Mathematics for Chemistry
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Lecture - 4

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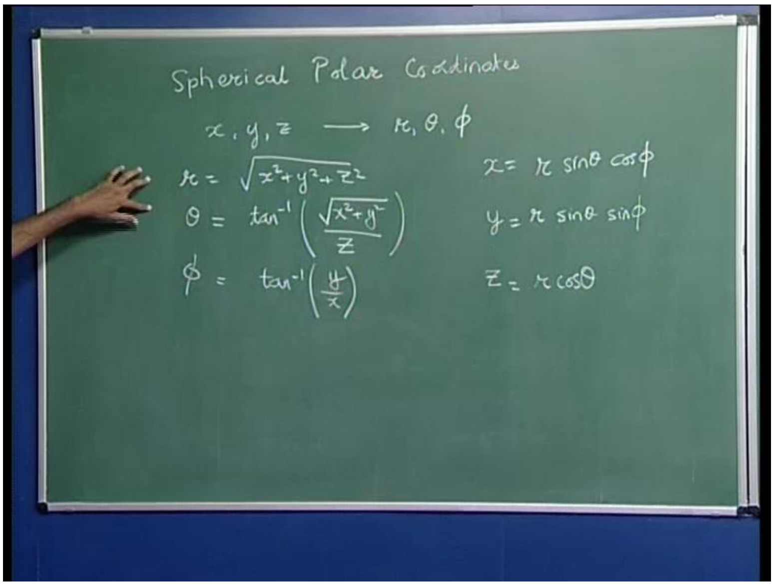

So, in the last class we discussed towards the end of last class. The spherical polar coordinate and the cylindrical polar coordinates, and this is the general field of change of coordinates. And in today's class, what I will do is try to give an application of what we have done so far; and the application that you will see is involves a change of coordinates it involves the change, it involves change of coordinates of a two body problem to the center of mass and relative coordinate system. Before we do that, let us recap what we thought. We said that the spherical polar coordinates and I will be using this in the class today, so I want to recap this part.

So, spherical polar coordinates; in this we have we go from x y and z to r theta and pi and the definitions are r is equal to square root of x square plus y square plus z square; theta is equal to tan inverse square root of, you can write it as tan inverse of square root of x square plus y square divided by z; and pi is equal to tan inverse y by x. So, this is the way you transform, you write r theta and pi in terms of x, y, z similarly, you can write x, y, z in terms of r theta and pi and we will just write down the value x is r sin theta cos pi y is r sin theta sin pi and z is r cos theta.

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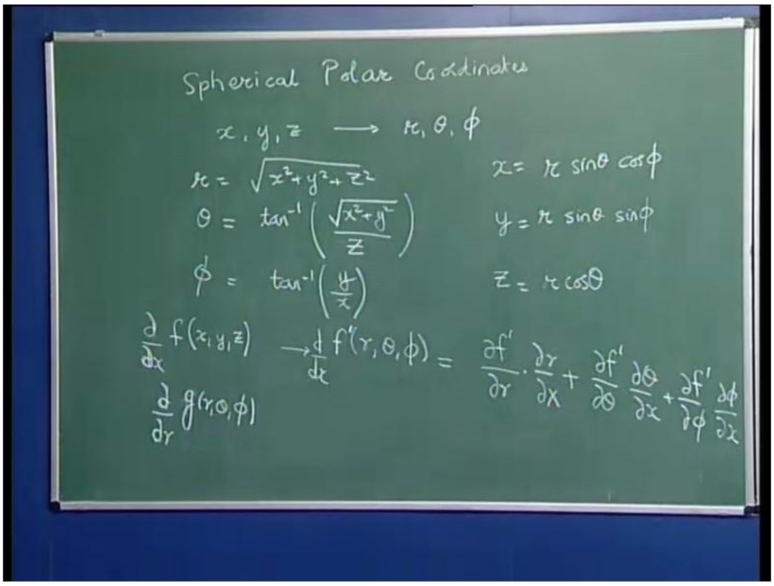

Now, I am emphasizing these relations, because these are the relations that you will use whenever you want to transform from one set of variables to another set of variables. And one set of transformations that you will do, will involve writing derivatives with respect to x, y, z in terms of derivatives with respect to r theta pi. So, I just want to briefly mention how you will do this transformation this is the usual calculus of any variables and I want to emphasize that when you do this transformation you have to be careful how you do it. So, suppose I have d by d x and I want to write it in terms of derivatives with respect to r derivatives with respect to theta and derivatives with respect to pi.

Now, I will be taking d by d x of some function and the function can be a function of x, y, z. Now, if wherever I have x I substitute this wherever I have y I will substitute this wherever I have z I substitute this value then my function will go from a being a function of x, y, z to a function of r theta pi and I will call it f prime r theta pi and I still have derivative with respect to x. Now, the point is how do you write this derivative with respect to x in terms of derivatives with respect to r theta and pi and to do this you know this that here I have a function of many variables and I am taking different shell with respect to some other variable.

So, I use the chain rule for partial differential equations to write this in the form dou, f prime by dou r into dou r by dou x. So, the dependence on r will be seen in this term and.

So, this is like if I only had a function of r then I would have only have this but, then since I also have functions of theta and pi I will have two other terms plus dou f prime by dou pi dou pi by dou x. So, we have used the normal chain rule for a partial differential equations and or and for a function of many variables to write derivative with respect to x in terms of derivatives with respect to r theta and pi similarly, I can write derivatives with respect to y and I can write derivatives with respect to z in terms of derivatives with respect to the other quantities.

Now, it is very important that, this should be written as a function of r theta and pi and nothing else it should be written as a function of r theta and pi there should not be any x y or z appearing in this f prime. Now you could ask a question what about going the other way. So, suppose I had a function suppose I will call it g of r theta pi and I am taking derivatives with respect to r of this function actually this should be a partial derivative, and the I will just step back here and say why this should be a partial derivative. So, this should actually be a partial derivative and we will look at the reasons why it should be a partial derivative?

