Variational Calculus and its applications in Control Theory and Nanomechanics
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Lecture 62 Introduction to Nanomechanics Part 2

Let me also introduce three other concepts. One is the integral form of the Hypergeometric Functions and also look at the Hypergeometric Functions for two variables x and y and also introduce certain special integrals known as the elliptic integrals.

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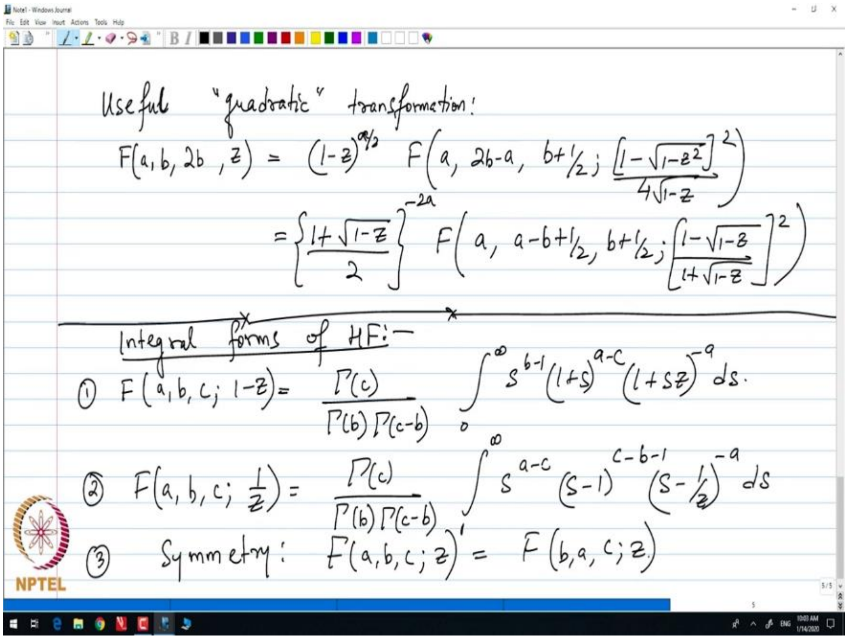

Useful "quadratic" transformation:

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

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

Integral forms of HF:-

① $F(a,b,c;1-z) = \dfrac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \displaystyle\int_0^\infty s^{b-1}(1+s)^{a-c}(1+sz)^{-a}\,ds.$

② $F(a,b,c;\frac{1}{z}) = \dfrac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \displaystyle\int_1^\infty s^{a-c}(s-1)^{c-b-1}(s-\tfrac{1}{2})^{-a}\,ds$

③ Symmetry: $F(a,b,c;z) = F(b,a,c;z)$

$$F(a,b,c;1-z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^\infty s^{b-1}(1+s)^{a-c}(1+sz)^{-a}ds$$
$$F(a,b,c;\frac{1}{z}) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_1^\infty s^{a-c}(s-1)^{c-b-1}\left(s-\frac{1}{2}\right)^{-a}ds$$

Then there is another relation that is the relation of symmetry that comes right from our series representation of the Hypergeometric function. We also see that there is a symmetry involved in this function i.e. $F(a,b,c;z) = F(b,a,c;z)$.

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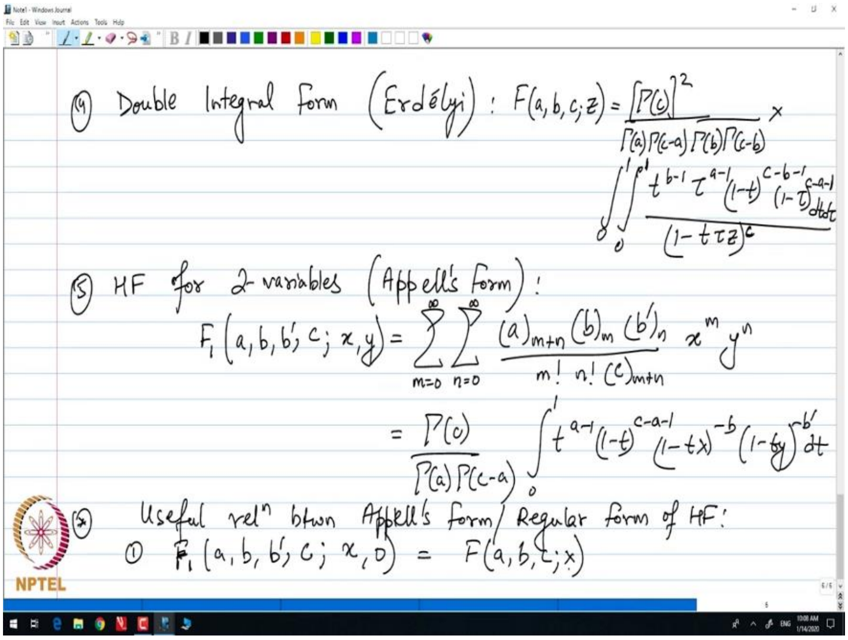

