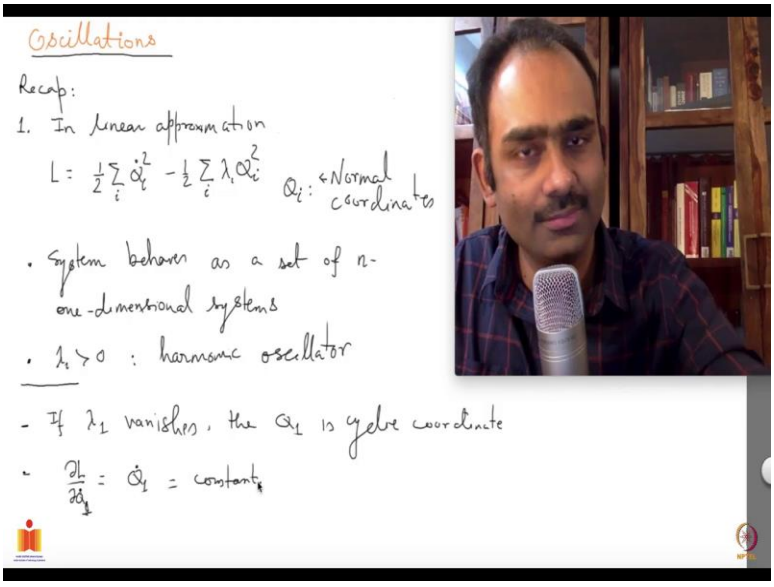
Introduction to Classical Mechanics
Professor Dr. Anurag Tripathi
Indian Institute of Technology, Hyderabad
Lecture 20
Oscillations, Triatomic Molecule

Last time we started looking at a System of n Degrees of Freedom near its equilibrium configuration, so we are assuming motion of the system when it is close to its equilibrium configuration and actually to be more precise but we started out was looking at that approximation under which the equations of motion near that equilibrium would be linear.

And then I mean that was given as an exercise and based on that we approximated the Lagrangian and we saw that, I mean that is what I wrote that the Lagrangian would have only if you expand the potential term, you only need to retain up to quadratic terms in the displacements and also for the kinetic energy, you need to retain only up to terms which are quadratic in the velocity generalized velocities. So, that is what you are doing, let me do a quick recap and then well proceed further.

(Refer Slide Time: 01:34)



So, let me write recap. So, as I said just now, in linear approximation the linear approximation for equations of motion, near the equilibrium configuration which was set at Q equal to 0, so all the generalized coordinates are 0 and the potential energy is also assumed to be 0 there or not

assume it is set to be 0 there then you can write down the Lagrangian in the following form dot square minus half summation over i lambda i Qi square, that is what we saw.

So, you can always go from one set of generalized coordinates to this set which we call normal coordinates, you can under which Lagrangian appears like this. This Qi's are called the normal coordinates that is good. And as is evident here and also I stated this last time, the system here is behaving as if it is a collection of n one-dimensional systems which are completely independent of each other, because they are no cross terms, there is nothing linking 1 Q, let us say Q1 to Q2, so or Q3 to Q7. So, they all are independent which is a very nice feature and if our maybe let me write that down also, so system behaves as a set of n one-dimensional systems.

