is in our previous example from example 1, that we discussed few minutes back, we see that the interaction energy of two cylinders per unit length is given by E_{cc} for cylinders of radius b_1 less than b_2 is:

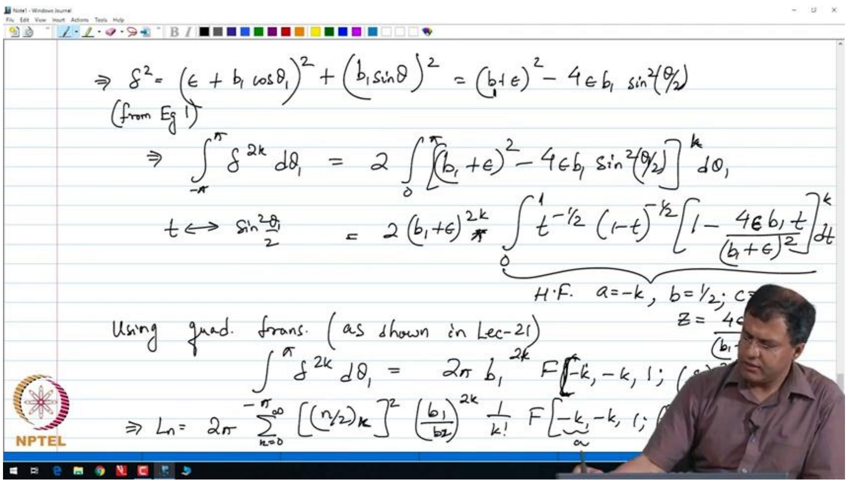
$$\begin{aligned} E_{cc} &= \eta_c \int_{-\pi}^{\pi} E_c(b_1 d\theta_1) \\ &= \frac{3\pi^2\eta_c^2 b_1}{4b_2^4}\Big[-AL_5 + \frac{21}{32b^6}L_{11}\Big] \\ \text{where,} \qquad L_n &= \int_{-\pi}^{\pi} F(n/2, n/2, 1; \delta^2/b_2^2)d\theta_1 \end{aligned}$$

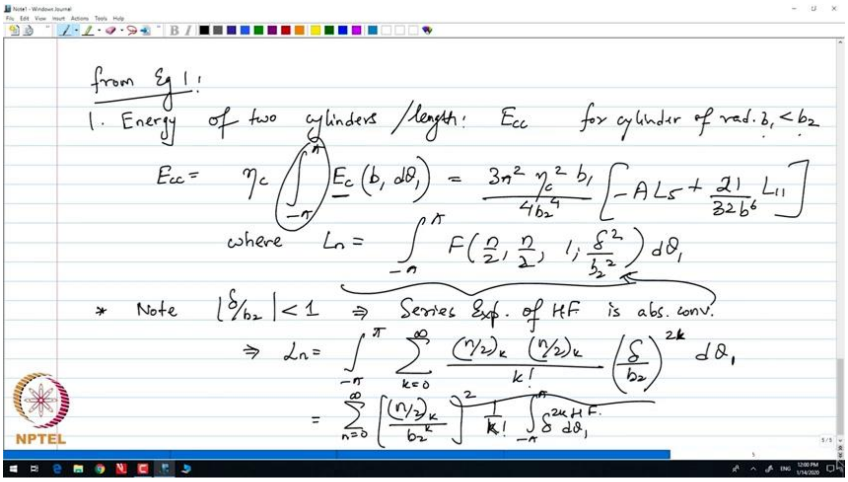
So notice we make few observations, note that $|\delta/b_2| < 1$ because δ is a point on the inner cylinder, which means that my series expansion of the hypergeometric function is going to be absolutely convergent. Let me write down this hypergeometric function now.

$$\begin{aligned} L_n &= \int_{-\pi}^{\pi} \sum_{k=0}^{\infty} \frac{(n/2)_k(n/2)_k}{k!}(\delta/b_2)^{2k} d\theta_1 \\ &= \sum_{n=0}^{\infty}\Big[\frac{(n/2)_k}{b_2^k}\Big]^2 \frac{1}{k!}\int_{-\pi}^{\pi}\delta^{2k}d\theta_1 \end{aligned}$$

So all I have to do is to integrate this inner integral and put it in this summation to sum it up.