④ Double Integral Form (Erdélyi) : $F(a,b,c;z) = \frac{[\Gamma(c)]^2}{\Gamma(a)\Gamma(c-a)\Gamma(b)\Gamma(c-b)} \times \int_0^1\int_0^1 \frac{t^{b-1}\tau^{a-1}(1-t)^{c-b-1}(1-\tau)^{c-a-1}dtd\tau}{(1-t\tau z)^c}$

⑤ HF for 2-variables (Appell's Form) :

$F_1(a,b,b';c;x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(a)_{m+n}(b)_m(b')_n}{m!\,n!\,(c)_{m+n}} x^m y^n$

$= \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 t^{a-1}(1-t)^{c-a-1}(1-tx)^{-b}(1-ty)^{-b'}dt$

(*) Useful relⁿ btwn Appell's form/ Regular form of HF:

① $F_1(a,b,b';c;x,0) = F(a,b,c;x)$

And then the fourth important relation is the relation by a mathematician Erdelyi which is the Double Integral Form. The Double Integral Form by Erdelyi and this is given as follows:

$$F(a,b,c;z) = \frac{[\Gamma(c)]^2}{\Gamma(a)\Gamma(c-a)\Gamma(b)\Gamma(c-b)} \int_0^1\int_0^1 \frac{t^{b-1}\tau^{a-1}(1-t)^{c-b-1}(1-\tau)^{c-a-1}dtd\tau}{(1-t\tau z)^c}$$

Now I am also going to introduce the Hypergeometric Function of two variables and we will look at a special form of these two variable functions known as the Appell's Form:

$$\begin{aligned} F_1(a,b,b',c;x,y) &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(a)_{m+n}(b)_m(b')_n}{m!\ n!(c)_{m+n}} x^m y^n \\ &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 t^{a-1}(1-t)^{c-a-1}(1-tx)^{-b}(1-ty)^{-b'}dt \end{aligned}$$

Now, some useful relations between the Appell's form or the two variable form and the regular form or the one variable form of the Hypergeometric Functions.

$$F_1(a,b,b',c;x,0) = F(a,b,c;x)$$

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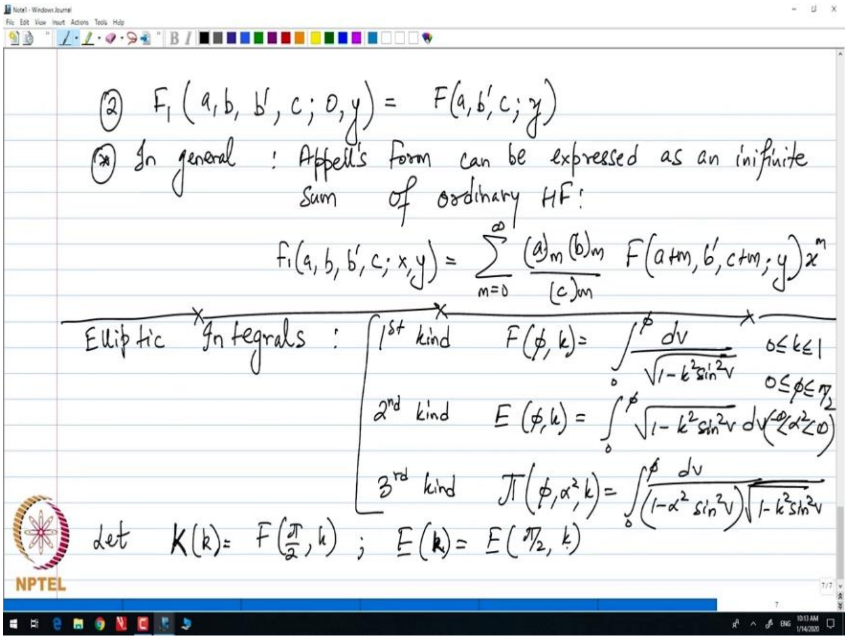