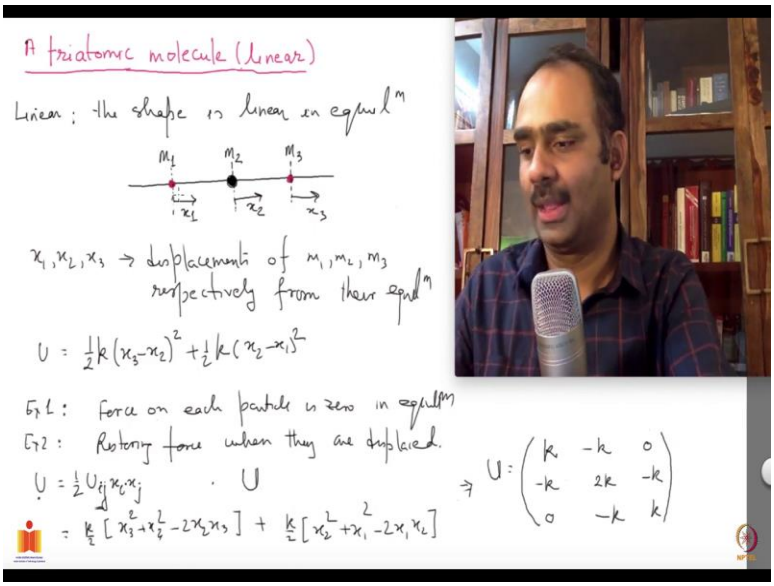
Also if our lambda i are greater than 0, so look at a particular generalized coordinate Qi and let us say for that particular coordinate lambda is 0, then the Lagrangian for the contribution to the Lagrangian which that can last coordinate is giving that is that of a harmonic oscillator, that is also what we saw. That is where we had stopped last time, very good I mean there are several things that can happen to lambda's one is they could be positive, they could be negative as well and they could vanish also, there are three such possibilities.

Because these are corresponding to real symmetric matrices this lambda i's is eigenvalues, so they will be real so it cannot be complex, that is one thing. Now it will be very nice if one of the lambda's vanishes and in fact, it will, so some of the lambda's will vanish as we are going to see soon and probably you can already tell why that will happen. Now, let us say lambda 1 vanishes, if that is the case, then Q1 vanishes, I mean Q1 does not appear in the Lagrangian, so if lambda 1 vanishes I am just taking such a case, then Q1 does not appear in the Lagrangian which means Q1 is cyclic coordinate, that we have talked several times earlier.

And if that is the case, then it is corresponding conjugate momentum will be a conserved quantity. And how do you get the conjugate momentum corresponding to Qi you have to take del L over del Qi Q1 in this case Q1 dot which is Q1dot and that will be a constant, that is one thing. Now, to appreciate what we have, let us take a specific example and things will be more clear when we take up a few examples and we study them in detail and we repeat what we have done in more abstract way in a particular context.

So, that is what the plan is for today. So, I am going to put all our manipulations algebraic manipulations that we have been doing since last two three videos in the context of the following example, which is very commonly found in textbooks, so I will take up maybe I should use some colour.

(Refer slide Time: 08:07)



So, a triatomic tri triatomic molecule, so that is what we want to study now. Actually, I want to be more specific, I want to take a linear molecule, linear molecule, so what I mean by that is the following, you see when you are looking at when I say a triatomic molecule I mean the molecule has three atoms, so let us say one here, one here and one here, that could be a configuration but what I am interested in is three atoms which are on the line on a given line, so they are always not always but they are in the line.

So when you say a triatomic molecule what you triatomic linear molecule, what you really mean is that the configuration is linear that the atoms are on a line when this molecule is in its equilibrium configuration. So, when it is in its minimum potential energy configuration all the atoms lie on a line, or when it does something it moves around the different particles are moving around of course they will not necessarily remain all in the line, one may go up, one may go down, one may do something.

So, when I say a linear molecule, I mean that the shape which it has in its equilibrium configuration, that is the meaning of linear here, let me take my, what happened? Black colour

back, very good, so let me write it down here what I said just now, when I say linear I mean the shape is linear in equilibrium.

So, here it is, let us say not a nice line, it is line but not beautiful anyway, so I have let us say three particles which are placed here like this, it will be nice if I can bring in some different colour, good, let me say that this guy is having a mass m1, that one has mass m2, this one has mass m3, so these are these are the equilibrium positions. Meaning that when the particles are situated here, they do not experience any force that is what an equilibrium position is, that is good.

Now, if the particles get displaced from their equilibrium locations which I have said that they are they are here, I will, let us say this m1 gets displaced by some amount the displacement from this place I will call x1, so x1 will give the displacement from this point from this location. Similarly, x2 will give the displacement of this particle from its equilibrium location and m3 from sorry x3 from this location. So, let me write down x1, x2 and x3, they are the displacements of m1 m2 and m3 respectively from their equilibrium positions.

