Classical Mechanics: From Newtonian to Lagrangian Formulation
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Lecture – 58
Small Oscillation – 6

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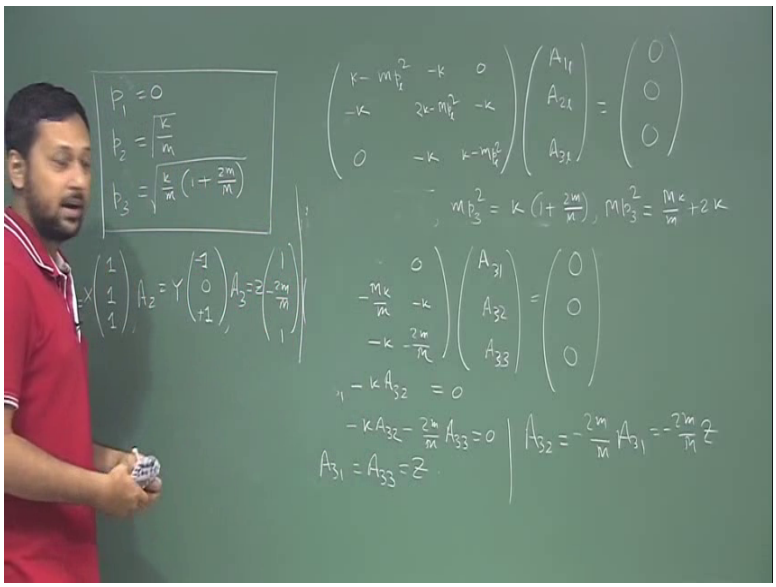

So, we continue our discussion and then we have found out that this is the third Eigen frequency or Eigen vector. And we see that the these two are equal and this one is negative opposite in sign, and there is a scaling factor. So, it means actually two masses they are going, so two outside the smaller atoms, they are going together like this or like that. And when they are moving on this side, the bigger mass moving in the opposite direction, where they are moving in like this, this one is moving in the opposite direction. So, we will give you a little more little detailed description of the same, but first let us try to normalize it. Now, this three you see there is an x, there is an y, there is a z and this three are arbitrary we have not given any we have not decided on any value of this matrices this quantities.

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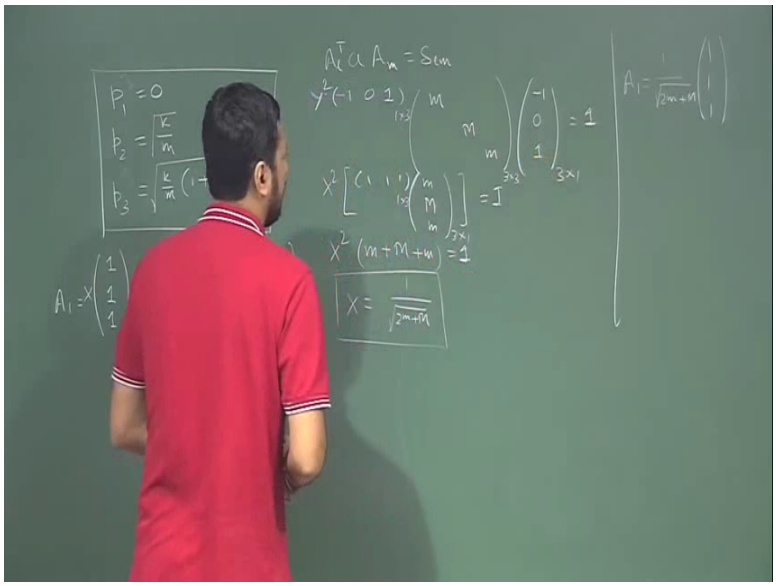

But what we can do is we can always find a means to normalize them. How do we normalize it? Please recall a sorry A l transpose a A m is equal to delta l m. So, this is our tool for normalization. What we are going to do is and if you so we are going to construct for example, with a 1 we are going to write x square 1 1 1 m capital M m 1 1 1 is equal to 1, this is just this relation open the, so I wrote it in an explicit form. Now, there will be an x from the transpose vector and x from this side vector. So, I just put an x square here. So, x square or x is a something, which we are looking to find out.