② $F_1(a,b,b',c;0,y) = F(a,b',c;y)$

(*) In general : Appell's form can be expressed as an infinite sum of ordinary HF:

$$f_1(a,b,b',c;x,y) = \sum_{m=0}^{\infty} \frac{(a)_m (b)_m}{(c)_m} F(a+m,b',c+m;y)\, x^m$$

Elliptic Integrals :

1st kind $F(\phi,k) = \int_0^{\phi} \frac{dv}{\sqrt{1-k^2\sin^2 v}}$ $0 \le k \le 1$, $0 \le \phi \le \pi/2$

2nd kind $E(\phi,k) = \int_0^{\phi} \sqrt{1-k^2\sin^2 v}\, dv$ $(-\infty < \alpha^2 < \infty)$

3rd kind $\Pi(\phi,\alpha^2,k) = \int_0^{\phi} \frac{dv}{(1-\alpha^2\sin^2 v)\sqrt{1-k^2\sin^2 v}}$

Let $K(k) = F(\frac{\pi}{2},k)$; $E(k) = E(\pi/2,k)$

Similarly,

$$F_1(a,b,b',c;0,y) = F(a,b',c;y)$$

So, in general I can write down my Hypergeometric Function of two variables for the general case as an infinite sum of Hypergeometric Functions of one variable. So in general, in general Appell's form can be expressed as an infinite sum of the ordinary Hypergeometric Function as follows:

$$F_1(a,b,b',c;x,y) = \sum_{m=0}^{\infty} \frac{(a)_m (b)_m}{(c)_m} F(a+m,b',c+m;y) x^m$$

So finally let me also introduce the relations of the so-called elliptic integrals. So, we have seen these elliptical integrals earlier when we were describing the solution of the bent beam problem or elastica. So, we will have the elliptic integrals of first, second and third kind.

$$\begin{aligned} F(\phi,k) &= \int_0^{\phi} \frac{dv}{\sqrt{1-k^2\sin^2 v}}, \quad 0 \le k \le 1, \quad 0 \le \phi \le \pi/2 \\ E(\phi,k) &= \int_0^{\phi} \sqrt{1-k^2\sin^2 v} dv, \quad -\infty < \alpha^2 < \infty \\ \Pi(\phi,\alpha^2,k) &= \int_0^{\phi} \frac{dv}{\sqrt{1-\alpha^2\sin^2 v}\sqrt{1-k^2\sin^2 v}}. \end{aligned}$$

So with regards to these three elliptic integrals, I have also some useful relations.

$$\text{Let} K(k) = F(\pi/2,k); \quad E(k) = E(\pi/2,k)$$

So, then I have some relations which we will be using while we solve, while we integrate our model equations.

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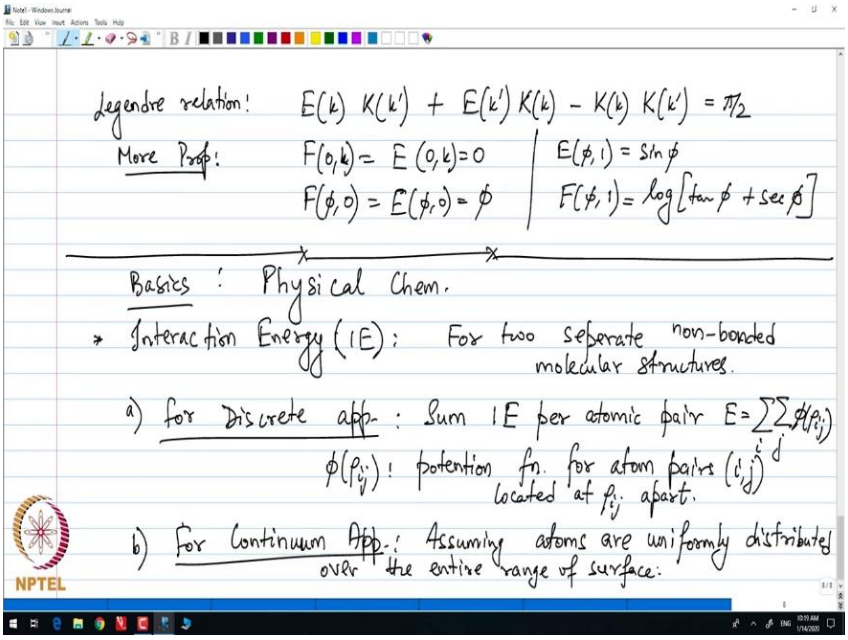

