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

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## Lecture 65 Introduction to Nanomechanics Part 5

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Since $a < 0$ ; the HF is represented as a terminating series! $F\left[-k, -k, 1; \left(\frac{\varepsilon}{b_{l}}\right)^{2}\right] = \sum_{j=0}^{k} \left[(-k)^{2}_{j}\right]^{2} \left(\frac{\varepsilon}{b_{l}}\right)^{2}_{j!}$
Modeling Nanotube inside Nanotube Oscillator:
* In this device, a DW CNT starts with (")
its inner tube extruded by a distrid, and the second secon
out of fixed, open-ended outer carbon Manotube. La Excess, van-der Waal force sucks inner nanotube back.
La Excess, van-der Waal force sucks inner nanotube back.
(*) Ly Reversal of dir" at the opposite end. of the outer nanotube. which returns oscillatory innortube back to its starting location.
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The questions is whether the motion is going to start? So what is the condition for the starting of the oscillatory motion and then the second question is what is the minimum energy that is required to start the motion of the oscillatory nanotube and finally how can we describe the motion of these oscillatory nanotubes. So, I am going to describe this model first by standard Newtonian mechanics and then later on I am going to describe the same model using our variational calculus and to come up at the same result that we began with. So, we are going to start our description of the model of the oscillatory nanotube inside nanotube oscillator. Let me just draw two nanotubes and I see that inner nanotube is as shown in figure above. So, this is at the a distance 'd' and this will be drawn outside and then also drawn inside. So, in this device what we have is a double-walled nanotube oscillator and it starts when we pull the inner nanotube by a certain distance, let us say 'd' and then we are going to assume in this motion that this pulling is not that much that the inner nanotube completely comes out of the outer nanotube or we are assuming that there are no edge effects of the outer nanotube with the inner nanotube, otherwise if the entire inner nanotube gets pulled out we expect that the motion is going to stop and the model is going to fail. So in this device a double-walled carbon nanotube starts with its inner tube extruded by a distance by a distance 'd' which means that the moment we pull out the inner nanotube we expect that the Van der Waals interaction energy or the Van der Waals force that is generated due to this pulling out effect is going to suck the inner nanotube back into the outer nanotube, however, due to inertia the motion will continue inside the outer nanotube and the the inner nanotube will go partially out from the other end and then due to inertia the motion is going to again repeat and we will get a cycle or the oscillatory cycle. So my excess Van der Waals force sucks the inner nanotube back and I see that there is a reversal of the direction at the opposite end of the outer nanotube because of the inertia itself, which returns the oscillatory inner nanotubes back to its starting location. So that is the motion that we are going to try to model.

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be sucked into outer manotube How much energy is picked up by the ascillation will be oscillatory freg. inner d po manortubes only interact Assume 100 of inner nested inner tube.  $(\Rightarrow)$ Ans. 91 🖿 🧿 🕺 🖬 🧶

Okay, so then as I said we have to answer three questions, let me write down those questions. So, the first question that is to be answered is, will the inner nanotube be sucked into outer nanotube and we call this as my acceptance condition and the second question is how much energy is picked up how much energy is picked up by the oscillating nanotube and the third question that we want to answer is what is how can we quantify this oscillatory motion or for example, what is the oscillatory time period or the oscillatory frequency of this motion.

So, what will be the oscillatory frequency of this motion. So the assumption is the two nanotubes interact so that they interact completely via the inner portion of the nested inner nanotube. So, which means that the outer portion of the inner nanotube does not contribute to the interaction energy of the motion of these nanotubes. So what I have is the assumption before I answer this question is assume the two nanotubes only interact along the inner portion of the two of the nested inner tube or it is equal into saying that the extruded portion of the inner tube does not contribute, so the extruded portion does not contribute. So, let us start answering all these questions. So, the first question is the acceptance criteria: will the nanotube be sucked into the outer one and the answer is yes, as long as the interaction energy is negative or attractive. So, consider the answer to this question is we need to consider the sign of the interaction energy, notice that we have evaluated the interaction of these two nanotubes and we call this cylinder-cylinder interaction as  $E_{cc}$ . So  $E_{cc}^{*}$  is:

$$E_{cc}^* = \frac{3(\pi\eta_c)^2 b_1}{4b_2^4} \left[ -AL_5 + \frac{21}{32B} / b_2^6 L_{11} \right]$$

We see that if I have, if  $E_{cc}^*$  is greater than zero, then the net interaction energy is repulsive and the inner nanotube will be pushed out of the outer nanotube, so we will not have the oscillatory motion. Now, second question is what is the suction energy? The moment we ascertain the sign of the interaction energy, which needs to be negative, the suction energy is equal to the work done on the system initially.