(Refer Slide Time: 29:24)





Thus,

$$
\begin{aligned}
\delta_2 &= (\epsilon + b_1 \cos\theta_1)^2 + (b_1 \sin\theta)^2 \\
&= (b+\epsilon)^2 - 4\epsilon b_1 \sin^2(\theta/2)
\end{aligned}
$$

$$
=> \qquad \int_{-\pi}^{\pi} \delta^{2k} d\theta_1 = 2\int_0^{\pi} [(b_1+\epsilon)^2 - 4\epsilon b_1 \sin^2(\theta/2)]^k d\theta_1
$$

Replace, $\sin^2(\theta_1/2)$ by t,

$$
= 2(b_1+\epsilon)^{2k}\pi \int_0^1 t^{-1/2}(1-t)^{-1/2}\left[1 - \frac{4\epsilon b_1 t}{(b_1+\epsilon)^2}\right]^k dt
$$

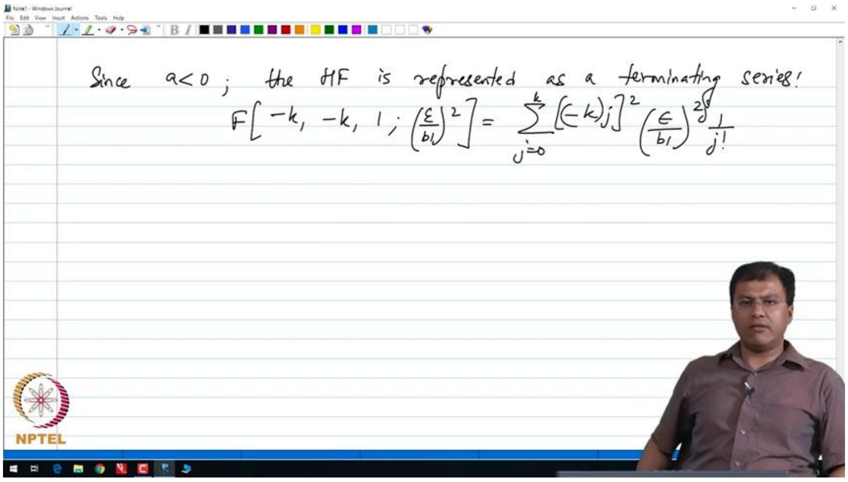
So notice that again we have been left with a hypergeometric function this integral is a hypergeometric function with the argument $a = -k, b = 1/2; c = 1$ and $z = \frac{4\epsilon b_1}{(b_1+\epsilon)^2}$. So then, I can rewrite my integral:

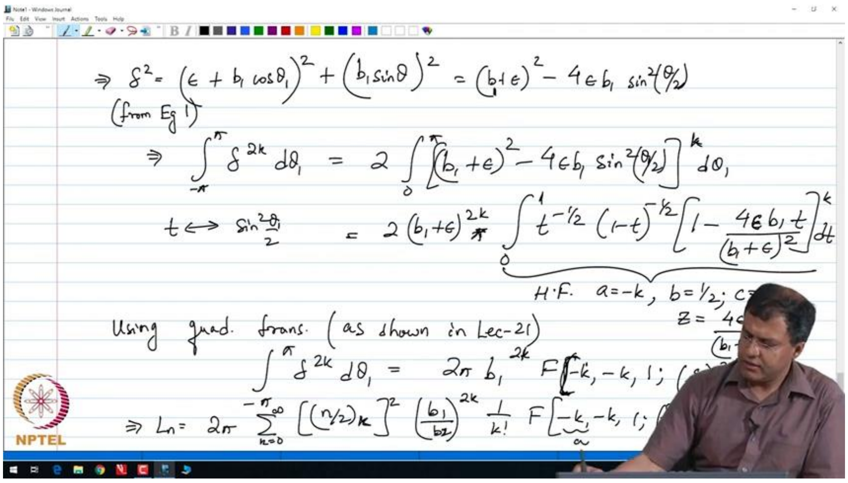
$$
\int_{-\pi}^{\pi} \delta^{2k} d\theta_1 = 2\pi b_1^{2k} F[-k, -k, 1; (\epsilon/b_1)^2]
$$

$$
\text{Thus,} \qquad L_n = 2\pi \sum_{k=0}^{\infty} \left[(n/2)_k\right]^2 \left(\frac{b_1}{b_2}\right)^{2k} \frac{1}{k!} F[-k, -k, 1; (\epsilon/b_1)^2]
$$

So to note that there is one last piece of observation note, so I have found the value of L_n and then I plug all these values of L_n into these expressions that I have found to begin with. Note that the argument here of this hypergeometric functions they are negative, which means that the hypergeometric function is going to terminate after finite number of terms.

(Refer Slide Time: 35:19)





Since a is less than 0, then the hypergeometric function is represented as a terminating series and I see that

$$F[-k,-k,1;(\epsilon/b_1)^2]=\sum_{j=0}^{k}[(-k)_j]^2\left(\frac{\epsilon}{b_1}\right)^{2j}\frac{1}{j!}$$

So that is what we have and then we plug all these hypergeometric functions into our previous result to figure out the value of a L_n's and then finally the interaction energy. So now, we are now quite set to describe the model of two oscillatory concentric carbon nanotubes.