Legendre relation: $E(k)\,K(k') + E(k')\,K(k) - K(k)\,K(k') = \pi/2$

More Prop: $F(0,k) = E(0,k) = 0$ | $E(\phi,1) = \sin\phi$

$F(\phi,0) = E(\phi,0) = \phi$ | $F(\phi,1) = \log[\tan\phi + \sec\phi]$

Basics: Physical Chem.

* Interaction Energy (IE): For two seperate non-bonded molecular structures.

a) for Discrete app.: Sum IE per atomic pair $E = \sum_i \sum_j \phi(\rho_{ij})$

$\phi(\rho_{ij})$: potention fn. for atom pairs (i,j) located at ρ_{ij} apart.

b) For Continuum App.: Assuming atoms are uniformly distributed over the entire range of surface.

One more relationship is the Legendre relation.

$$E(k)\ K(k') + E(k')\ K(k) - K(k)\ K(k') = \pi/2,$$

and we have more properties of the form

$$\begin{aligned} F(0,k) = E(0,k) &= 0 \\ F(\phi,0) = E(\phi,0) &= \phi \\ E(\phi,1) &= \sin\phi \\ F(\phi,1) &= \log[\tan\phi + \sec\phi] \end{aligned}$$

So, these are my relations that we will be using in our later development of the model. So, this is so far the basics that I have covered in terms of the special functions. Now my next set of lectures are going to cover some basics in physical chemistry, namely the introduction of interaction energy, the Van der Waals interaction energy and the so-called Lennard-Jones potential. So let me just introduce some basics in physical chemistry. So again, these basics are extremely rudimentary in the form that almost all students taking this course must have done in certain high school science courses. So I am just revising some of these basics of physical chemistry. Let me start with the concept of interaction energy. So, when I talk about interaction energy, I talk about the interaction of 2 non-bonded structures. We do not talk about bonds like covalent bonds, ionic bonds and so on. We just talk about the energy of interaction between 2 structures, e.g. 2 molecules, 2 compounds which are not bonded to each other. So I denote it by IE and these are for 2 separate non-bonded molecular structures. So if I want to find the interaction energy of many structures, we could either use the discrete application where we can individually sum the interaction energy or if this distribution of these structures are nearly homogeneous and the distance is infinitesimally small, then possibly we could use as the interaction energy in the form of an integration rather than a summation. So for discrete applications I can sum the interaction energy per atomic pair or sum the interaction energy per structure where my net interaction energy is E is given by $E = \sum_i \sum_j \phi(\rho_{i,j})$, where $\phi(\rho_{i,j})$ is defined as the potential or the interaction potential function formy atom pairs (i,j). So, $\rho_{i,j}$ is the interaction potential for atom pair (i,j) and located at $\rho_{i,j}$apart. So then for continuous applications, I can change my double summation as double integral. For continuum applications, I can assuming that atoms are uniformly distributed over the entire range of surface, essentially, we do not want non-uniform distribution otherwise some integration may not hold or may not make sense.