Now, if I perform this calculation this will be x square, see the first one it will be 1 1 1 m capital M m equal to 1, which will be X square m plus M plus m this is equal to 1. I am just doing it explicitly probably you already know how to this do this calculation. Please recall that it is a 3 cross 3 matrix please note is that it is a 3 cross 3 matrix, it is a 3 cross 1 matrix, it is a 1 cross 3 matrix. So, this will reduce it to a 3 cross 1 matrix, this is a 1 cross 3 matrix. So, eventually the final answer will be a single number 1 cross 1. So, x is 1 by root over this is 2 m plus m right. So, this is the value of x let we have put.

Now, in this case it is not terribly important because any way this is a translation it is not a true vibration, but just to show you just to demonstrate how it works this is the value of x. So, if you want to write the normalized value, so you have to write a 1 is equal to 1 by 1 by root over or just write little closer that is easier for the camera 1 by root over 2 m

plus m 1 1 1 good. Now, let us repeat the same procedure for this one, it will be Y square capital Y square, it will be minus 1 0 1, similarly it will be minus 1 0 1.

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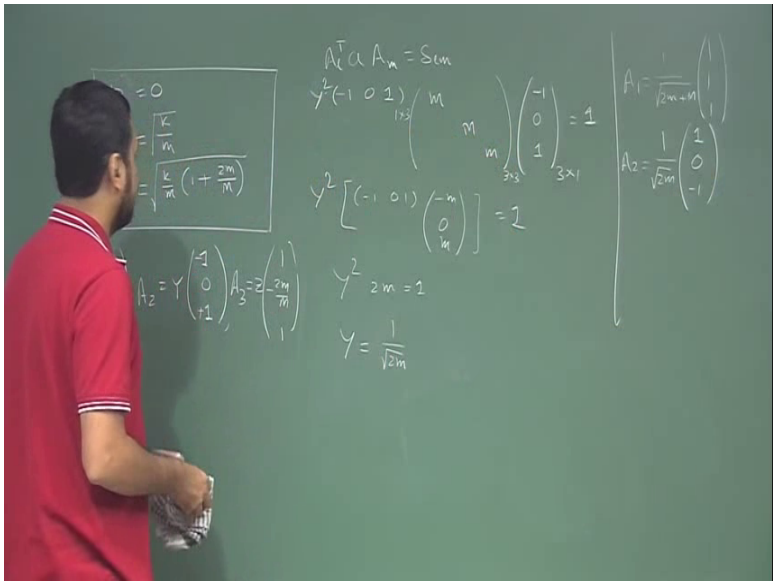

So, following the same procedure, we get Y square is equal or Y square times it will be m, so first it will be minus 1 0 1; second it will be minus m and m 0 it will be equal to 1. So, y square times, so it will be m plus m - 2 m, which will give you Y is equal to 1 by root 2 m. So, in this normalization the capital M does not enter, because there is no motion as I said for this mode it will go both together out or together in the side molecules, the central molecule will remain stationary. So, understandably there is no scaling there is no association of capital M with the normalization constant. So, if I write it, it will be 1 by root twice m 1 minus 1 or it could also be plus 1 minus 1 here, and there is a 0 in the middle.

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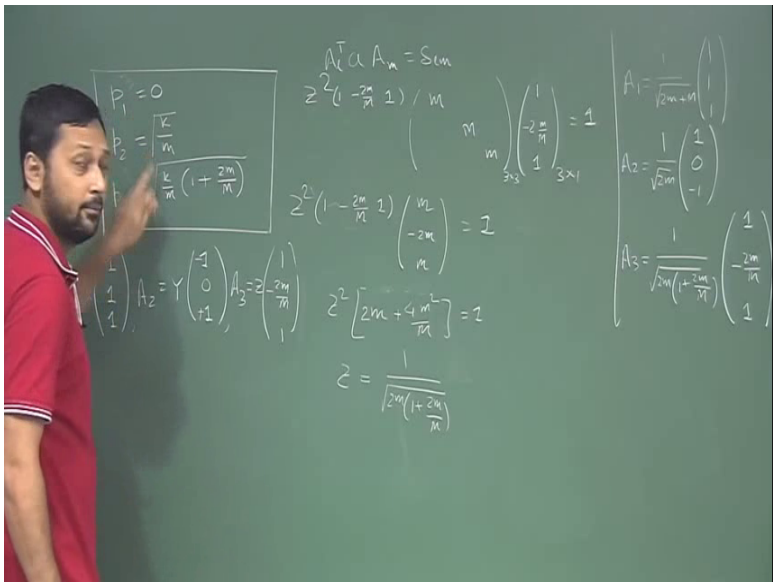