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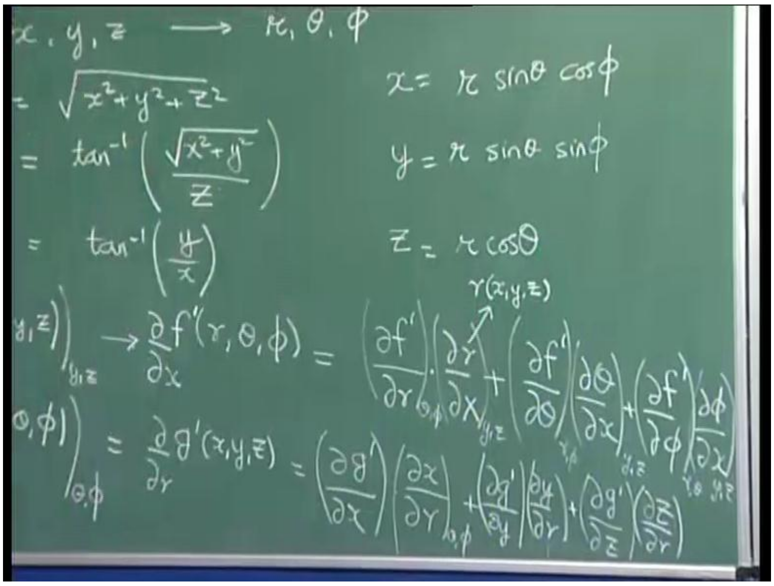

So, the reason it should be a partial derivative is that we want to take the derivative with respect to x keeping y and z fixed. So, when I take this derivative I keep y and z fixed and I would not bother saying that when you take the derivative with respect to x you have to keep y and z fixed but, that is understood. Now in this case here when I take the derivative with respect to r I have to keep theta and pi fixed and here when I take derivative of r with respect to x I need to keep y and z fixed similarly, here I will keep r and pi fixed and here I will keep y and z here.

Again, I will keep r and theta and here y and z. So, the point is we will always deal with partial derivatives and we would not bother writing this sub indices. So, because it will make our notation a lot simpler but, the point is that when you are taking derivative of r with respect to x you have to keep y and z fixed and that means your r has to be expressed as a function of x y and z. So, you should use r as a function of x, y, z, you should use this relation now similarly, when you write theta as a function of x you should use this relation when you take derivative of theta with respect to x and similarly, when you take derivative of pi with respect to x you should use this relation and it is important to keep track of which variables you are differentiating with and which variables are kept constant, and that will also tell you which relations you should use here now similarly, if you had a partial derivative with respect to r here the assumption is that theta and pi are kept fixed.

So, this is at fixed theta and pi and what we want to do is to write this in terms of derivatives with respect to x, y and z. So, you can follow exactly the same procedure. So, what you do is wherever you have r you use this relation wherever you have pi you use this relation. So, you go from a function of r theta pi to another function of x, y, z we will call this g prime of x, y, z and now your derivative with respect to r can be expanded in a chain rule just like this. So, what you had is derivative with respect to r keeping theta and pi fixed. So, you can write this as dou g prime by dou x this is this is keeping y and z fixed into dou x by dou r dou r. So, we are taking derivative with respect to r and this is keeping theta and pi fixed plus dou g prime by dou y into dou y by dou r plus dou g prime dou z dou z by dou r and as usual here you will keep theta and pi fixed here also you will keep theta and pi fixed now if you want to calculate dou x by dou r then you need x as a function of r theta and pi. So, you should use this relation. So, when you calculate dou x by dou r you use this relation when you calculate dou y by dou r you use this relation and when you calculate dou z by dou r you should use this relation.

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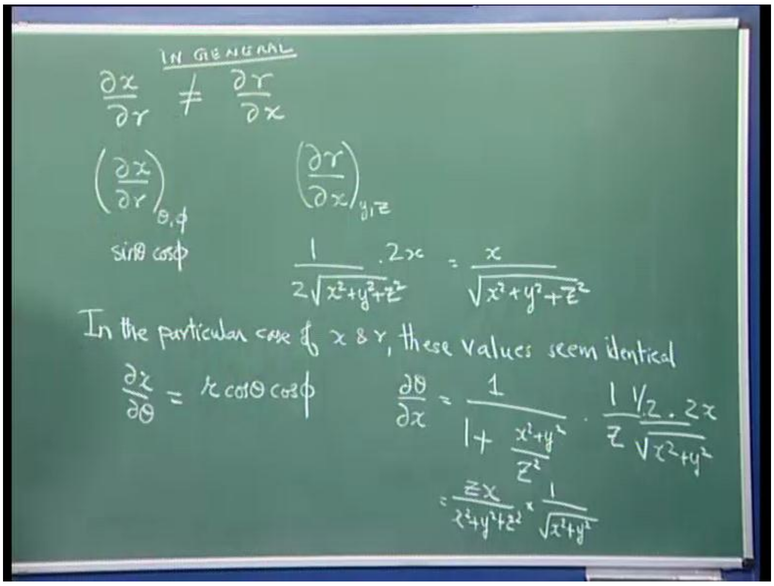

Now remember in this notation it is not true that dou x by r is not equal to dou r by dou x. So, this is very important to remember it is not like the usual ordinary derivatives in this case the partial derivative of x with respect to r is not the same as partial derivative of r with respect to x and the reason for that is when you write this derivative when you write dou x by dou r then the variables that you are keeping fixed you have to write x as a function of r theta pi. So, the fixed variables are theta and pi. So, when you take partial derivative with respect to r you are keeping theta and pi fixed and in this case when you are taking partial derivative of r with respect to x you have to keep y and z fixed and in general these two are not equal they may be equal in some special cases but, in general they are not the same. So, for example, I want to calculate dou x by dou r then I will be using this relation.

And so, if you use that relation what you get is dou x by dou dou r is equal to this is in general. This is not true in this particular case what you will get is that dou x by dou r is just sin theta cos pi cos pi in this case dou r by dou x if you use this relation you will get 1 over two square root of x square plus y square plus z square and you will get a 2 x. So, you will just get x divided by square root of x square plus y square plus z square, and the confusing part is that. In this special case these two seem to have the same value because this is x by r which is sin theta cos pi. So, in general this is not true.

So, that is why i am emphasizing that in general you take derivative of one quantity with respect to another, and you do the same partial derivative you would not get the same answer but, in the particular case. So, in the particular case of particular case of x and r these values seem identical. However let us look at dou x by dou theta. So, if you want to calculate dou x by dou theta you use this relation and what you will say is that, this is equal to r cos theta cos pi and if you take dou theta by dou x dou theta by dou x. So, in this case you will get 1 over 1 plus if you take the derivative of tan inverse you will get 1 plus x square plus y square divided by z square times the derivative of this argument and the derivative of that argument is just 1 over z into 2 divided by square root of x square plus y square into sorry half square root of x square plus y square into 2 x. So, dou theta by dou x in this case will be this is equal to z divided by x square plus y square plus z square z square into 1 over square root of x square plus y square, and you can easily show that this is not the same as this quantity in fact this has dimensions of r whereas, this has dimensions of 1 over length. So, even dimensionally these quantities are not the same. So, it is important to keep in mind that this need not be true.