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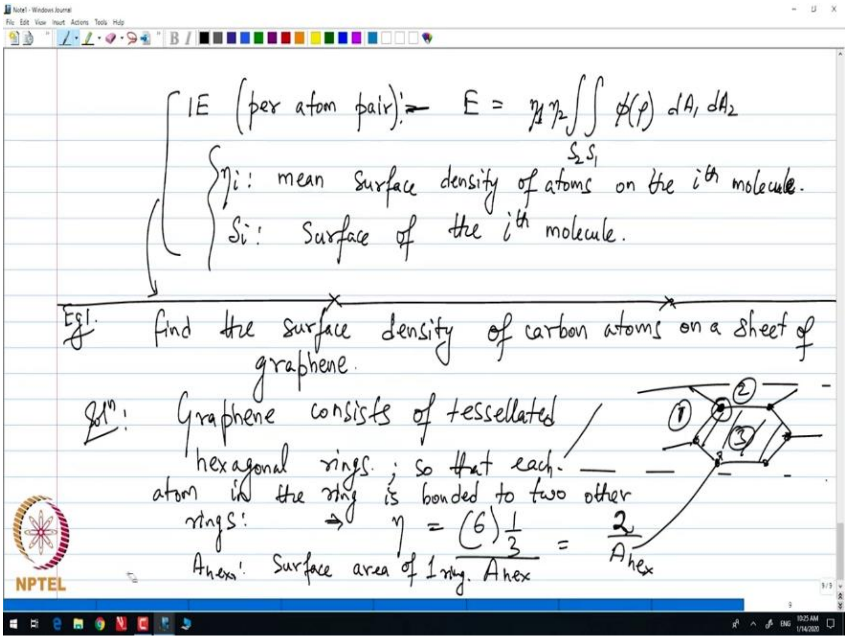

IE (per atom pair): $E = \eta_1 \eta_2 \int_{S_2}\int_{S_1} \phi(\rho)\, dA_1\, dA_2$

η_i : mean surface density of atoms on the i^{th} molecule.

S_i : Surface of the i^{th} molecule.

Eg 1. Find the surface density of carbon atoms on a sheet of graphene.

Sol^n: Graphene consists of tessellated hexagonal rings; so that each atom in the ring is bonded to two other rings: $\Rightarrow \eta = \dfrac{(6)\frac{1}{3}}{A_{hex}} = \dfrac{2}{A_{hex}}$

A_{hex}: Surface area of 1 ring.

So, assuming that the atoms are uniformly distributed over the entire range of the surface, then I can describe my interaction energy IE per atom pair as follows. So

$$E = \eta_1 \eta_2 \int_{s_1} \int_{s_2} \phi(\rho) dA_1 dA_2$$

So, I am talking about the atomic or the 2 pair structure interaction and then I take the integration of these pair structures. And also, these are multiplied by the number of atoms per unit surface or number of structures per unit surface where my η_i is the mean surface density of atoms or structures on the ith molecule and my s_i is a surface, surface of the ith molecule which means η_i is the number of atoms per unit surface of the structure and we are considering the ith structure. So that is the interaction energy per pair. So let me highlight this concept with an example. A very, very basic example of a graphene sheet. We know that graphene has at the molecular level, a hexagonal structures and also graphene is arranged in such a way that each of these structures are arranged in sheets. So, we have the arrangement of graphene in the form of sheets and that is why graphene is very slippery. So, let me look at a hexagonal structure of graphene. So let us see in figure above, a sheet of graphene.

We have hexagonal structures of graphene where each of these vertices of the hexagon are occupied by carbon atoms. Let me just extend this structures. Notice that if we were to look at each of these joints, this one joint which is occupied by one carbon atom is shared by 3 hexagonal rings. So, ring like 1,2,3, which means that since there are 6 carbon atoms in 1 ring, so essentially the number of carbon atoms per ring will be 6 times one third or 2 carbon atoms per ring because each carbon atom is shared by 3 rings. So, which means that the atomic density per molecule of the graphene is 2. So the example says find the surface density of carbon atoms on a sheet of graphene. Graphene consists of the hexagonal rings or the so called tessellated, tessellated hexagonal rings, so each atom in the ring is bonded to 2 other rings which means that my atomic density Eta will be 6 atoms times one third because shared be 3 different rings divided by the surface of 1 ring, let us say A_{hex}. So, I see that my Eta comes out to be $2/A_{hex}$ or where area is the area of 1 hexagon and that gives me my surface or the number of atoms per unit area of the ith ring of the graphene. Once we have introduced the concept of interaction energy, let me also look at the specific interaction energy known as the Van der Waals interaction. So again, Van der Waals interactions are non-contact interaction unlike the interaction like covalent or ionic interactions. So, these are non-contact interactions.