And for the third normalized Eigen vector, we have to write Z square with 1 minus 2 m by m 1 1 minus 2 m by m 1. So, second step will be m minus 2 m m equal to 1 and then we have z square times m minus 4 m square by m plus m. So, it will be 2 m 2 1. So, z will be equal to 2 m 1 by root 2 over 2 m 1 plus 2 m by m is it correct oh I have made it I did it correct great, I am doing well today, very good. So, A 3 is equal to 1 by root over 2 m 1 plus 2 m by m and 1 minus 2 m by m 1. So, this is the third Eigen vector.

Right now we have so we started with three frequencies 0, root k by m, and root k by m plus 1 by 2 m by m, and we have found out three normalized Eigen vectors. So, that means, the problem is in principle solved kind of not completely yet because we still have not you know officially declared what is I mean as in mathematically we have not proved what is normal modes and all. But let us once again let us look into the details of this motion. See I am taking time in this example because if something which is very intuitive, this example is easy to grab its calculations are slightly longer, but it is not complicated and also it is very visual this one. The other examples might not be that visual.

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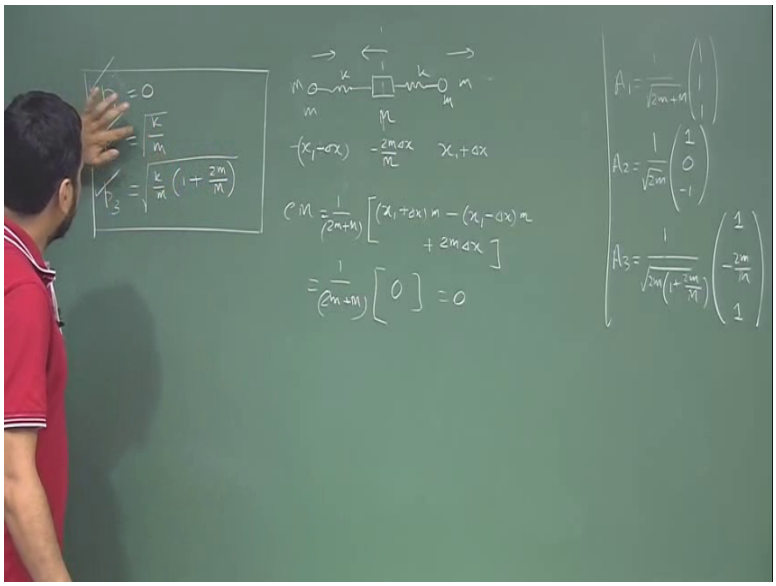

So, this is my molecule once again. So, we have m, m and capital M here. Now, what happens when there is a translation, there is a translation means all three moving in the same direction either this direction or that direction that is very straightforward. So, this we understand. For this one, we have seen that two are moving in opposite direction and one is stationary, so the central atom is stationary. Let say this one is heavier and this two are lighter. So, this one moves out or move in whatever they do, they do it in a synchronized manner with the frequency k by m and that is also very easily understood. Because see k by root k by m is the frequency if I replace this with a solid wall the frequency of this spring mass system will be root k by m, because this central atom is not moving in this particular frequency mode. So, this is a definition of a normal mode normal mode is a particular type of in a very particular motion in which system oscillates with one single frequency, there is no multiple frequencies in normal mode.

So, when the system oscillates with only one frequency then only this particular frequency then we have this one stationary as if this you can think of it as if you replace this with a wall solid wall and this two masses are moving independently, but not exactly independently. Because there is a very steady phase relation of 180 degree between this two. So, either again that is also relative because there on other sides of this particular molecule we are thinking that they are going out 180 degree, but if you think of it as a two independent systems, they are exactly synchronized any way. So, this is one motion.

And for the third motion with, so we understand this for this one you see two molecules two atoms they are moving in a same direction at a given instance of time. And the middle mass what is it doing it is going opposite with a scaled amplitude if I try to explain this right. So, these two are either going like this or going like this, and if these two are going like this the middle one is moving this way; if they are going like this the middle one is going this way with a scaling in amplitude which is given by 2 m by m.

