Introduction to Classical Mechanics
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Lecture 21
Triatomic molecule normal coordinates

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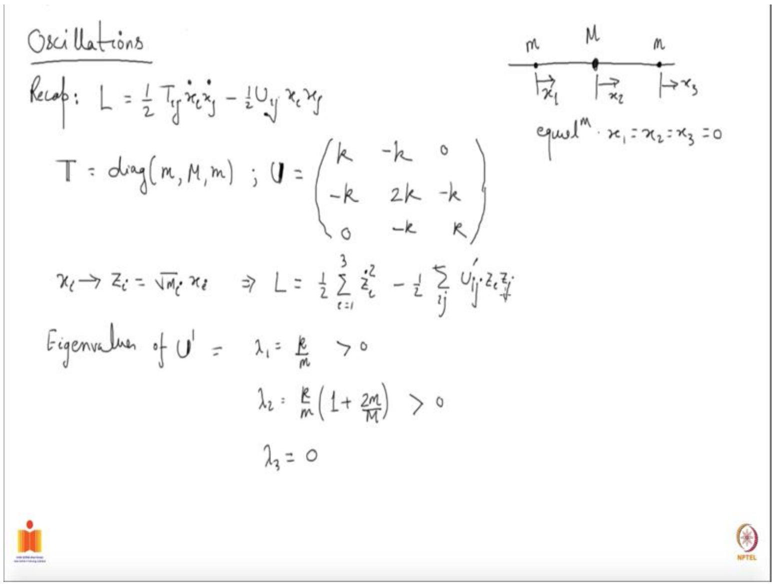

Hello, we were talking about linear triatomic molecule last time. So, I will start by doing a quick recap and then we will continue from there. So this is the, this is the plan for today, so we were saying that we have a molecule which is linear and by that I mean that in its equilibrium configuration all the atoms of the molecule are aligned in a line. So we were writing like the following, so let us say this is the line on which all the particles are aligned. This is particle number 1, this is particle number 2, this is some mass capital M and the two at the ends have the same mass.

And we also said that, we are going to measure their displacements from these positions, these are the positions of equilibrium. So if this particle gets displaced from its position either this direction or that direction I call it x1, similarly x2 and x3. And our equilibrium is at x1 equal to x2 and that is equal to x3 and they all are 0. Now we had written down the Lagrangian of the system as half Tij xi dot xj dot minus half Uij xi xj.

Let me also remind you what the Tij is, the matrix corresponding to Tij I was writing as this T this is just diagonal, diagonal matrix with these entries. And we had written down U maybe I should write it down again, the matrix corresponding to Uij I was denoting by this U bold face basically. This U is equal to k minus k 0, we should check that what I am writing is symmetric 0 minus k, k looks symmetric, so it is good.

So this is the matrix we have and then we said if we do a transformation from x so this x is a basically a column vector to z. Let me write the components here or maybe I should write the components of the x. So xi so this is same as before let me write it again, xi if I do the transformation that instead of xi's I start using zi's which are related to the xi's by this transformation. So you just absorb the square root of mass in the corresponding x and that is the definition of z.

If you do so then your Lagrangian becomes the following, then your Lagrangian becomes half zi square zi dot square, that is the kinetic term minus half ij they all run from 1 to 3 Ui Uij prime zi zj. And U prime will still be symmetric matrix and then we had found the Eigen values of U prime. That is what we did last time we found the Eigen values of U prime, by U prime I mean the matrix, U prime which corresponds to these elements.

And, we found that it has three Eigen values which we except because our equation was cubic and the Eigen values are the following. Lambda 1 is k over m, lambda 2 is k over m times 1 plus 2 m the entire thing divided by capital M and lambda 3 was 0. I have change the order in which I mean what I am calling lambda 3 I was calling in the last lecture is lambda 1 but now we will follow this naming.