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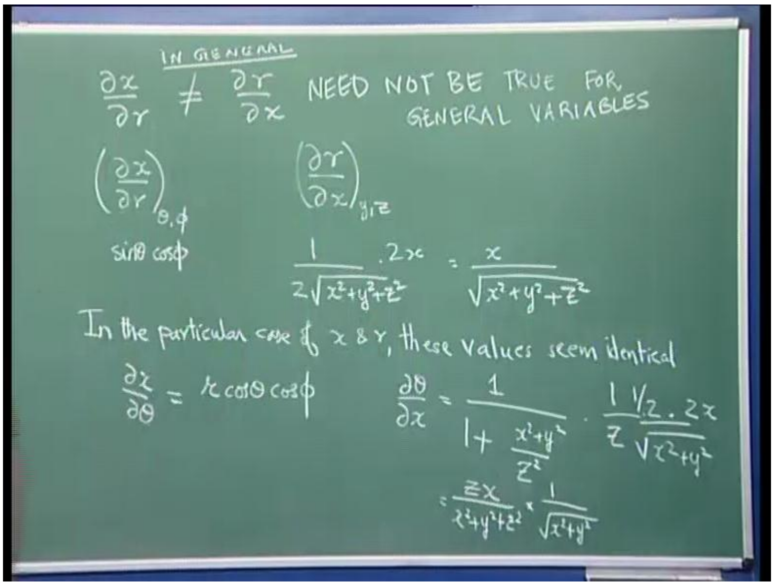

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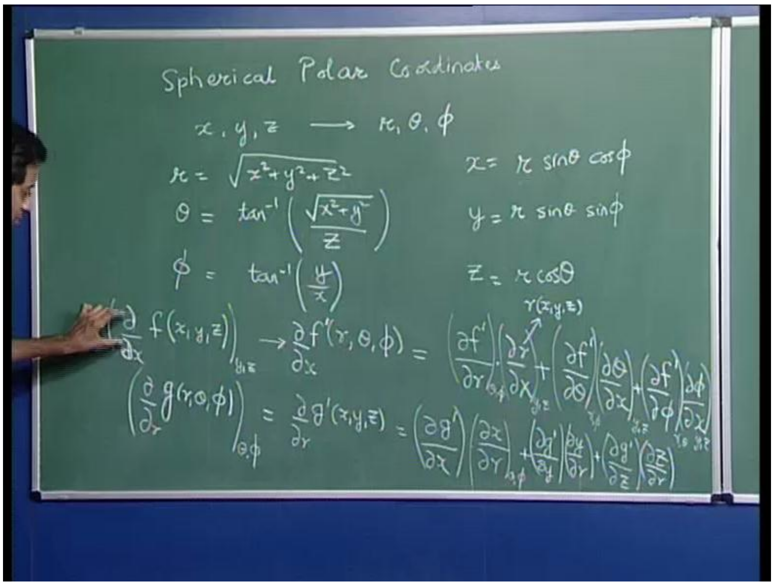

So, I again emphasize need not be true for general variables. So, anyway at the end of this what you get is that you can transform a function of x, y, z to a function of r theta pi. You can transform derivatives with respect to x y and z to derivatives with respect to r theta and pi and with these transformation rules you can completely change from 1 coordinate system to another coordinate system here we have taken the examples of spherical polar coordinates but, the same method of the transformation of coordinates can be used for any 2 sets of coordinates.

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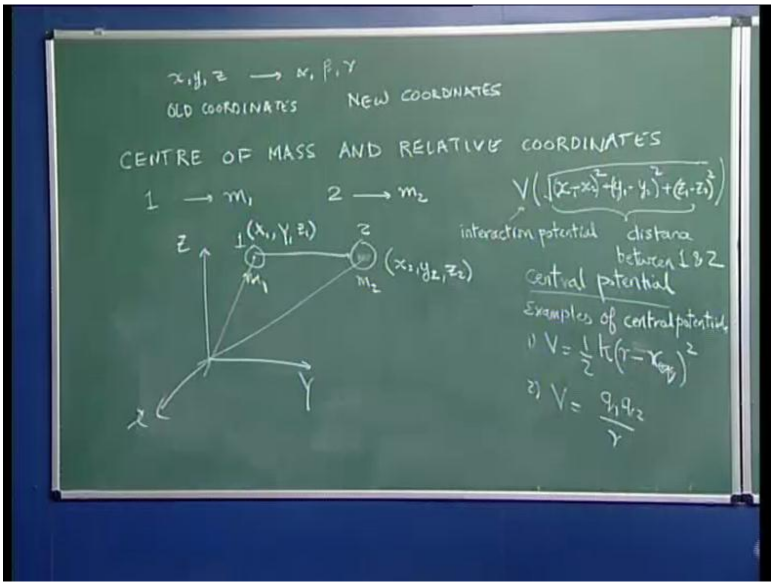

So, here once again I emphasize that we have taken the special case of spherical polar coordinates but, if you go from x, y, z to some arbitrary coordinates you can still use the same transformation rules. So, we can go from a set of coordinates x y and z to another set of coordinate's alpha beta gamma. So, these are the new set of coordinates. So, old coordinates to new coordinate and when we do this transformation. We know? How to transform functions of x, y, z to functions of alpha beta gamma and vice versa? And we also know how to deal with derivatives involving x, y, and z. And write them in terms of derivatives involving alpha beta gamma. So, let us take particular example of this and this is an example, that you probably have seen in the quantum chemistry courses it is related to the center of mass and relative coordinates.

And this is classic way of solving a converting a two body problem into single body problem. So, let us consider a quantum mechanical system that consists of the two particles is particle 1 of mass m 1 and particle 2 mass m 2. So, and these two particles have an interaction between them. So, the interaction potential. So, the potential of interaction of the two particles depends only on the scalar distance between them. So, it depends only on x 1 minus x 2 square plus y 1 minus y 2 square plus z 1 minus z 2 square just depends on the square root.

So, this is a interaction potential and when the interaction potential depends only on the scalar distance between the particles distance between the particles and when you have this case where the interaction potential depends only on the distance between the particles you say that, this potential is called a central potential. So, such a potential of interaction is called a central potential and there are many such examples of central potentials in fact all the potentials that we deal with are mostly are usually central potentials. So, what does this look like you have a particle of mass m 1 and you have another particle of mass m 2 this is particle 1 particle 2 mass m 2.

Now, the coordinates of this particle could be in the coordinate system, the coordinates of this particle are written as x 1, y 1, z 1 and the coordinates of this particle are written as x 2, y 2, z 2 all small letters here. Now we have specified the system. If we specified the form of the potential then we have completed the specification of the problem. So, examples of central potentials so, we can say V is equal to half k r square. So, it is as how these two particles are connected by a spring of spring constant k and. So, when you stretch the particles the potential energy changes and in fact more correctly.

What we will say is r minus some equilibrium length r equilibrium length square. So, the spring has some equilibrium length, and if you stretch it beyond that then the particles feel some force the other example is if these two of the interaction between the two particles is columbic in nature then you can say V looks like and it looks like if Q 1 and Q 2 are the charges on the particles Q 1 Q 2 by r. So, where r is a distance field in the particle and depending on the sign of Q 1 and Q 2 it could be attractive or repulsive. So, these are examples that you will see in your courses on quantum chemistry.