Now, why so, this is why because there is another very interesting property of normal oscillation or normal mode vibration, please remember this properties specific to vibration. For translation and rotation, it might not be valid and that particular property is the center of mass in a vibration normal mode vibration should not move. So, what is happening here when for the first one it is a translation, so it is not a vibration that particular property is not a valid property. For the second one when they are this one is stationary and this two are moving, see by symmetry of this system if they are all identical if we have two identical masses with two identical spring constants k, the center of mass is exactly on this particular atom. So, when this two are moving out or coming in together this overall center of mass position is not changing.

Let us try to formalize it a bit lets us say I will just call them this is my origin, let us call this x 1, let us call this x 2. If this is the case or please remember that if it if this is x 1 sorry if this is x 1, this will be minus x 1, because this is my origin. I am just taking this just for convenience, so that center of mass at equilibrium position will be m what is the relation for center of mass sum over i m i r i divided by sum over i m i. So, the lower sum will be 2 m plus m and we have from here we have x 1 minus x 1 times m plus 0 capital M this will also cancel which will give you 0. So, center of mass at equilibrium is at 0. Now, if you for the first type of motion, if you boost the center of a boost the position of this to increase the position of this 2 by delta x. So, this will be x 1 plus delta x and this is minus of x 1 plus delta x, it remains the same because this two anyway cancels out.

Now for the third motion, what happens for this particular frequency, if this has gone by delta x let us say if this is gone let us say in this way x plus delta x. So, this one will be x 1 minus of x 1 minus delta x. And from the normalization from this relation does not matter if it is normalized or not from this relation we know that. So, we are discussing a situation once again we are discussing a situation do not be confused. We are discussing

a situation where this one is going this way, this one is going this way and this one is coming this. Now, this one will not be 0 anymore, but it will be minus 2 m delta x by capital M, because this one I will just open the bracket and write here if this one was minus x 1 or plus x 1 this is minus x 1 plus delta x this is plus x 1 plus delta x. So, this is minus 2 m by m delta x.

Now, you calculate the center of mass, total mass I am not interested that will remain the same anyway; I will just put 1 by 2 m. So, let it be there does not matter really. Now, this one is x 1 plus delta x m minus x 1 plus x 1 minus delta x m plus 2 m delta x this capital M and m will cancel out. And if you do that after this see first term will cancel out, second term will cancel out, so it will give you a 0 once again, so it will be equal to 0. So, and this x delta x we have taken at any instant of time, we can also take x 1 minus x is the calculation we will not change. So, whatever we do the center of mass for this frequency it is very intuitive, because this one is not moving at all and this two are moving out simultaneously you are coming in simultaneously, so the center of mass is stationary. This one both all three masses are moving even then we can show you we could have shown systematically that we have shown systematically that the center of mass is stationary, so that is another property of normal coordinates.

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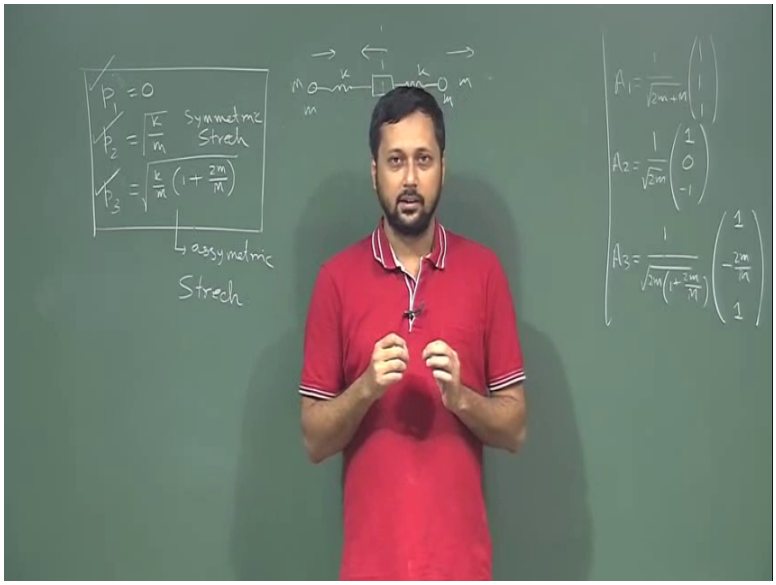

I will come back to that in a moment formalize the normal coordinates, but let us first tell you let me tell you that these two modes where the two atoms two site atoms are moving

in or out simultaneous, it is called the symmetric stretching. And this one where two are moving in one direction the other one is moving in opposite direction it is called asymmetric stretch of a linear triatomic molecule. Now, it is so happens that this modes for certain molecules for example, carbon dioxide molecules, they can be measured exactly using spectroscopy. And these modes are what some of this modes are responsible for the carbon dioxide laser. So, we have certain frequencies in laser right. So, in what happens in a laser we is that we have an optical cavity we have certain frequency, and if that frequency matches with the natural resonance frequency of this optical cavity then we can boost you know by stimulative absorption of radiation, we can boost this particular frequency and we can send a spark.

