Variational Calculus and its applications in Control Theory and Nanomechanics
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Lecture 61 Introduction to Nanomechanics Part 1

Okay, good morning, everyone. So, in today's lecture I am going to discuss yet another new applications of the calculus of variations, namely the one arising in nanomechanics.

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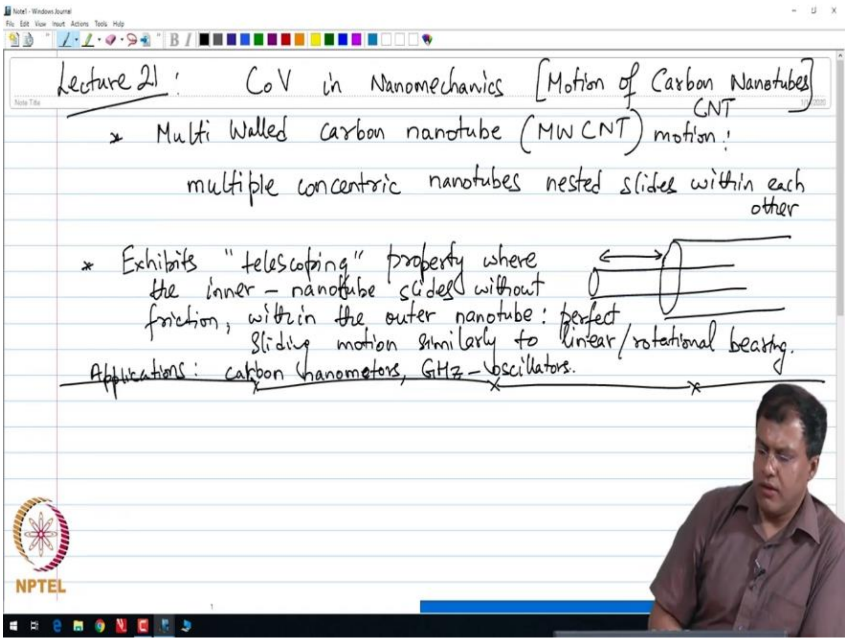

So, today's lecture, we will talk about the applications of calculus of variations in Nanomechanics, and specifically, I am going to look at the motion of carbon nanotubes. I call it as CNT. So let us introduce some background. In today's time, we have the revolution of data science but before the revolution of data science, it was all about the revolution of nano science, namely the motion of small scale or the prevalence of small-scale machineries and the heart of all these small machineries were these so-called nano motors or small-scale bearings which used to drive these small machines. Now I am going to talk about the motion of one of the small bearings in the form of 2 concentric carbon nanotubes. So, to describe the motion, we will look at the Hamilton's equation in this description of the motion of these carbon nanotube. But before we do that, I will have to build some background.

Here, we are going to look at in particular Multi Walled carbon nanotube also known as MWCNT motion. So, in this situation we have the set-up is we have multiple concentric carbon nanotubes which are sliding within each other. So the setup is we have an outer nanotube, an outer cylinder perhaps made of a material like carbon or graphite and and we have an inner nanotube which is moving back and forth inside this outer tube and this oscillatory motion of the inner nanotube generates the necessary mechanical energy. So, we are going to look at how to quantify this mechanical energy of this carbon nano motors.

Notice that, these oscillatory tubes exhibit the so-called telescopic properties or the sliding motion in almost perfect condition i.e. without any friction. So, the set up exhibits the telescoping property, where the inner nanotube slides without friction within the outer nanotube and it creates a perfect sliding motion, also the so-called bearings, similar to the motion of the bearings. So, it creates a perfect sliding motion similar to linear or in fact, sometimes rotational bearings. So, the sliding motion of these concentric nanotubes is the source of mechanical energy which drives these nano machines. Now to describe the motion of this oscillatory nanotubes we need some background in applied maths, specially some basic descriptions of special functions we will be using e.g. Hypergeometric Functions.