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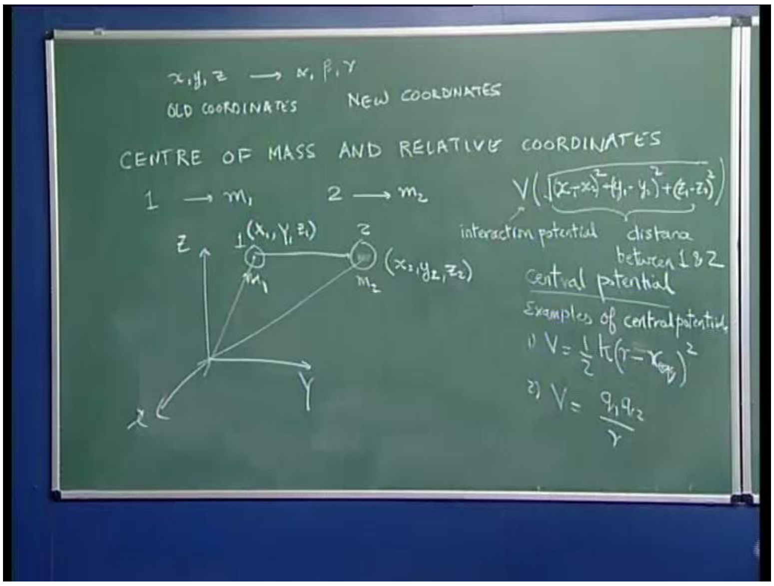

And what I want to show you is to take the general case of a two body problem where the interaction potential only depends on the distance between the particles. So, in other words of i take these two particles I keep the distance a same but, I place them in this way if. So, long as i keep the distance as same the energy of the system will not change. So, I can take this particle put it here, I can do all these things and it would not change the energy of the system and this is something that makes physical sense.

So, it should not matter which way the particles are oriented. So, long as the distance between them is the same. So, what is typically done in your quantum chemistry courses is to solve what is called the time independent Schrodinger equation for this problem and we would not go into solving the time independent Schrodinger equation for this problem but, you should be familiar with an object called the Hamiltonian which appears in quantum chemistry. So, what we will do is we will write the Hamiltonian for this system in the old coordinates and then see how transform that Hamiltonian into the new coordinates.

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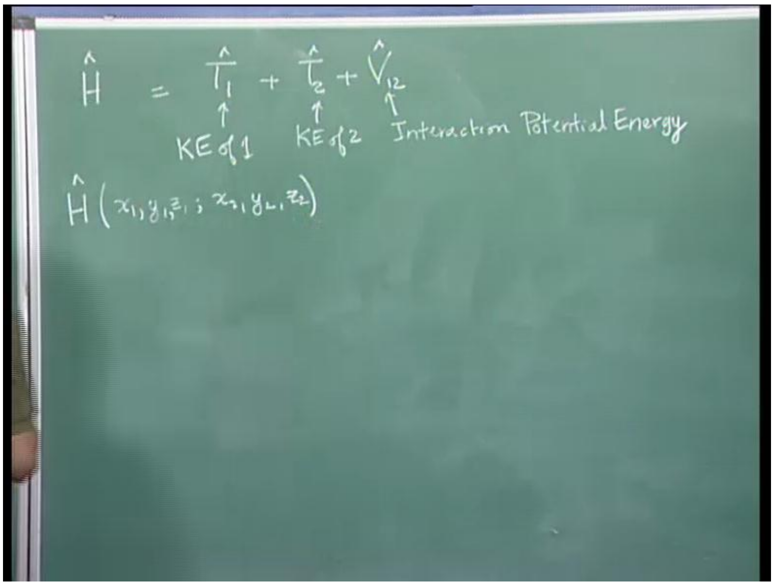

So, we start with the Hamiltonian as you must be familiar from your quantum chemistry courses is an operator for the total energy. So, the Hamiltonian it can be written as in this case. So, this is the total energy operator. So, it involve the kinetic energy of particle one it will involve the kinetic energy of particle two and it will in involve the interaction the potential energy of interaction between the two particles. So, I will write this as V 1 2 this is kinetic energy of 1 kinetic energy of two this is the interaction potential energy. So, the point is we know the form of the operator for kinetic energy of 1 and this form of operator in the in the x, y, z coordinates or a or rather x 1 let me get back to this.

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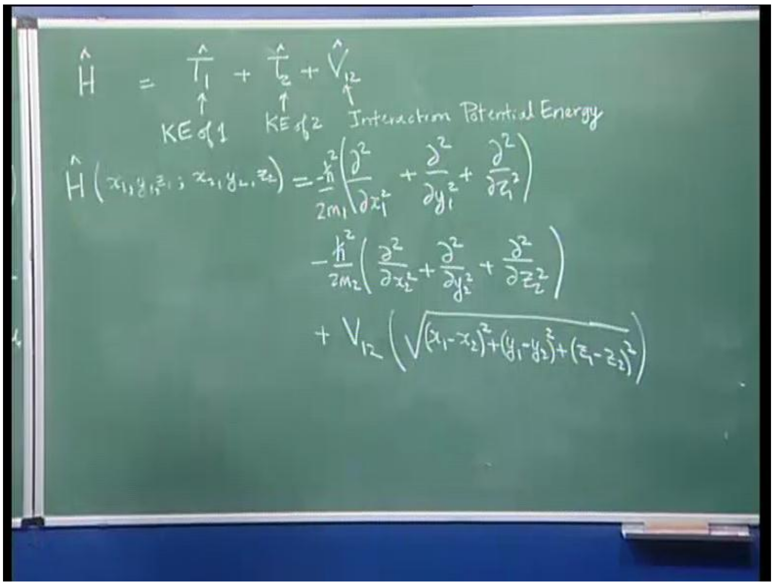

So, the Hamiltonian is an operator that operates on the variables involving the positions of both the particles. So, this involves this operates on the positions of particle 1 and particle two. particles 1 has three position coordinate x 1 ,y 1, z 1, particle two has three coordinates x 2 y 2 z two. So, this Hamiltonian operator operates on these positions. So, it involve it operates on these positions and it involves and it operates on functions of these positions.

Now, what we want to do is to take this form and write it instead as something that operates on what are called a center of mass and relative coordinates in order to do that let us first look how the Hamiltonian looks for a for these two particle system and you will be familiar with this you will be able to write this as d square minus h cross square by two m 1 d square by d x 1 square plus d square by d y 1 square plus d square by d z 1 square. So, this is the kinetic energy of particle 1 then you write the kinetic energy of particle two as minus h cross square by 2 m 2 and what you have is and in addition you have to have the interaction potential energy and we will just write it as V 1 2 of and this is a function only of the only of the scalar distance between the two particles. So, if the distance between the two particles is r this is the function only of this distance and this distance can be written in this form.