So, these modes the symmetric stretching modes and axisymmetric stretching modes and also bending modes of carbon dioxide molecules are responsible for different frequencies of carbon dioxide laser. Now, in molecular spectroscopy also for many triatomic molecules, we can actually measure the symmetric and axisymmetric matching modes. So, this is something which is more practical. So, more than theoretical aspect of it and it is been found out although they are very small systems, they are quantum mechanical in nature. The classical picture is not very far in terms of frequencies to describe the motion. So, we will if possible we will take up some of this I will show you some of this examples of real world spectroscopic data, but let us first the finalize our discussion on normal modes.

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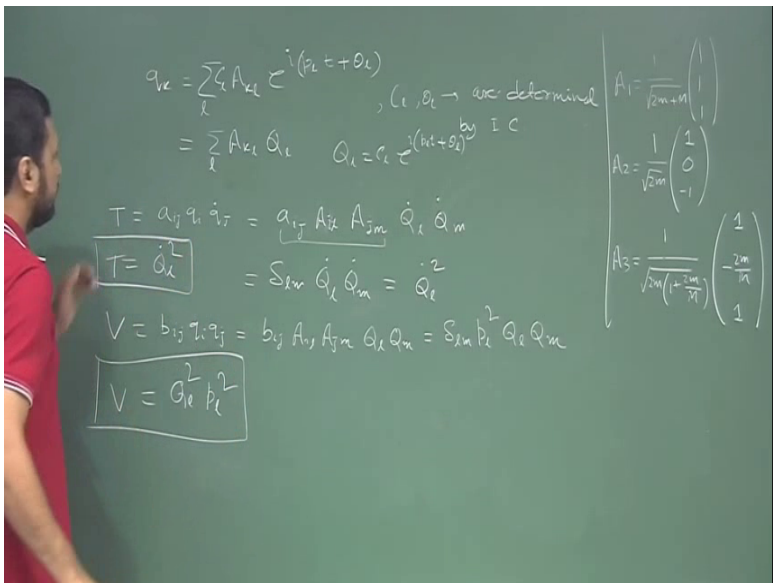

So, keep this in mind. We will come back and use this relation see q k is given by sum over l A l e to the power i p l right is it right, that is what we have written so far, but let me tell you this is not completely right, there are two terms missing. First of all they will be c l here I will explain this and secondly there will be a theta l here why these two constants additional constant see what we have what we have found out so far at the normalized part. So, this is something which will give you the quantitative description or rather qualitative description of the problem. Right now we have just just now we have discussed the symmetric stretching and axisymmetric stretching for a triatomic molecule. I can tell you by virtue of this normalized Eigen vectors, I can and tell you that what will be the proportion I mean what will be the relative motion between this molecules.

But what is a magnitude of it, no where in this discussion no in this expression you cannot find any you know the any number which is responsible for the amplitude the amplitude could be 5 millimeter, it could be 5 centimeter, it could be 5 meters nothing is mentioned here we do. So, nothing is associated with the system size except system masses are include definitely, but the lens scale is not included that lens scale you will be included there. Also I can look at it this way we have certain boundary conditions to begin.

So, let us say one molecule even triatomic molecule is in equilibrium position. So, if we start the oscillation, if we just displace one of the masses from equilibrium and let it go only then it will oscillate and that leads to some initial condition. Now, that initial conditions has to be included somehow in the final solution. Right now we have found out only this part A and p l, A l and p l, which is which gives you a very good qualitative idea of the motion, but not give you a single idea of what is the actual magnitude of vibration, also there is a face factor.