Also, I am assuming that I am not assuming I am going to do the approximation which we have been talking about meaning retaining only the quadratic terms in the Lagrangian as far as the potential is concerned, also for the kinetic. And I am going to assume the following potential so I say that the potential energy of the system when it is displaced is this. So, half k some constant and so it take displacement of x3 and x2.

So, if both x3 and x2 are 0 meaning the particles are here and here then there is 0 potential energy associated with this and similarly if these guy is here the entire potential is 0, but the moment this and this and this they get displaced there is a restoring force which is going to create the potential energy and which will be just x3 minus x2 square because that is how much the separation has changed and that is why this will be x3 minus x2 square and similarly here x2 minus x1 square.

And I am assuming that the strength of the forces are same, so that is why the k the spring constant is same here in both the cases, this one assumption I have made and also I have neglected any interaction between m3 and m1's which is happening any direct interaction between m3 and m1 that I have neglected. So, you can do two small checks, you can do the

following exercise, check that the force on each particle is 0 in equilibrium which will be easy to check. And check that there is a restoring force, when they are displaced.

So, these checks you can do quickly, that is good. Now, what I will do is I will write down U the potential energy as half Uij xi xj and the matrix which will correspond whose corresponding elements are Uij I will denote by maybe I will denote like this, I will put one more line to distinguish it from this U, otherwise it is confusing. So, when I talk about these elements in matrix form I mean the matrix formed by these elements I will denote it by this.

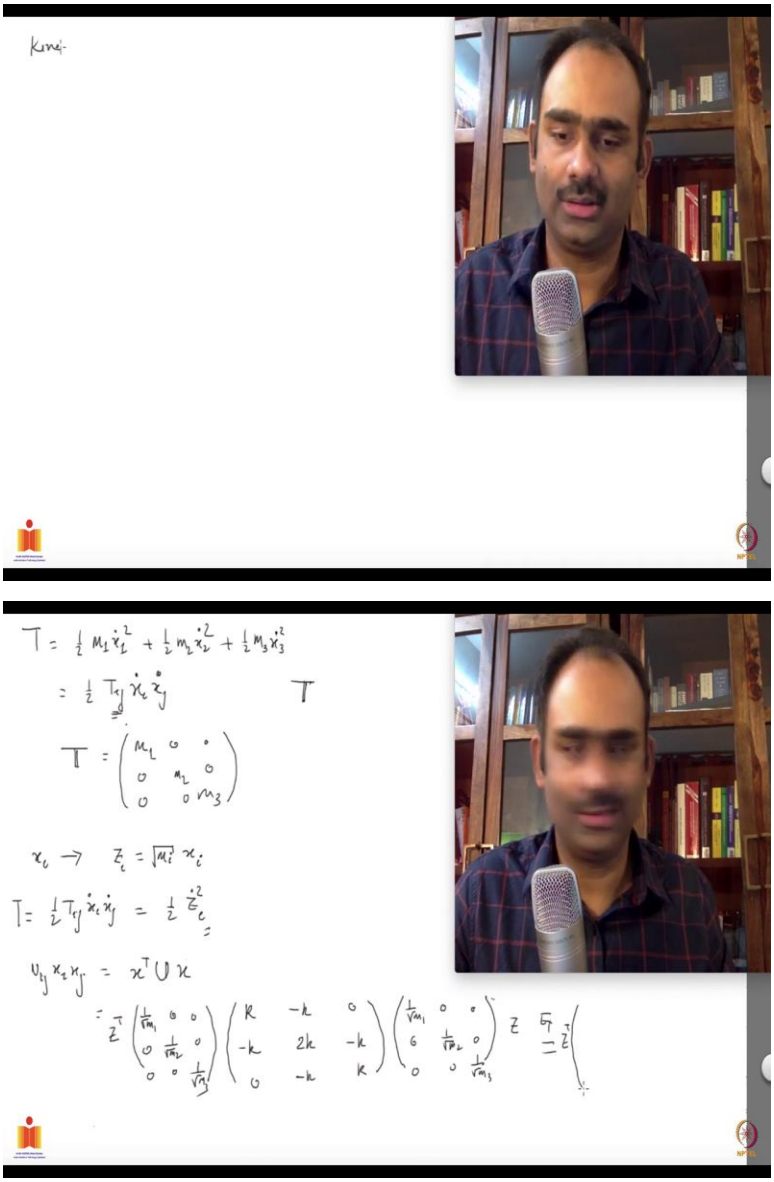
So, you can write this as, k over 2 x3 so I am just opening up these two squares x3 square plus x2 square minus 2 x2 x3 plus k over 2 x2 square plus x1 square minus 2 x1 x2, correct? Check that this corresponds to the following U. So, your U is k maybe on the next sheet, will it be better, I think it will be better, let me let me write down here itself k minus k 0, minus k 2k minus k and 0 minus k and k.