So, V which is a function of square root of and the operator for this is just a functional form of this. So, if this form is half k r minus r equilibrium square the operator form of this will just be multiplying by half k into this square similarly, if this form involves a 1 over r the operator form will also involve multiplying by 1 over r. So, this is the entire Hamiltonian and what we will do in the next fifteen or twenty minutes is to take this Hamiltonian and write it in terms of transformed variables and the variables that we will choose to transform them are what are called the center of mass and relative coordinates.

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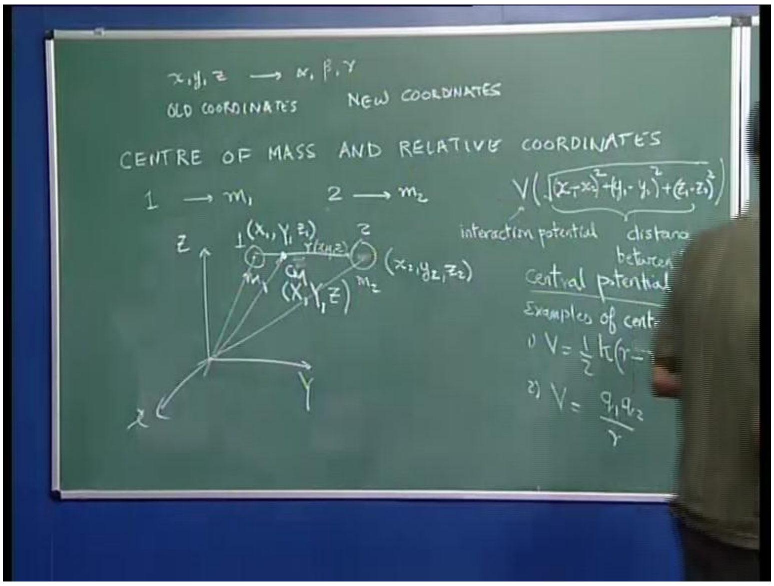

So, before we see how this is to be done lets define the center of mass and relative coordinates. So, you can say that. So, our goal is to go from x 1, y 1, z 1, x 2 y 2, z 2 to two coordinates and the two coordinates 1 will be the center of mass coordinate. So, if the center of mass is of the system is here center of mass and that will have coordinates capital X, capital Y, capital Z and the other coordinate is the relative coordinate which we represent by r that is x, y, z little x, little y, little z. So, this is the transformation we are going to do and we will see that center of mass and relative coordinates.

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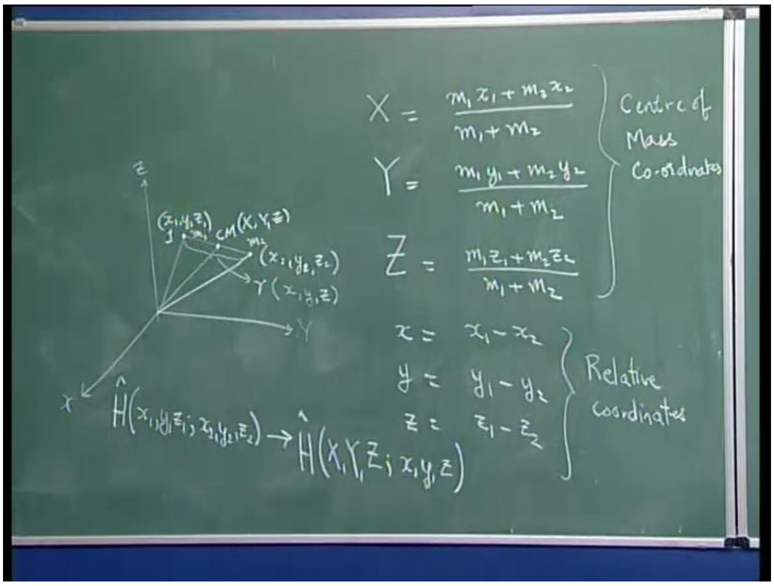

And once again let me remind you. So, we have two particles this is the x coordinate you have first particle located at x 1, y 1, z 1 this is particle one and particle two is located at x 2, y 2, z 2 and we are going to a system this particle has particle one has mass m 1 this has mass m 2 we are going to a coordinate system in which instead of using x 1, y 1, z 1, x 2, y 2, z 2 we will use the center of mass coordinate. So, if this is the center of mass coordinates are typically represented by capital X, capital Y, and capital Z, and we have the relative coordinates. So, this is r and this is represented by little x, little y, little z.

So, the meaning of these will become clear when we define this transformation. So, the transformation is defined in the following way capital x coordinate is the coordinate of the center of mass of these two particles and that is given by m 1 x 1 plus m 2 x 2 similarly, capital y is given by and capital Z is given by. So, these define the center of mass coordinates. So, these three together are called. So, this tells where the center of mass of this two body system is located. Now if you want to write the Hamiltonian operator since we had six variables here you need three more variables and the other three variables are what are called the relative coordinates they are given by little x is equal to x 1 minus x 2 z and these three are what are called the relative coordinates. So, we have set up the problem.

Now, we went from a coordinate system involving x 1, y 1, and z 1 to a coordinate system involving x 2, y 2, and z two. So, we went from a coordinate system involving these two to a coordinate system involving capital X, capital Y, capital Z and little x, little y, little z. So, the next target is to write your Hamiltonian which is written in terms of an operator on functions of x 1, y 1, z 1, x 2, y 2, z 2, to a Hamiltonian which can be written as an operator on functions of these x variables. So, we want to go from here to a Hamiltonian which is a function of these x variables. So, I will just write it down here. So, you want to go from h operating on x 1, y 1, z 1, x 2, y 2, z 2 to h operating on x, y, z little x, y, z. So, the question is, we how will we do this transformation and the answer is that you will do exactly what we did when we went from center of mass to a spherical polar coordinates, only thing instead of three coordinates.