This will be, I mean that is how I want to do, note that this quantity lambda 1 is greater than 0, the lambda 2 is also greater than 0 and lambda 3 is anyway 0. So, this is where we had stopped last time and let us proceed from here. Now what I want to do is, I want to put the second quadratic form which is here, see this is anyway diagonal now, not only diagonal the options are unity. But this quadratic form I want to put as a sum of squares. And that is the that is the plan, so let me go to the next slide or may be, may be next slide, let us go, so just remember you have a U, half U prime zi zj.

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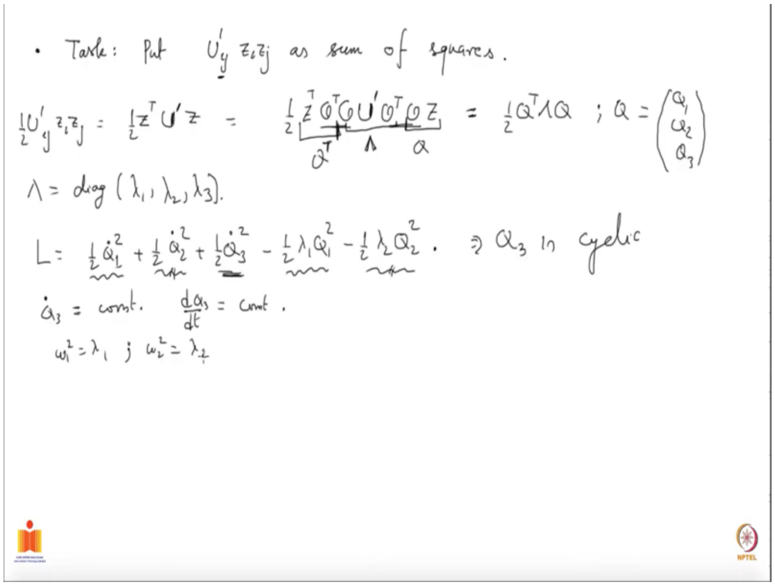

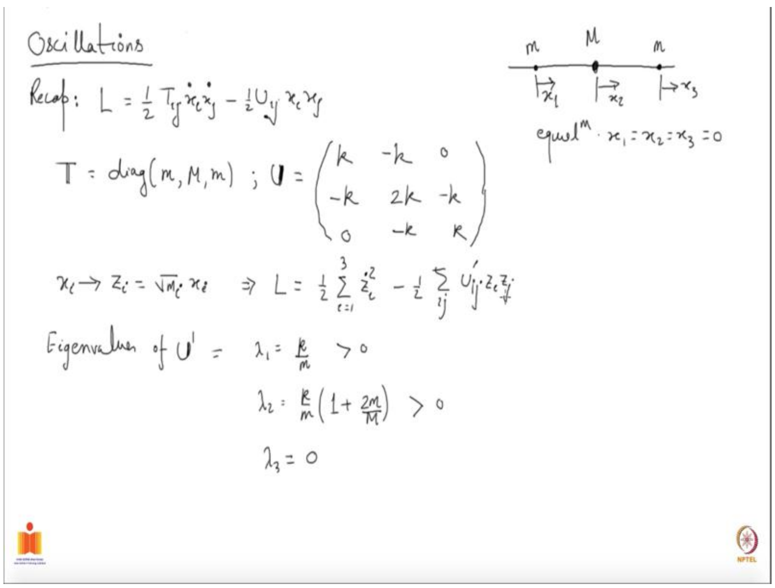

So now, our task is put this quadratic form Uij U prime ij zi zj as sum of squares. See I am just following the steps which I took when I was talking about the mathematical these two videos where I discussed about the sum of the mathematical quantities which I will be using in this course, so there we had done all this, in general I am just applying those things for the specific case of this triatomic molecule as the sum of squares, very good. So what we have to do is so let me write this using column vectors and matrices.

So I will write U prime ij zi zj as column vector or row vectors that transpose matrix U prime column vector z and the entries are z1, z2 and z3. Now this I know that I can diagonalize U prime by a orthogonal transformation which means that there are matrices I mean which means that there is matrix o, which and, which when I put o transpose and o next to U prime it will become a diagonal matrix. So that is what I am going to utilize here, so let me write as U prime o transpose o o o transpose.