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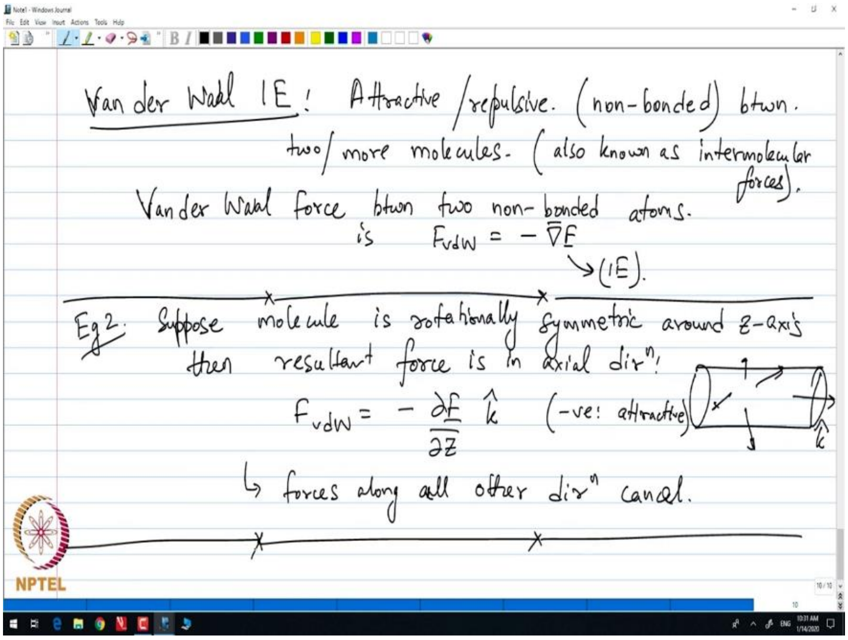

Van der Waal IE: Attractive/repulsive. (non-bonded) btwn. two/more molecules. (also known as intermolecular forces).

Van der Waal force btwn two non-bonded atoms. is $F_{vdW} = -\overline{\nabla}E$ $\searrow$ (IE).

Eg 2. Suppose molecule is rotationally symmetric around z-axis then resultant force is in axial dir^n:

$F_{vdW} = -\frac{\partial E}{\partial z}\hat{k}$ (-ve: attractive)

$\hookrightarrow$ forces along all other dir^n cancel.

So we will talk about Van der Waals interaction energy. These are either attractive or can be repulsive. We will look at a specific form of the interaction potential which models this attractive/repulsive interaction energy. Namely we will see that the, if the atoms come very close to each other or almost touch each other, this interaction energy becomes strongly repulsive and when they move slightly away from each other, eventually they become attractive and then the amount of attraction, it falls away exponentially. So, as I just said these are attractive or repulsive interactions and these are non-bonded between two or more molecules. So, I am not going to go into extreme depth of these interaction energy. I am going to just highlight the basic mechanism or the philosophy of these interactions which is useful for our model development. Students who are more interested, again, can look at some of the basic school text books in Physical Chemistry. So these are non-bonded interaction between two or more molecules, also known as the intermolecular forces. So then once we have the Van der Waals interaction energy, I can describe my Van der Waals force. Van der Waals force between two non-bonded atoms is the gradient of Van der Waals interaction energy(E) i.e. $F_{vdw} = -\overline{\nabla}E$. I have put a minus sign so that to represent that this force is an attractive force. So let me highlight this interaction energy with a quick example. Suppose we are given a cylinder, let us say a carbon nanotube and we are also given the interaction energy of the carbon nanotube with some surrounding particles. So, these are all cylindrically symmetric objects and I want to find the interaction of the Van der Waals force of the carbon nanotube with its surrounding objects. Note that due to cylindrical symmetry, the radial components of the force completely balance out each other and the only force that we will have will be along the axial direction or F_z. So suppose my molecule that we are after is rotationally symmetric around the z axis. My molecule is rotationally symmetric around the z axis then the resultant force is in axial direction and

$$F_{vdw} = -\frac{\partial E}{\partial z}\hat{k}$$

Notice that along r, all the components of the force, they cancel each other. So negative sign means attractive and along all other directions. So once I have described my Van der Waals interaction energy, let me also describe the so-called Lennard-Jones potential which describes these Van der Waals interaction energy. So, Lennard-Jones potential has a very specific form and it represents this attractive, repulsive type of an interaction versus the distance between the 2 atoms or structures.