This as I said I will denote like this, this you can read up from here. So, for example, this half is here that goes away and if you look at x3 square, this is the only place it where it appears. So, this is the k coefficient is k and that is why, here you have k.

Similarly, for x1 square you have a k here, but x2 square appears at two places here and here, so it has a total 2k and that is why there is a 2k and similarly you can read off the other off diagonal elements.

And also note that this matrix is symmetric as you expect, you see these are this is a symmetric matrix, if you take the transpose you get back the U. And also this fact that this is a symmetric matrix is independent of your choice of the labels you have put here for the particles. So, even if you start calling this one as x2 and this one as x1 the matrix will change but it will still remain symmetric, that good.

(Refer Slide Time: 19:37)



Let us, look at the kinetic energy term or just the T your T is now half, half m1 x1 dot square plus half m2 x2 dot square plus half m3 x3 dot square. And again if I write T as half Tij xi dot xj dot in this case it just let me write it that way, that is the actually correct way of writing it, then if I similarly denote by T the matrix whose components are Tij then I get that matrix T to be the diagonal matrix of course because it has only diagonal entries m1, m2 and m3 and other entries are 0, m2 0, 0, 0 and m3, that is quite easy.

Now, this is good. So, let us, now let us do a change of basis and put T as not only diagonal but make the entries on the diagonal as 1, which is what we have been talking earlier when we were

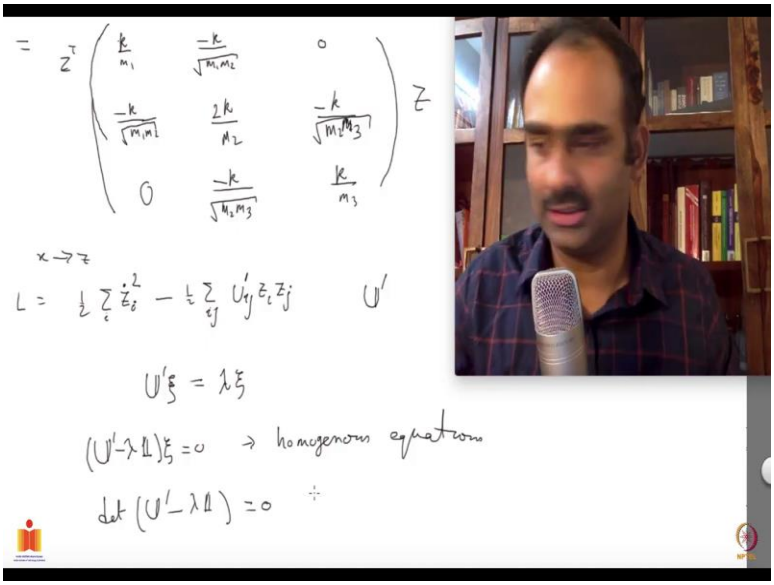
talking about simultaneously putting simultaneously diagonalization of two quadratic forms as sum of squares. So, we had put the 1 which is positive definite as the corresponding matrix as the identity matrix. And we have already talked about why T is a positive definite matrix.