So basically, I have done nothing because o transpose o is unity, this is also unity. So I have done nothing and you have z transpose. So I have written this original thing again, so this is identically equal to this, I have done nothing. Now as I know that, by the way this o is one which diagonalizes, so this matrix here I will call lambda and lambda will be a diagonal matrix. And, this quantity I will call Q and this then becomes Q prime, Q, not Q prime, so Q transpose. So what we get here is Q transpose lambda Q, Q is a column vector where Q is Q1 Q2 and Q3.

And my lambda is, let me write it here diagonal lambda 1, sorry, lambda 1 lambda 2 and lambda 3, that is good. So what do I have for my Lagrangian, now my Lagrangian looks like this, half Q1 dot square and then from here there was a half already. Let me write down first all the kinetic pieces, so half Q2 dot square plus half Q3 dot square, then the potential terms will give you minus half lambda 1 Q1 square is that clear, so this so this is a half already it was there which I have not written here, maybe I should write half, half and a half and a half.

So this is Q, if you write it in components it will be Q1 lambda 1 Q 1 plus Q2 lambda 2 Q2 and so forth, which is what is giving us this terms minus half lambda 2 Q2 square. And then, you have the lambda 3 term and lambda 3 is 0 so I am not going to write this so that term is gone. Which means that Q3 is cyclic as I mentioned last time. Which also means that Q3 dot this is the momentum corresponding to Q3 is a conserved quantity so it has to be constant. Which means the derivative dq over dt this is a constant, that is one thing. And if you look at the Lagrangian apart from the appearance of Q3 which we will talk about later, it is trivial actually what you have is the sum of two harmonic oscillators which I mentioned last time.

So if you look at this piece and that piece they together form a harmonic oscillator and these two form a another harmonic oscillator. With frequencies given by, the frequencies of two oscillators given by omega 1 square is lambda 1 and omega 2 square is lambda 2. That is good, there was something which I wanted to say, let me see do not remember now anyway. This is fine now so here is my Lagrangian. Let me go to the next slide.

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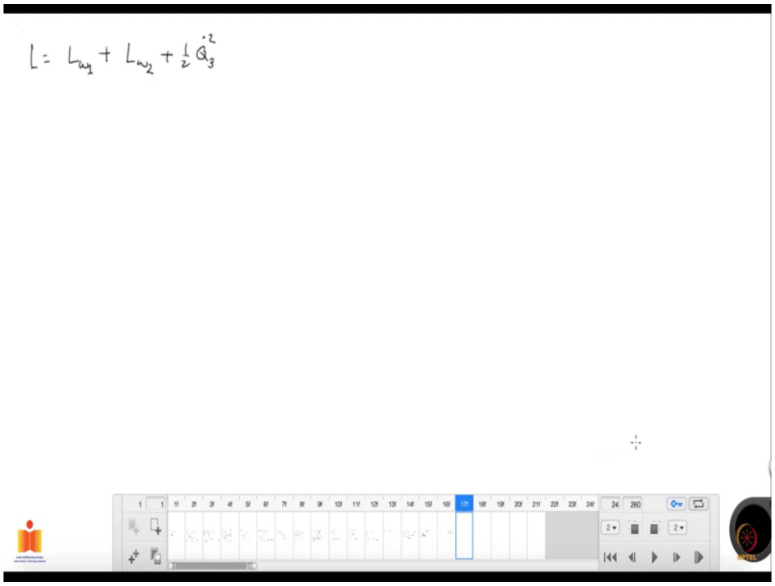