We will also look at some basics in chemistry, namely, the type of interactions that we have to look at and these basics are just simple perhaps almost all covered in class 12th or high school. For example, Lennard-Jones interaction energy and interaction potential and finally with all these basics we will look at the modelling of this nanotube motion via the regular Newtonian mechanics and also compare the motion of these nanotubes via the Hamiltonian dynamics leading to our Hamilton'fs equation. As we can see this is a highly applied area and the application of these models lies in developing efficient nano motors as well as gigahertz oscillators. So, the applications of this part of the course lies in developing efficient carbon nano motors and fast oscillators or gigahertz oscillators.

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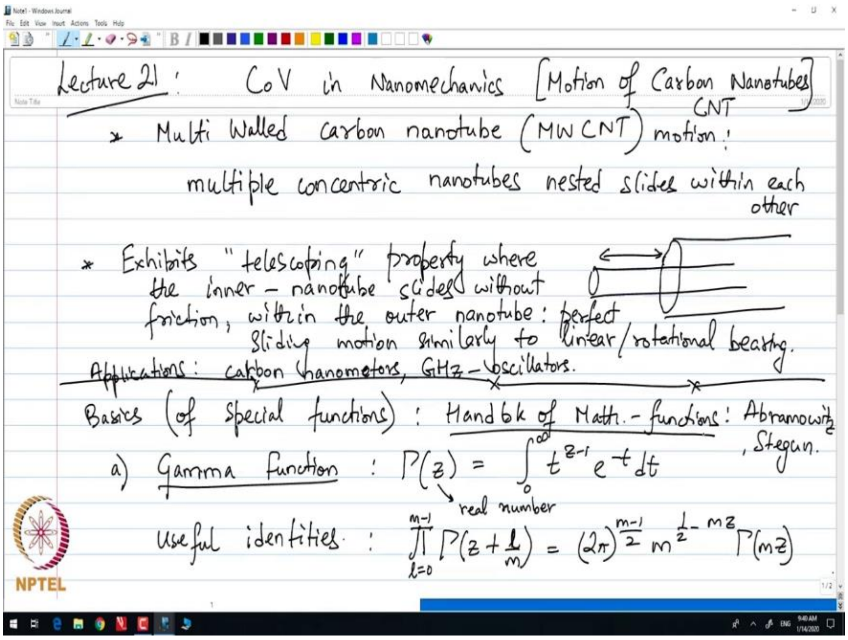

Let us start with some basics. To begin with, let me give all the students the source from where all these basics are picked. So that students can look at it in more detail. I am going to write down only those results which will be relevant for our discussion in this lecture, without any proof or argument. So students are constantly requested to look at this textbook which is known as the Handbook of Mathematical Functions by Abramowitz and Stegun, two Russian mathematicians. So the functions that we would like to consider are the first and the simplest function is the so-called Gamma function. Here the Gamma function is defined for any real number z as:

$$\Gamma(z) = \int_0^\infty t^{z-1} e^t dt$$

Now I know that this, this can be shown that it reduces to to a ratio of 2 factorials when z becomes a natural number or a positive integer. So then, some of the useful identities that I will be using while in the description of the motion of this carbon nanotubes is the following:

$$\prod_{l=0}^{m-1} \Gamma\left(z + \frac{l}{m}\right) = (2\pi)^{\frac{m-1}{2}} m^{\frac{1}{2}-mz} \Gamma(mz)$$

Let me denote Gamma function integral as (a). Again, the students are frequently requested to look at the source mentioned above to see how we are able to come to these results. So, I am just stating some of the basics in the form of these results. Once we have introduced Gamma function, the other necessary and important function is the Beta function which can be described in terms of Gamma function.