So, if we move it you know if let us say we have this as my initial configuration, so if I initially let us say I have taken this one in this direction, and this one in this direction. So, that means, we are stretching this spring and you know compressing that spring and then I let it go which mode of vibration will that be I mean which mode will be activated, will it still remain in the anti. So, moment we release it this two masses the this mass will start going inside and this mass will start moving outside so that means, they are going anti phase axisymmetric stretching. But also what we can do is we can also give a displacement arbitrary displacement of this and let it go. So, we do not know what will

be the phase relation unless and until and phase relation due to the initial condition unless and until we include this theta l here.

So, most general description will include of c l and theta l where c l theta l are determined by initial condition IC means initial condition. So, now that is something which we which gives you a complete description of the motion. So, we can write this as A l sum over l. So, there will be a k l all this time A k l q l. So, we can define Q l which is equal to C l e to the power i p l t plus theta l. Now, some of the books you will see that instead of this only the cos term cosine term has been taken that is also valid description, because the people use logic like the for real measure I mean for real life measurement we are interested only in the cosine part. The sin part is imaginary which is there, but which we will not be able to measure, so that is also a valid description. So, we define Q l like this.

Now if I try to look at my kinetic energy matrix which will be q k dot or rather a i j q i dot q j dot, now in terms of this representation, I can write this as a i j A i l A j m yeah Q l dot Q m dot. Now, look at this term this is nothing but delta l m, so that we have seen this is from the normalization this is how we normalized A ls. So, delta m Q l dot Q m dot which is because l equal to m is the only possible solutions, so we can just write it as Q l dot square.

Similarly, potential energy equal to b i j q i q j which will be b i j A i l A j m Q l Q m which will be delta l m p l square Q l Q m which will be V will be simply Q l square p l square. So, you see that both kinetic energy and potential energy. So, T is once again Q l dot square and V is Q l square p l square. So, in the in this new defined coordinate Q l which is given by this if I define this as a coordinate which is also valid definition because there is the only one running index l which is here and here as well here and here as well. So, c l and theta l are from the initial condition and p l is the normal frequency that we have to determine by solving this determinant. Now, if we do that in that representation T and V these matrices are completely diagonal.

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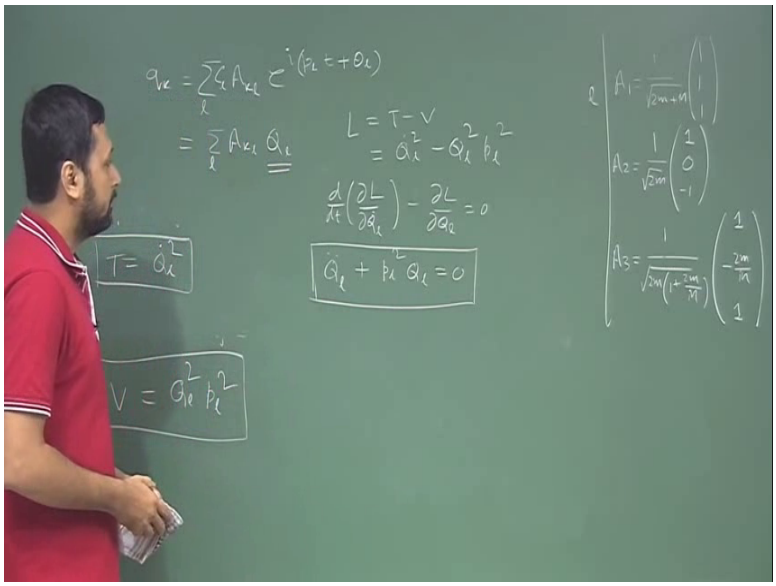

Not only that if I now construct this now this toward the matrices. Now, if I construct this Lagrangian, which is T minus V, which will be given by Q l dot square minus Q l square p l square. Now, in this Lagrangian, d dt of del l del q l dot dot minus del l del q l will be equal to 0. Now, if you do that you will get Q l double dot plus p l square Q l equal to 0. And this is kind of obvious the way we have defined Q l, this has to happen. So, if we work in a new set of coordinate q l the by the way this is a point transformation the same Lagrangian which we which we wrote in terms of Q ys and Q js we have reduced in terms of Q s capital Q s.

And in this particular after this point transformation not only the Lagrangian becomes a diagonal I mean Lagrangian becomes totally diagonal and each of this is a discrete independent equation. So, what we have here using this particular coordinate capital Q l, we have diagonalized not only the we have not only we have diagonalized the kinetic energy and potential energies, but also we could distinctly you know we could write independent differential equations for different frequencies and these are the theoretical definition of normal modes right. So, we will do one thing we will take it up from we will go back to this example of linear triatomic molecule and I try to find out what are the normal modes here right.