So, what we want to do is we want to go from the bases xi from these coordinates to a new basis which we will call Z and which will be related to our x by the following, this is the same thing which we did when we were talking about the mathematical aspects some videos ago. So, this is what we want to do and if you do this transformation, then your quadratic form Tij xi xj becomes half Zi dot square, that is what you will get because you would absorb the mi's into the Zi's.

So, this is nice, now I have put the T as this, so my kinetic term T is now this one, which is now is, so when I have done this transformation my Uij xi xj the other quadratic form has turned into the following so to make it slightly easier to understand let me write in this manner U x, this has turned into the following. So, you have you had this let me write here, you had k maybe this is equal to so first I have my U which is k k minus k 0, minus k 2k minus k, 0 minus k k, is it symmetric? It is so, it is correct, that is our U and we have gone from x to Z, which makes it the following.

This is what we have talked in detail earlier, so it should be quite understandable what I am doing, 1 over square root of m1 0 0, 0 1 over square root of m2 0, 0 0 1 over square root of m3 and here also the same thing, very good that is what it is and you can do the following simple exercise that this is left as an exercise that you can write this as Z transpose and then a matrix here, which I will write down maybe on the next sheet will be better.

(Refer Slide Time: 25:49)



So, you please check that the following is true, that whatever I wrote before is same as the following if you do the matrix multiplication you get the following. k over m1 minus k over m1 m2 square root there has to be a square root because look at this, this has mass dimension m in the denominator I mean mass dimension 1.

So this should also have so if I have m1 m2, they should be square root and 0 minus k over m1 m2 which is also correct because for it to be symmetric this is what you should get here, 2k over m2 at least dimensionally this is correct minus k over m2 m2 m3 square root, the bracket should go some like something like this, then you have 0 minus k over m2 m3 square root k over m3.

And then you will have a Z here, please check that this is correct. Let us look at the matrix k 2k m2 m3 minus k this 0, so this matrix is symmetric, which is what you expect, because all these transformations are not going to change the symmetry property of the matrix you have, so which means I have not made any mistake because if you if I had made any mistake the symmetry property will be the first thing to get spoiled and we would note that there is a mistake.

But anyhow, now that I have gone from x to Z what I have in my Lagrangian is this, half summation over i Zi dot square minus half summation over i and j U prime, let me call it prime ij Zi Zj, so that is what we have now. Now, the last step that I choose I mean I do one more transformation and go from Z to Q capital Q is under which this part will get diagonalized or

become sum of squares, but when that happens this will just go over to Q dot square Qi dot squares.

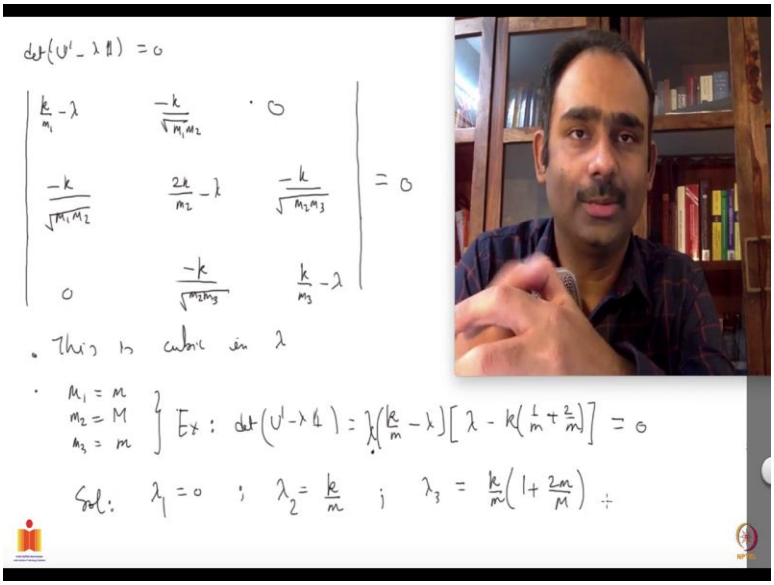
Because the transformation that is going to diagonalize U will be an orthogonal transformation and under that this will still remain the sum of squares that is what we have talked earlier, so that is will do now. So, let us say the matrix corresponding to U prime is denoted by this which is again a symmetric matrix. So, how do you do the transformation? Of course you have to search for the eigenvalues of the matrix U prime, because that is how you construct the diagonalizing matrix.