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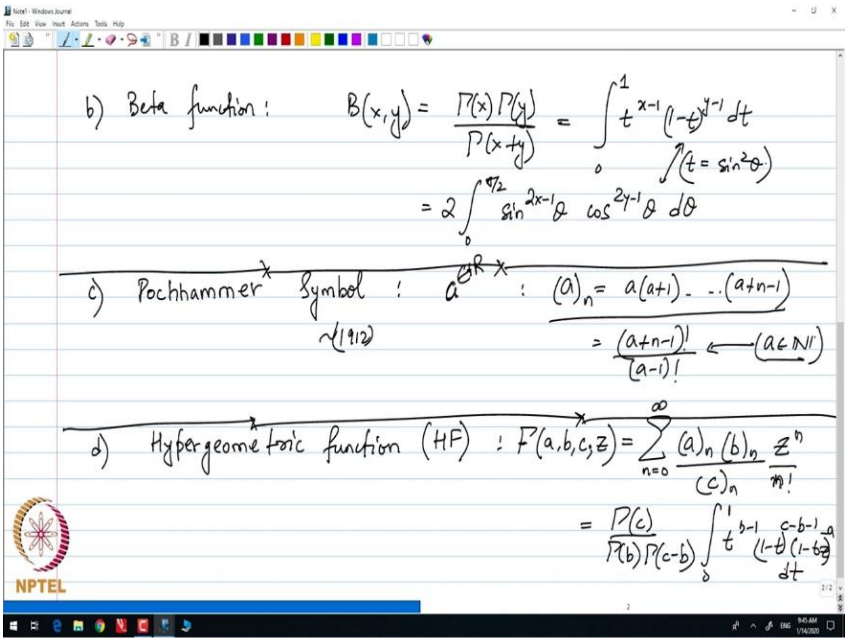

So, let me continue numbering and assume (b) is Beta function.

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^1 f^{x-1}(1-t)^{y-1}dt$$
$$= 2\int_0^{\pi/2} \sin^{2x-1}\theta \cos^{2y-1}\theta d\theta, \qquad \text{(assuming: t=}\sin^2\theta)$$

So the third important relation that we will be using is the so called Pochhammer symbol. Pochhammer was a Prussian mathematician who developed this notation around 1912. For this let us suppose a is a real number, then it is denoted as:

$$(a)_n = a(a+1)\cdots(a+n-1)$$
$$= \frac{(a+n-1)!}{(a-1)!},$$

where this is only true when a is a natural number. Notice that the way the Pochhammer symbol is defined, if a becomes negative, then we expect that one of the factor is going to disappear or will be equal to 0 for some value of n and suppose a is negative, the Pochhammer symbol is going to disappear at certain value of n. Now I am ready to describe the most important Hypergeometric function. So, let me use a shorthand notation HF for Hypergeometric Function.

$$F(a,b,c,z) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!}$$
$$= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}dt$$

So, when we are using the description of Hypergeometric Function, we are going to regularly switch between the series and the integral notation.

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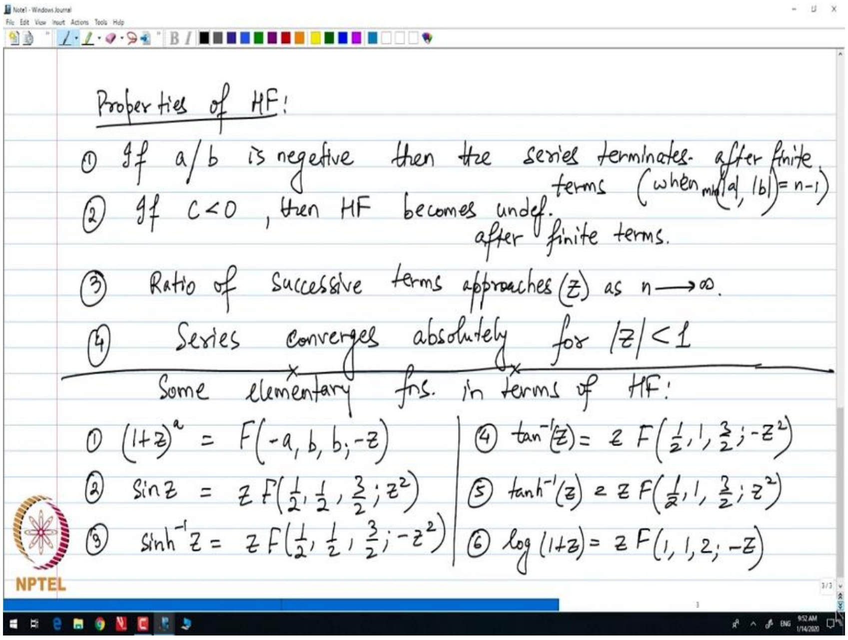