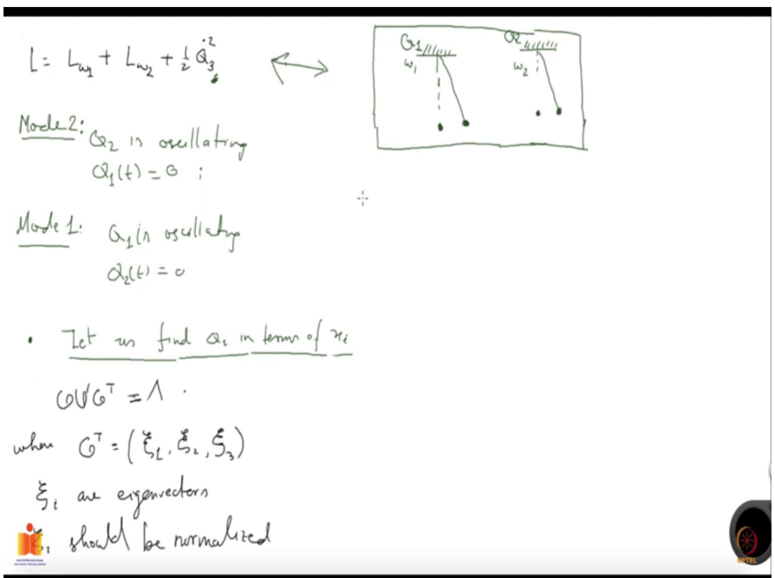

So the Lagrangian that we have I will write down as L of, I mean L is harmonic oscillator here we have describe by frequency 1, Lagrangian of harmonic oscillator describe by frequency 2 plus the term which is half Q3 dot square that is what we have. And this just a second let me remove this animation timeline, now this system I can pictorially represent like this. So my system is equivalent to that of having 2 harmonic oscillators, let us say I have 2 pendulums, one with corresponds to the coordinate Q1 and has frequency omega 1which is square root of lambda 1 basically.

And you have another harmonic oscillator described by your normal coordinate Q2 and which, this pendulum has frequency omega 2. I will tell you that later this is really an unimportant so that is why I am worried about it I will show you later. But anyway the Lagrangian for our system is this I mean the system is equivalent to this. Do not worry about what algebra we have done and what system we started with. As far as where we stand now this is the Lagrangian of the system and it is equivalent to this thing. That this is the system which we are having now in front of us.

Now if this is a system that is given to you then it is your choice which pendulum or which oscillator you want to set in motion. So you may choose to keep this one at rest so that this one does not move at all. So the mass keeps sitting here and only this oscillator is oscillating. So let me write that is one option you have so you can put the coordinate Q1 to be 0 at all the times and only Q2 is oscillating.

That is one, so I say that my system is in mode is oscillating in mode 2. If I should have written mode 1 first but anyway no problem. If I put Q2 to be 0 at all the times meaning this guy is just standing still here at rest and only this one is oscillating. Then of course Q1 is oscillating then my system is oscillating in mode, normal mode 1 that is what we say. So and of course you can do this because these two oscillators are in independent they are not coupled.

And that is what a normal mode is and that is how you can choose to set these, choose to make your system oscillate in one mode or the other. So, you may simultaneously put all other modes. Let us say your system was equivalent to having hundreds of oscillators. So you may choose to excite only one normal mode an all other modes you can keep at rest.

Now, that is all good, looks nice but you might be wondering how you are going to put your molecule to oscillate in first mode or in the second mode? What should you do that your triatomic molecule is oscillating in the first mode or second mode? So, for that you need to know how your normal coordinates are related to the coordinates X1, X2 and X3. So this what we are going to address, so let me write down in short that, to, I hope you are understanding what we are saying. So let us find Q i's in terms of Xi's, that is our task now.

Let me use black, good and that is not difficult. Let me put a, anyhow. So you know I already said that if I look at my matrix U prime it is diagonalize by an orthogonal transformation which is this. And that will put it in this form where lambda is diagonal and our, the diagonalizing matrix O or O transpose, let me write down for O transpose are the Eigen vectors xi1, xi2, these xi1, xi2 and xi3 are Eigen vectors of U prime. That you will already know from your matrix, understanding your matrices.