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My suction energy is, so if I provided my interaction energy is the cylinder-cylinder interaction energy is negative, then my let me call this as SE, then my suction energy is work done in extruding the cylinder out of the outer cylinder. I see that the inner cylinder has been extruded initially by a distance 'd', so my suction energy will be equal to the work done, which is also equal to  $-E_{cc}^*$  times 'd'. Note, that I have put a minus sign so that I can get a positive work done. So, this is the work done in extruding out the inner cylinder by a distance 'd'. So what is the suction energy which will drive the system. The third and the most vital question is describing the mechanics of the setup. Okay, so then to describe the oscillatory motion of the two nanotubes let us look at these two tubes of a certain length, which are in which the initial tube is extruded via distance 'd', so let us say that in general I have the outer tube, let us say it is of length L2 and let me also show that the inner tube is of length L1. They are all coaxial, so that is the assumption and let us say that the center of L1, I am going to call this distance as 2L2 and this distance as 2L1. We see that for convenience I have the center of all the axis is the origin and the center of the inner cylinder is at a distance (Z,0). The setup is as following: To look at the oscillatory dynamics, let us assume inner and outer nanotube of length 2L1 and 2L2. We also assume the center of the outer nanotube is at the origin so the outer nanotube of length 2L while the center of the inner nanotube is at initial point (Z,0), so it is slightly shifted. So, Z is going to be our distance from the center through which we are going to describe the oscillatory motion. So we expect that at equilibrium Z is zero, otherwise in the oscillatory motion Z changes its value. Notice that outer cylinder is of length 2L, so the ends of the outer cylinder or the inner or the outer nanotube is at length plus minus L2 and my inner cylinder is of length Z plus minus L1. My outer cylinder is of length L2 and my inner cylinder is of length Z plus/minus L1 and then in my oscillatory motion we will see that we have five different cases where the center of the inner cylinder can remain with respect to the origin.

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(ase 1: 2 < - (4+62) : inner tube fully extruded along portially " along -ve z-axis fully inside outer tube. (ase2: -(L+L) < Z < -(L2-L1) : " () lase 3 :- (12-4) < 2 < 12-4 ! Case 4: 12-4 < Z < 62+4 ! partially extended in the Z-axis " " Z > Lath : fully extended along the Z-axis. 2=  $\pm L_1 \pm L_2$ points ! Abbume : fully (1) & (5): extended states Ec=0 W increases for other states : times b Interact  $\begin{cases} E_{cc}^{*} (L+L_{c}+z) \\ E_{cc}^{*} (L+L_{c}-z) \\ E_{cc}^{*} 2L \end{cases}$ case 2 ⇒ - W= Carse 4 case 3 e 🖬 🧿 <u>N</u> 🖬 🦉 🦻

I am going to describe the motion in five different stages. Let me call this is in the form of five cases. My case one is when the center of the inner cylinder is extremely far apart or when my  $Z < -(L_1 + L_2)$ so it is outside the outer cylinder so that there is no edge effects as well which means that the inner tube in this case is fully extruded along negative Z axis. And then in case two I have that  $-(L_1 + L_2) < Z < -(L_2 - L_1)$ , so it is partially inside to  $-(L_2 - L_1)$ , so Z is partially inside the inner tube is partially inside the outer tube, but still in the positive along the negative Z axis, along the negative axial direction. In this case we have the inner tube partially extruded along along negative Z axis. The inner tube is partially extruded along the negative Z axis. Then my third case is when it is completely inside the outer tube, so suppose I have that  $-(L_2 - L_1) < Z < (L_2 - L_1)$ , so here I have the inner tube is fully inside the outer tube, so these are my various positions of the center of the inner tube. Then, I could also have that the inner tube is partially contained inside the outer tube, but along the positive Z axis, so which means that  $(L_2 - L_1) < Z < (L_2 + L_1)$  and then this is where the inner tube is partially inner tube is partially extruded in the positive Z axis and then fifth case is I have that  $Z > (L_2 + L_1)$  and this is the case where the inner tube is fully extruded out of the outer tube, but in the positive Z direction, so inner tube fully extruded along positive Z axis and to describe the oscillatory motions these five cases are repeated twice, so these five cases are going to be repeated once for half the motion of the nanotube or half the time period of the nanotube. Then, the next stage is to describe these stages of motion using the interaction energy. So, note that in case one and case five there is absolutely no interaction so we can assume that in one and five there is interaction energy zero, so assume before we do that note that these five cases involve four boundaries, one boundary is this point, the other boundary this point, the third boundary this point and the fourth boundary this point, so my cutoff points cutoff points or my boundary points are given by Z is equal to plus/minus L1 plus/minus L2, so there are four cutoff points, so that is the point we will note.

Then notice that we are going to assume that in case five and case one the interaction energy is zero because there is no interaction with our assumption. So, assume fully extruded states one and five gives ECC equal to zero and for other states the work done increases by ECC star times the length or the distance that the nanotube travels. For other states for other states for other states W increases W increases by ECC star times the interaction length. We see that in this case W will be in case so we have three more cases left so in case two W will be ECC star times L1 plus L2 plus Z and in my case in my case four in my case four, so case two and case four are very similar, one in the negative Z axis, the other in the positive, I see that this is ECC star times L1 plus L2 minus Z and finally instead three or case three where the tube is completely inside I see that the work done is ECC star times the length of the inner tube which is 2L1 times the length of the inner tube which is 2L1 and what I have is the following. Well, so what ECC star now is negative by its definition because it is a suction interaction energy, the attractive interaction energy, so what I have I have written down is negative of the work done. If I were to plot this negative W if I were to plot this W with respect to Z, I will see that we have the following five stages, so this is my Z axis, so let me know break down into following five stages. I have three, I have four so I have three and four, stage number three, stage number four and stage number two and stage number one stage number one and stage number five. I have divided into five different stages, so let me remove all these arrows because the diagram becomes little clearer, so this is my negative W axis and I see that I see that I get the following curve, so this times this, this, this and this so this is my stage three, these are my stage two and my stage four and my stage one and five are given by this. We can see that in stage one and five the work done is zero and in stage two the work done is decreasing with Z and in stage well in stage four the work done is increasing with Z. In stage three or in case three the work done is constant, we can see that it is independent of Z which is given by ECC times 2L1. So, the diagram here is important because we can see that there is zero acceleration of the particle or the nanotube at in for case one, case three and case five. The only acceleration is/deceleration is in case two and four.