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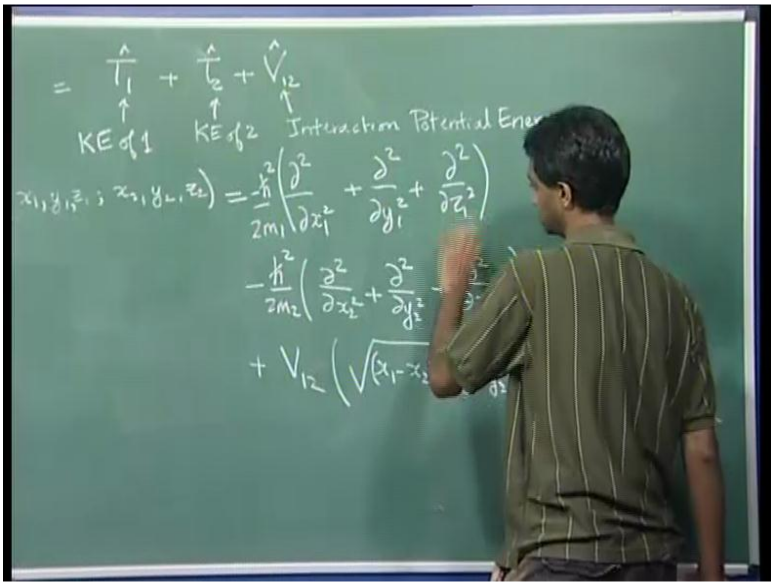

Now, you have to do it or with six coordinates. So, here we wrote capital x capital y capital Z in terms of and little x little y little z in terms of in terms of x 1, x 2, y 1, y 2 and z 1, z 2 what we want to do is to take this operator and transform from x 1, y 1, z 1, to a x 2, y 2, z 2 to those coordinates. So, whatever we have to write in terms of in terms of capital x capital y capital Z little x little y little z.

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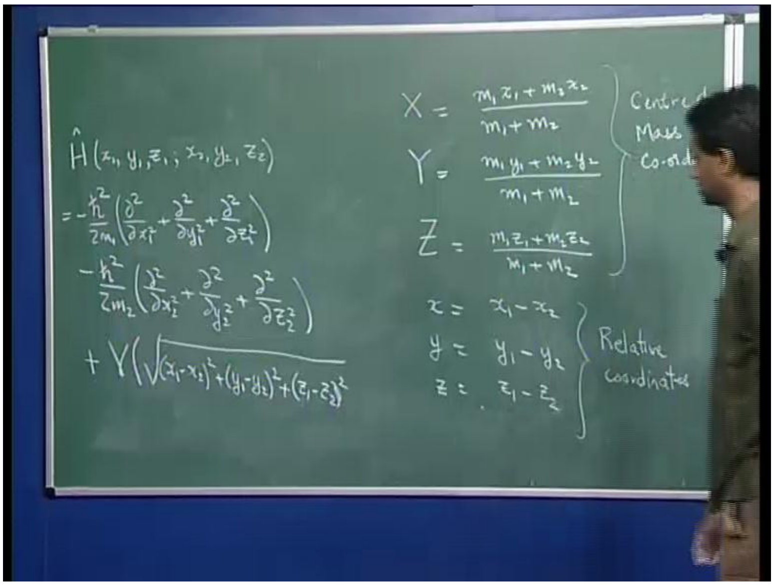

So, let us see how that is done center of mass and relative coordinates and our target is to take the Hamiltonian which is written as a function of x 1, y 1, z 1, and x 2, y 2, z 2 as this is written in the form minus h cross square by 2 m 1 d square by d x 1 square minus h cross square 2 m 2 plus V which is a function of square root of. So, we want to go from a function of x 1, y 1, z 1, x 2, y 2, z 2 to a function of x, y, z and let me remind you once again that, this is the kinetic energy of particle one this is the kinetic energy of particle two and this term is the interaction potential energy of the two particles in order to do this what we will do is that.

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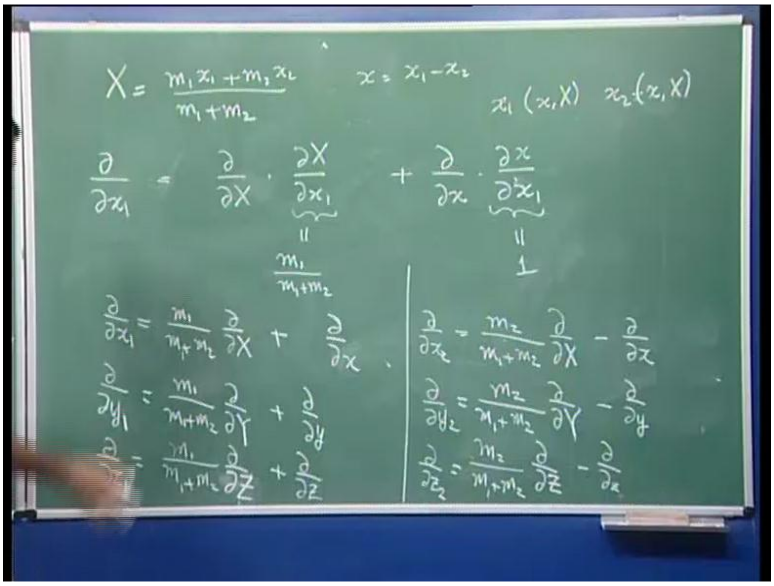

What we will say is that wherever we have d by d x 1 we want to write it in terms of d by d capital x and in terms of d by d little x. So, let us we have the equation x is equal to m 1 x 1 plus m 2 x 2 divided by m 1 plus m 2 and we have little x is equal to x 1 minus x 2. So, the first thing first thing you will say is that is that if I have this involves d by d x one. So, if I want to express d by d x 1 in terms of d by d capital x and d by d little x then I will write this as d by d x 1 is equal to d by d capital x into d capital x by d x 1 plus d by d little x into d little x by d x 1.

So, here whatever function I had I can express using these two expressions I can express x 1 in terms of capital x and little x and x 2 in terms of capital x and little x I can write x 1 as a function of x capital x I can write x 2 as a function of x 2 as a function of little x and capital x and I have once my function my this Hamiltonian operates on some function, and if I can write that function as a function of little x and capital x then I can use the chain rule for partial derivatives which we used earlier to write the derivative with respect to x 1 in this form and. So, if this operates on function you it will operate on the same function here and that function will appear here.

So, let us then the question is what is this and in order to calculate this, that you will say that I am taking the partial derivative of capital x with respect to little x one. So, that should keep all the other variables fixed the other variables will be y 1, z 1 and x 2, y 2, z two. So, if you do that, then I just have to take the derivative of this with respect to x 1 keeping everything else fixed and. So, I can write and if you take the derivative you will just get m 1 divided by m 1 plus m two. So, we will get exactly just m 1 divided by m 1 plus m 2 similarly, if I take the derivative of little x with respect to x 1 little x with respect to x one, I will just get one.

So, then I can write d by d x 1 is equal to is equal to m 1 divided by m 1 plus m 2 d by d capital x plus d by d little x. So, that takes care of d by d x 1 here. Now similarly, I can write d by d y 1 as m 1 by m 1 plus m 2 into d by d y plus d by. So, I can write d by d y 1 is equal to m 1 m 2 dou by dou capital y plus dou by dou little y and I can write d by d z 1 as m one. So, I have expressed derivatives with respect to x 1 y 1 and z 1 in terms of derivatives with respect to little capital x and little x capital y and little y capital Z and little z this is capital z. So, what I should have here is capital Z now this completes only half the problem the other half of the problem is to express is to express derivatives with respect to x 2 and z 2 in terms of derivatives with respect to capital x and little x and. So, we will do that right here we do not I mean it is it should be fairly obvious if I take the derivative with of with respect to x two then, what I will have is d by d capital x into d x by d x two.