Which we also talked about couple of videos ago. So these xi1, xi2, xi3 are the column vectors. So this is a column, this is a column, this is a column, that is how you get a matrix. And as we talked sometime back these are Eigen vectors. Also remember that xi i's should be normalized, I hope you understood why you see when you solve the Eigen value equation you get Eigen vectors but any multiply of Eigen vector is also an Eigen vector with same Eigen value. And you also remember that when we were talking about diagonalization we when we look at orthogonal matrices, the matrix for the matrix to be orthogonal all not only all the columns should be orthogonal to each other each column vector should be normal.

So it is the magnitude of that each column vector should be 1. So whatever Eigen vectors you get you should normalize them. So that their magnitudes is, magnitude of that each vector Eigen is 1, so that is what this xi i should be. Now I will give you a set of simple exercises to do so that you can get arrive at the final result.

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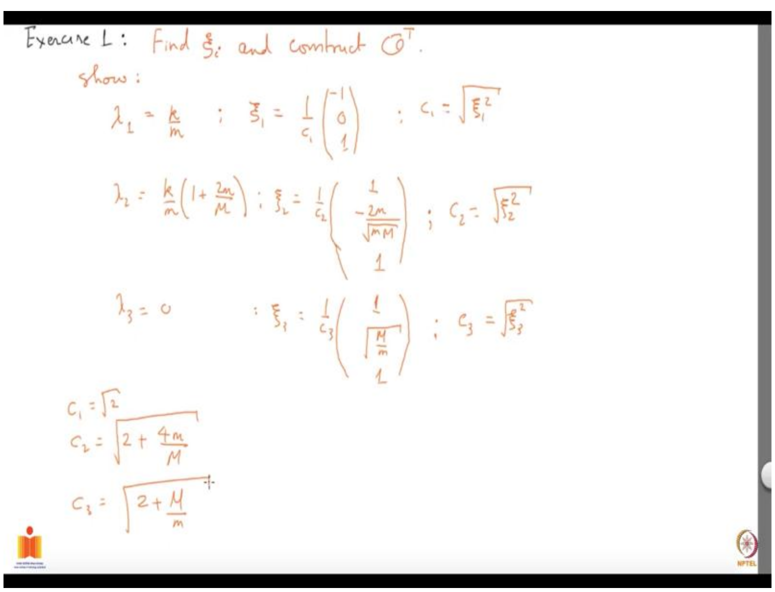

So let me list them down exercise 1, maybe some. So find xi i and construct O transpose, the transpose which I talked just now, so that is what you have to do which basically amounts to do in the following. So you should show that is you show that for lambda 1 equals k by m for this Eigen value and the corresponding Eigen vectors xi 1 is minus 1. The color is changed anyway I will write let me try to change the color, minus 1 0 1, and as I said we should normalize it which means I should divide it by constant c1, where c1 will be just xi 1 square underfoot.

If you do so then the vector xi 1 will be normalized. And also please find the Eigen vector corresponding to this Eigen value which I am writing now, these are the ones which we found earlier. So just find xi 2, xi 2 is again you have to normalize so I am dividing by 1 over c2 which you should find, and you will find when you calculate the Eigen vector, this is minus 2 small m over m capital M in square root. Fine, I will tell you why I had stopped for a second, you see I was checking the dimensions.

So all the time you should be checking for dimensions, so this is dimensionless, this is dimensionless so which is good. So this guy should also be dimensionless, otherwise clearly we have made a mistake. So here you have one mass and here you have two but then it is a square root so it cancels the mass dimension and that makes it perfectly fine dimensionless, dimension wise. So hopefully, that is correct.

Then you should find out the c2, c2 is again xi 2 square, if you divide by this this will be normalized vector the xi 2. And for lambda 3 equal to 0 you will get xi 3 1 over c3 1 then you have capital M over small m in the square root and then you have 1 here. And as before c3 is xi 3 square under root. Now it is trivial but I will never the less write down your c1 is root 2, c2 is 2 plus 4 m over M in the square root and c3 will turn out to be 2 capital M over m. So please do these exercises, fine and then what, then next exercise is the following.