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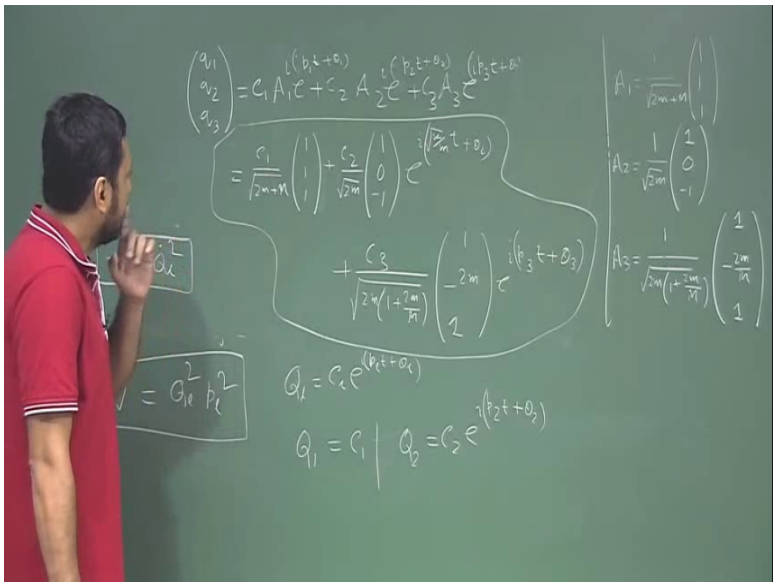

So, for linear triatomic molecules, we have not written the final solution. We have written three frequencies which was p 1 equal to 0, p 2 equal to root k by m, and p 3 equal to root k by m 1 plus 2 m by m. Am I right just give me a second, I will just check here yes good. So, these are three. So, we can write in terms of the Cartesian coordinates q 1, q 2 and q 3, we can write them as C 1 or rather we can write them as C 1 A 1 plus C 2 A 2 C 1 A 1 e to the power i p 1 t plus C 2 A 2 e to the power i p 2 t plus C 3 A 3 e to the power i p 3 t. Now writing explicitly it will be C 1 by root 2 m plus m 1 1 1, this will be 0 because p 1 is this will be 1, because p 1 is 0 plus C 2 by root twice and 1 0 minus 1 plus C 3 by root twice m 1 plus 2 m by m 1 minus now e to the power i i wrote k by m t 1 e to the power i, I will just write p 3 t.

So, in principle, we can write q 1 expression for q 1, q 2, q 3 of course, there will be a theta 1, there will be a theta 2, and there will be a theta 3. So, it will be plus theta 2, i will be outside i will be outside plus theta 3, so that is the most general solution get rid of this ones. So, these is my most general solution for a linear triatomic molecule. Any motion if we are given boundary condition, they are initial conditions in terms of C 1s and theta ones, we can find out the instantaneous position of any of this coordinate.

Now, in terms of normal mode, so what will be the normal modes in this case, we have to write Q ls, if I have to write Q ls my q 1 will be, what is the definition go back to the definition once again which is sorry Q l is equal to c l e to the power i omega l t plus

theta l or other p l p l t plus theta l. If I follow this definition, my Q 1 will be C 1. I am not writing it explicitly forget about the amplitude it will be C 1 there will be no amplitude term plus C 2 e to the power i root k by m t plus theta 2 plus C 3 e to the power i this big term this third frequency whatever p 3 t plus theta 3.

So, this is my one normal mode. Similarly, I can write expression for two other sorry it will be oh sorry it will be C 1 right C 1 e to the power i p l t plus theta l. Q 1 will be simply C 1 sorry my mistake Q 2 will be C 2 e to the power i p l or p 2 t plus theta 2, and same for Q 3. So, these are my three normal coordinates k. So, now, we have solved this problem in principle in terms of both normal modes and we have found out the normalized amplitudes. So, this problem is in principle solved. Of course, unless and until we have boundary conditions we cannot determine C 1s and theta ls which will be which will take up in one of the next problems. So, we have a few more problems in the problem set, and we have two more lectures in hand we will see it we will try to find it we will try to solve it as soon as possible. And once these are solved if we still have sometime probably we will revisit some of our previous discussion and go little bit more into the details.

For now thank you.