Since we will be using these functions very often in our model description, let me just state some properties of Hypergeometric Function. So first of all, as I just said few minutes back, if one of my arguments a or b is negative integer, then the series terminates. Notice that if a is negative, there will be a value of n for which $(a+n-1)$ becomes 0, which means that if n is for larger and larger values of n, beyond that particular critical value this summation gives me 0. So the series terminates after finite terms. That will be when I have that the absolute value of a or b equals $(n-1)$. That is when the series is going to terminate. So, in fact, it will be minimum of the absolute value of a and b. Now the other important property is if I have $c < 0$, the quantity in the denominator of the series is negative and we expect that the series is going to blow up after finite number of terms. So, if c is negative then, then the Hypergeometric Function becomes undefined after finite terms and then the ratio of successive terms approaches z as n goes to infinity. The ratio of the successive terms approaches z as n goes to infinity. So, if we were to take the ratio and take n tending to infinity, we are only going to get z because all these constants, they become equal to each other in the limiting scenario. So, which means we can also say something about the series being convergent or divergent via the ratio test. So, which means that if the ratio of 2 successive terms approaches z and if the absolute value of $z < 1$ then I can say for sure that the series is absolutely convergent. So I can quickly say that the series converges absolutely within this range $|z| < 1$. Thus all the properties that we will be using in our model development and then let us also note down some useful relations for these Hypergeometric Functions. First let me highlight how to write certain basic functions in terms of Hypergeometric Functions. It turns out almost all continuously differentiable functions can be written in the form of series and the series eventually can be written in the form of this Hypergeometric Functions. So let me show some elementary functions in terms of the Hypergeometric Functions:

1. $(1+z)^a = F(-a, b, b; -z)$
2. $\sin z = zF(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; z^2)$
3. $\sinh^{-1} z = zF(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; -z^2)$
4. $\tan^{-1}(z) = zF(\frac{1}{2}, 1, \frac{3}{2}; -z^2)$

5. $\tanh^{-1}(z) = zF(\frac{1}{2}, 1, \frac{3}{2}; z^2)$

6. $\log(1+z) = zF(1,1,2;-z)$

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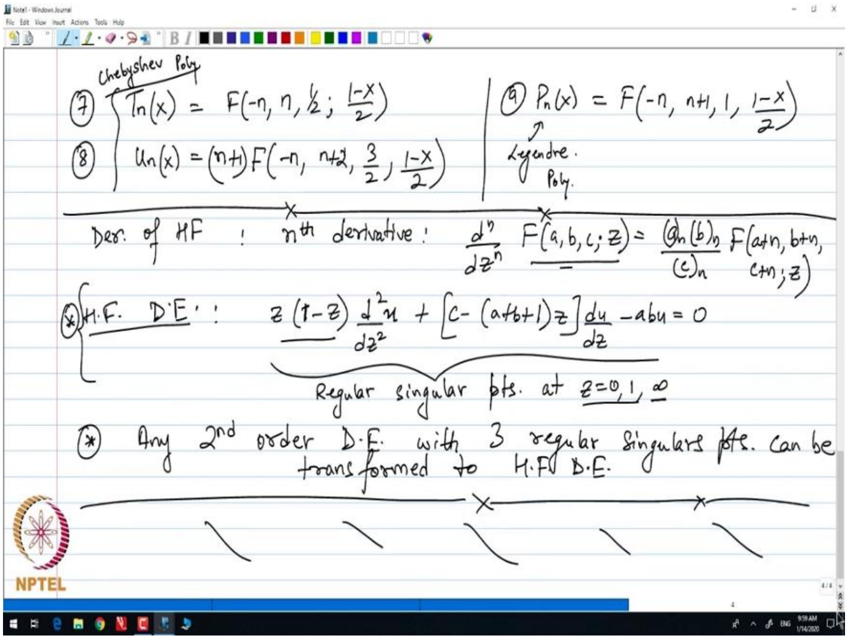

I also want to represent some special Orthonormal functions. For example, the Chebyshev polynomials Tn and Un. These can be written in the following form:

- $T_n(x) = F(-n, n, \frac{1}{2}; \frac{1-x}{2})$
- $u_n(x) = (n+1)F(-n, n+2, \frac{3}{2}; \frac{1-x}{2})$
- $P_n(x) = F(-n, n+1, 1; \frac{1-x}{2})$

The last one is the Legendre polynomial. I also want to introduce the differential equation whose solution is the Hypergeometric Function. Before I do that, let me also describe how to take the derivative of these Hypergeometric Functions with respect to the variable z. So, the nth derivative is as follows:

$$\frac{d^n}{dz^n}F(a,b,c;z) = \frac{(a)_n(b)_n}{(c)_n}F(a+n, b+n, c+n; z)$$

Then I have the differential equation whose solution is this Hypergeometric Function with the argument a, b, c, z. So the Hypergeometric differential equation (HF DE) is

$$z(1-z)\frac{d^2x}{dz^2} + [c-(a+b+1)z]\frac{du}{dz} - abu = 0$$

Notice that this differential equation has a singularity at $z = 0$, $z = 1$ and also at $z \to \infty$. So this has regular singularities. If I replace my variable z by $\frac{1}{z}$ and take the limit z tending to 0. We will see that the solution is not going to be defined. Now, the next statement that I am going to make is without any argument or proof, which says that any second order differential equation with any 3 regular singular points can be transformed to Hypergeometric Differential equation. This is something we will be using and also one final relation that is very important in our modelling is rewriting. Can we rewrite very complicated Hypergeometric Differential Equation into a simpler form? We will introduce the so-called Quadratic Transformation.

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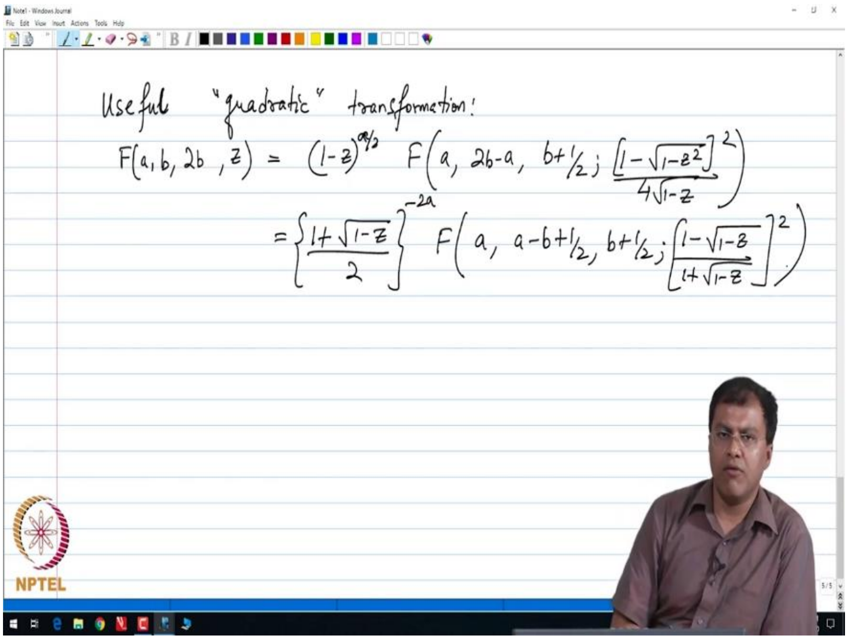

So, this is one last relation. In fact there are many such relations. The one that I will be using in our lecture discussion is the one that I am stating i.e. Useful quadratic transformation.

$$F(a, b, 2b, z) = (1-z)^{a/2} F\left(a, 2b-a, b+1/2; \frac{(1-\sqrt{1-z^2})^2}{4\sqrt{1-z}}\right)$$
$$= \left(\frac{1+\sqrt{1-z}}{2}\right)^{-2a} F\left(a, a-b+1/2, b+1/2; \left[\frac{1-\sqrt{1-z}}{1+\sqrt{1-z}}\right]^2\right)$$

So, these are some useful relations we will be using in our model development later on.