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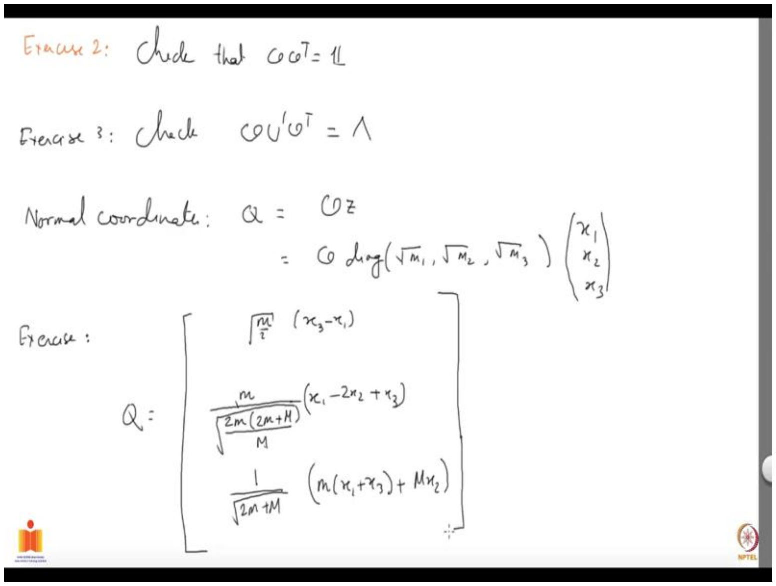