So, you find out the eigenvalues and you construct the diagonalizing matrix by putting the eigenvectors as the column vectors for example, so let us say xi denotes the eigenvectors of U prime with that is strange it is fine lambda and this is nicer, this eigenvalue equation now because this is a set of homogeneous equations this will have so this is a set or let me write it this way it will be more familiar I think I can write this as U prime minus lambda, so I am bringing what you have on the right hand side to the left is equal to 0.

Now, this is a set of homogeneous equations, total n number of equations if n degrees of freedom we have for our system. And this set of equations will have a non-trivial solutions xi only if the determinant of U prime minus lambda i vanishes, that is the condition for having non-trivial solutions and that is what we have to solve now, at least to find what are the possible lambda's that are allowed, for our system for the triatomic molecule linear triatomic molecular system. I think I have forgot to mention that in this analysis I am only looking at those motions in which the atoms of the molecule remain on the line.

So, I am restricting myself to those motions. So, I am not looking at those molecules going off the line, so it could happen that particular number 1 goes up, particle number 3 goes down something of that sort, I am not looking at that, I am just looking at things moving along the line, I should have mentioned this earlier, I forgot, that is good. So, now this you see where is my let me write it down in more explicit way.

(Refer Slide Time: 32:13)



So, determinant of U prime minus lambda i equal to 0 that is the following equation. So, what I am going to do is just insert the lambda's so you have by m1 minus lambda minus k over m1 m2 0, then you have minus k over m1 m2 square root 2k over m2 minus lambda and then you have minus k over m2 m3 square root, then you have 0 here, it is a same thing I wrote earlier but now I have explicitly I mean just the only additional thing is that I have put the lambda's on the diagonal entries minus lambda and the determinant of this should be 0.

Now, if you see this is a cubic equation in lambda, because you are you see you take this and then you have to multiply these two and you can see clearly that this is going to be cubic, so let me write down that thing, this is cubic in lambda and in generally expect three routes. Now, what I will do is I will make the molecule to be a little more symmetric, so I will put m1 to be m, m2 to be a different mass capital M and m3 to be same as m1 small m.

And it's should be easy to show that with this this will be an exercise, please check that you get the following, determinant of U prime minus lambda 1 is k over m minus lambda there is a lambda before and then you have one more lambda minus k 1 over m plus 2 over m. And that is what you should get and this is 0. So, what do we have here for solutions, so we got three routes for lambda and the solutions are lambda is equal to 0, which is coming from here, then you have lambda equals k over m that is what you would get if you had one oscillator of mass m, a simple harmonic oscillator of mass m would have lambda equal to k or m and it is interesting that we

are getting it here and you get another solution, so let me put lambda 1 lambda 2 lambda 3 m 2m over m.

So, these are the three solutions which you will get and please do this exercises, these are easy and show that this these are indeed correct what I have written down. Now, so we can, so one we are noticing that we are getting one of the eigenvalues to be 0. And one appears to be that of a simple harmonic oscillator and one is different case in the next video we will talk further about this problem and try to understand why we are getting such solutions and using these we will write down our Lagrangian in the normal coordinates we are almost there, because we have found the eigenvalue so we can diagonalize with eigenvectors and these are the eigenvalues which are going to appear in the Lagrangian.

So, we will write down our system using normal coordinates and from there we will do more analysis of the system and see how I can interpret the system as this triatomic molecule the linear one as independent harmonic oscillators, so that is what we would like to see and understand the meaning of the normal coordinates in this context. So, that will be for the next video. So, see you in the next video then.