So, partial of capital x with respect to x 2 and you can see from this expression that, this is just m 2 divided by m 1 plus m two. So, this will just be to d by d capital x. So, once again what the first term if I had instead of x 1 if I had x 2 then the first term would be d by d capital x into d capital x by d x 2 and that is just this expression the second term would be d by d small x into d small x by d x 2 and so that you can show that d small x by d x 2 if you look at this expression if I take the derivative with respect to x 2 then I will just get minus one.

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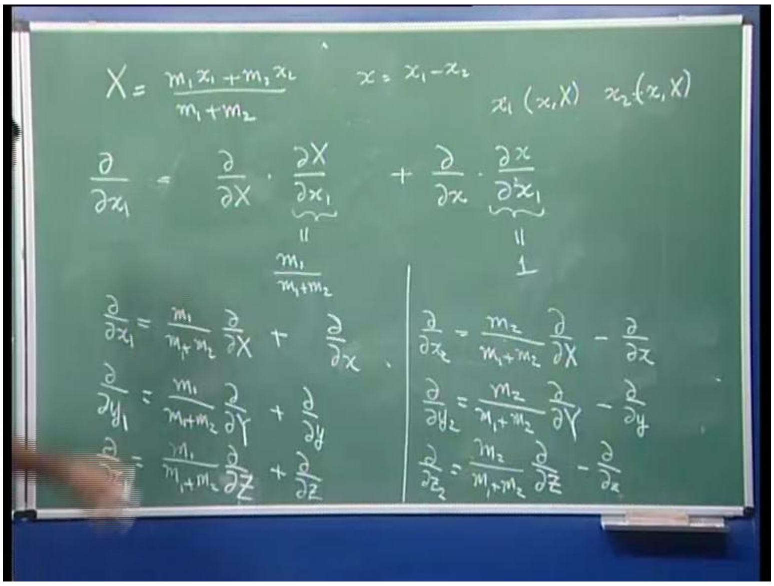

So, then this second term will just look like minus d by d x and. Similarly, I can write d by d y 2 as m 2 divided by capital y and I can write d by d z 2 as m 2 ok. So, this completes the first part of the exercise is where we wanted to express functions with respect to x 1 y 1 and z 1 and x 2 y 2 z 2 in terms of derivatives with respect to x, y, z a little x little y little z now. So, the next part is to just take this expression substitute it here in order to do this you have to calculate the second derivative. So, this gives us the first derivative. Now the next task is to calculate the second derivative with respect to x 1 and if you do that what you will see is that you will have two derivatives with respect to capital x 2 derivatives with respect to small x and 1 derivative which mixes capital x and small x. So, let me do that next. So, we have the first derivative now we have to calculate the second derivative.

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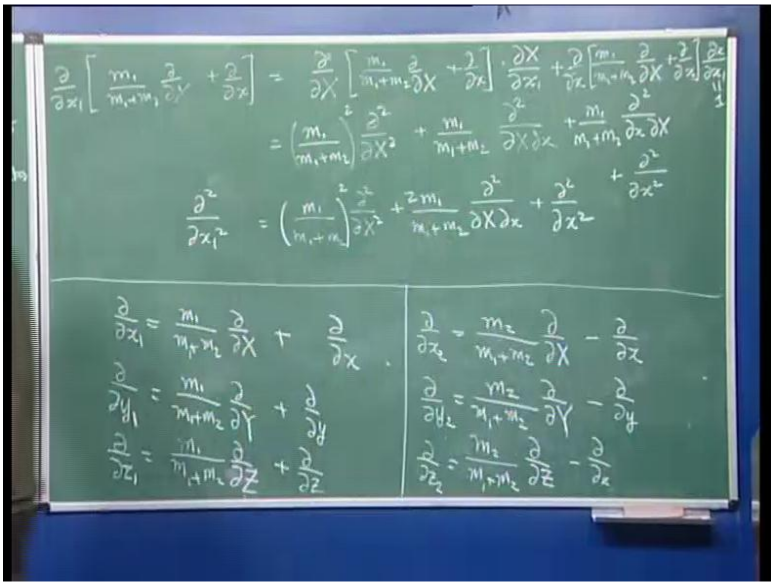

So, if I take the second derivative that is just like taking a first the derivative of this. So, if I do that can I have dou by dou x 1 of m 1 over and if I go ahead and do this. Then I write this as d by d capital x of the first derivative that is m 1 into d x by d x one. So, I just take this thing and put it here plus I get d by d little x of x into d x by d x one. So, I have the. So, I am using the chain rule again for partial derivatives. So, d by d x 1 I am writing as d by d capital x into d capital x by d x 1 plus d by d small x into d small x by d x 1 and you already know these values. So, I can write this as I can substitute for this and I will I would not go into the details but, you can show that this is equal to m 1 over m 1 plus m 2 square dou capital x square. So, that is the first term and the second term will be m two. So, this will give me a quantity m 1 over m 1 plus m 2 and what I will have is I have a 1 d by d x and I have 1 d by d little x due to d square by d capital x to little x plus I will have a term and here I have m 1 by m 2 now what I have is d by d x of.

So, this quantity is just one again. So, the first term will just be m 1 over m 1 plus m 2 dou square by dou little x dou capital x and the last term will just be d square by d x square. So, we will have these four terms now notice that in these two terms it is only the order of the differentiation that is changed and if your function is a continuous function of both these variables then the order of the differentiation does not matter. So, I can write this as m 1 plus m 2 dou square by dou x square.

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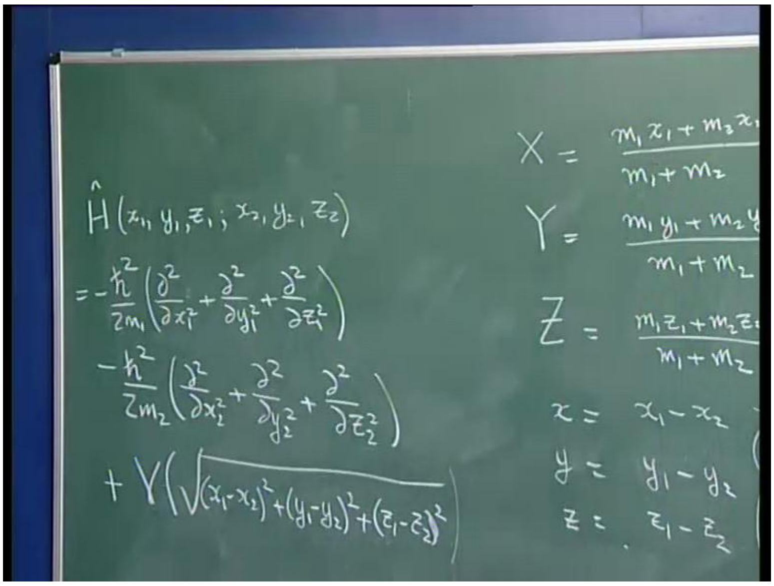