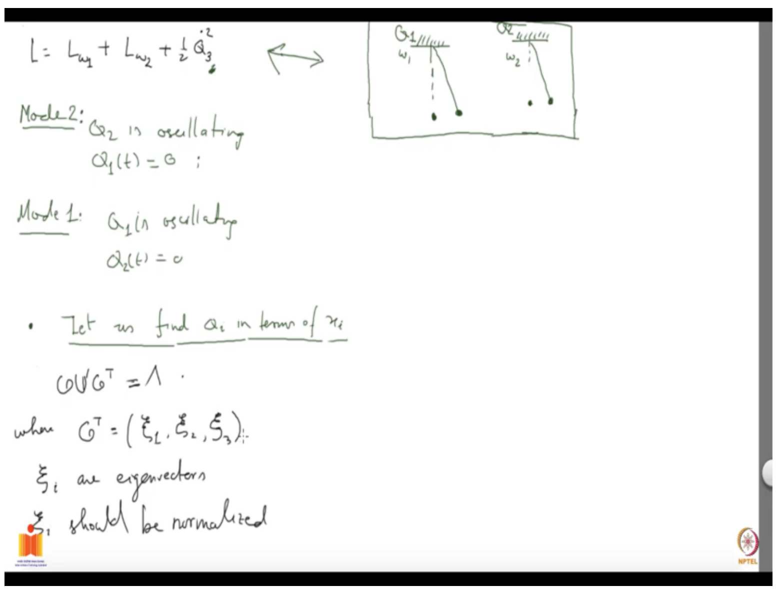

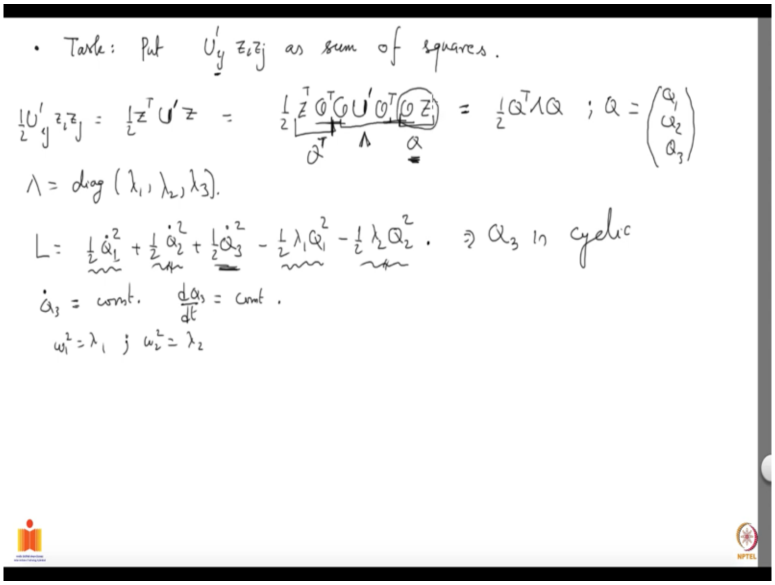

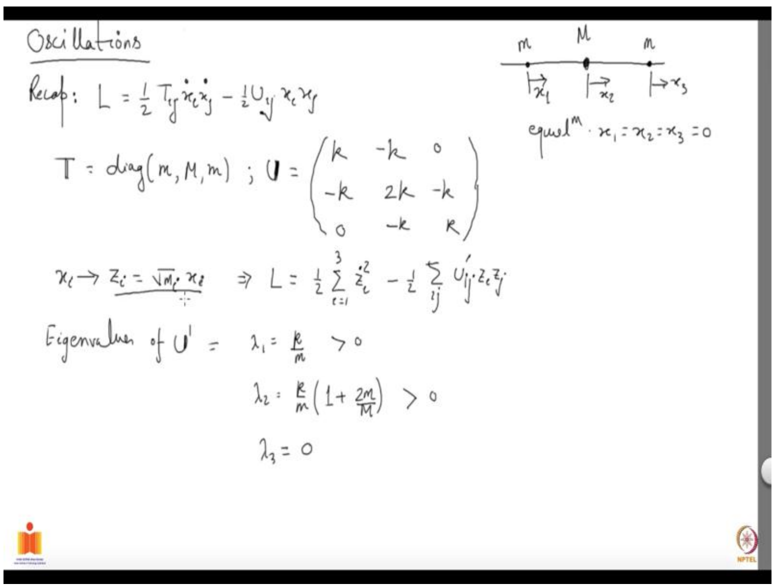

Exercise 2, I want to switch back to black color. Now you have to form O and O transpose and as I showed earlier our O transpose is just xi1, xi2, xi3 these three columns, column vectors placed together and check that when you have placed all these normalize xi1, xi2, xi3 into a column into a matrix they satisfy this.

This will give you confidence that the calculation you have done is correct or the results that I am giving to you is are correct. Now let us look at exercise number 3, so also check that UOU prime O transpose that comes out to be the diagonal matrix which we have been writing so, that will be another check. Now let us look at the normal coordinates. We wanted to know what Q is in terms of our x1, x2 and x3, and that is easy to find out because your Q is O times z where z is the column vector containing z1. z2 z3, let us go back and see that.

Somewhere here I should have written it, here, you see the Q is O times z. And if you also recall what z was, z was obtained by multiplying a diagonal matrix m1 square root of m2 square root of m3 where m1, m2, m3; m1 and m3 are small m and capital M is m2. This times x1, x2, x3 let us go back and check somewhere here should be, here you see the z is related to x by this which is what I am writing now in terms of a diagonal matrix.

So again, another exercise, check that when you multiply all this O the one, the O you have found already this diagonal matrix and this x1 you get the following. So you get the Q to be this x3 minus x1 m over 2 in the square root then you get x1 minus 2 x2 plus x3, and the coefficient is square, not square root m over 2 m 2 m plus capital M entire thing is divided by capital M and this is in the square root. Let us check dimension wise this and this piece have same dimensions and here it is a square root of m so we should have a square root of m here as well.

Now see this is m times m m square divided by mass it becomes m so the there is a mass in the square root and there is a mass in the numerator and so this works out. And then the third one is and that looks no it does not look strange it is fine, 2m plus M, I will tell you why I was surprised for a moment. I saw this factor in the denominator which is 1 over square root of m and I thought I am doing something wrong, but then I have a mass here which these together make the same as here. So it is all fine, there is no mistake I believe, so that is the Q. So you know what your normal coordinates are in term of x1, x2 and x3. That is good let us see what next.