So, m 1 by m 1 by m 1 plus m 2 square plus m 1 twice m 1 over m 1 plus m 2 dou square by dou x dou x plus dou square by little x square. So, this whole thing is equal to dou square by dou x 1 square. So, you have three terms for dou square by dou x 1 square similarly, we will have three terms for dou square by dou y 1 square and you will have three terms for dou square by dou z 1 square and again three terms for each of these now as far as a V goes V is V can be expressed simply using x 1 x 1 minus x 2 equal to little x y 1 minus y 2 equal to little y and z 1 minus z 2 equal to little z in terms of x y z. So, let us put all this together and see what we get and what you will realize is that what we get is something very familiar to it will be quite familiar to many of you.

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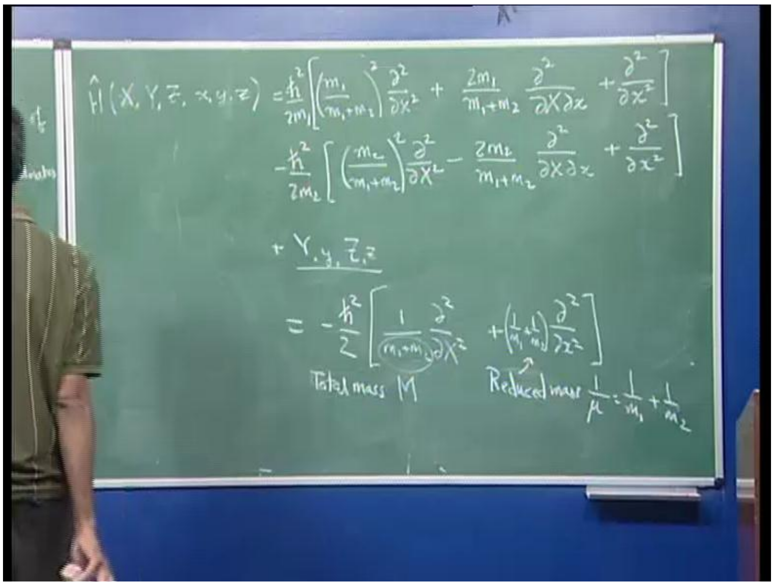

So, when I put all these together what I will get a Hamiltonian which is a function of little x of capital X, capital Y, capital Z, little x, little y, little z, and each of these will have various terms. So, when I take the second derivative with respect to x 1 I saw we saw three terms here and I want. So, what I will do is I will collect the various terms in a convenient ways to write this in the following form plus m 2 square d square by d x square into. So, this is minus h cross square by 2 m 1 into this plus. So, this whole thing is just the contribution from this first term.

Now, you can show for yourself that the contribution from this term from the x 2 term you will have a contribution that looks like m 2 what you will get is m 2 divided by m 1 plus m 2 square and then this will change to a minus sign. So, minus 2 because you remember in the derivative with respect to x 2 the component involving d by d x came with a minus sign. So, 2 m 1, 2 m 2 and you have. So, similarly, you will have plus for y z and z. So, you will have terms involving all these. So, we would not bother writing that. So, let us look at this part now if I add these two terms here I have a 1 by m 1 here I have 1 by m two. So, then m 1 square becomes m 1 and you have m two. So, you have m 1 plus m 2 divided by m 1 plus m 2 square and.

So, I can write this whole Hamiltonian as minus h cross square by 2 and. So, have 1 over m 1 plus m 2 and m 1 plus I have 1 over m 1 plus m 2 dou square by dou x square then what you notice is that these two terms will cancel each other because here I am dividing by m 1 here I am dividing by m two. So, I just get plus 1 over m 1 plus m 2 and I get minus 1 over m 1 plus m 2 and they will cancel each other and if you take these two terms these two terms they will give you just. So, I have d square by d x square 1 over m 1 m 2 and for those who are familiar this term is called a center of mass capital m center of mass or the total mass and this is called the reduced mass or it is a actually 1 over the reduced mass is 1 over m 1 plus 1 over m two.

So, this looks like 1 over reduced mass d square by d x square and this 1 over total mass d square by d capital x square and I would not go into the details of the remaining parts but, you can show that you can write similar expressions for y which will be exactly the same instead of d by d x you will have d by d y instead of d by d little x you will have d by d little y and similarly, for z.

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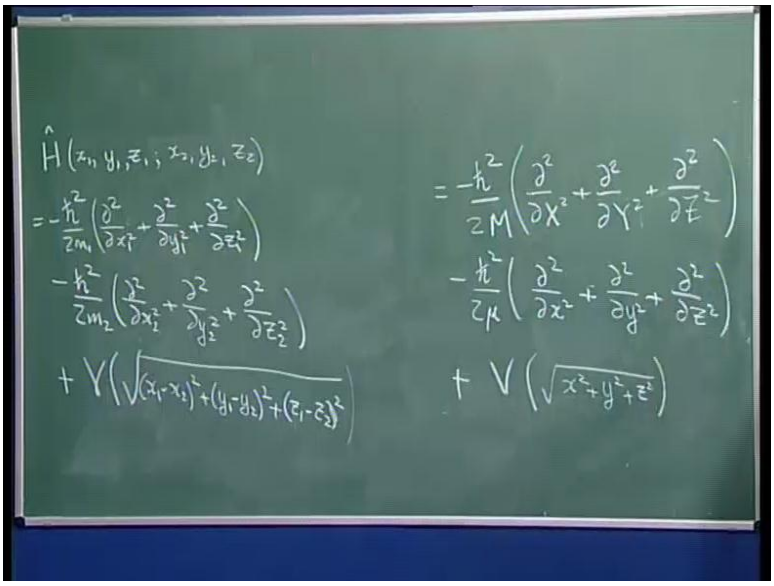

And so, you can finally, write this Hamiltonian in this form. So, you can finally, write the same Hamiltonian as minus h cross square by two capital m dou square by dou capital x square plus dou square by dou capital y square plus dou square by dou capital Z square minus h cross square by 2 mu dou square by dou little x square plus dou square by dou little y square plus dou square by dou little z square plus you have the interaction potential. So, the interaction potential is just written as V which is a function of square root of x square plus y square plus z square. So, we wrote the Hamiltonian from x 1, y 1, z 1, x 2, y 2, z 2, to coordinates involving capital X, capital Y, capital Z, little x, little y, little z, and this is a standard center of mass and relative coordinates that is used in your chemistry courses.