Quantum Mechanics
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Lecture - 26
Classical vs Quantum Mechanics - II

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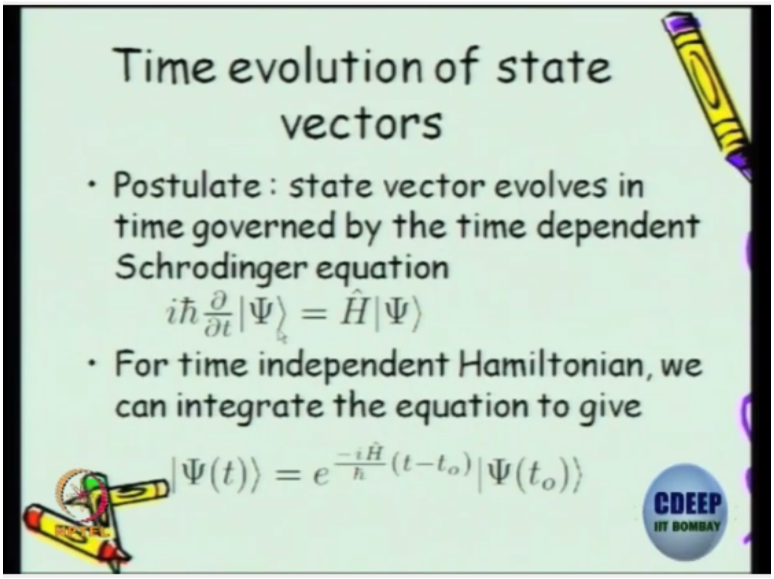

Okay what was the next one; we had a Hamilton's equation in classical mechanics. Similarly, we need to give a time evolution of the state vectors. So that is the equation which is your familiar time dependent Schrodinger equation and that Schrodinger equation again depends on Hamiltonian. Here it will be an operator. So this is an operator equation operating on any state vector psi and this equation will tell us how the state vector psi evolves in time okay.

So that is where the dynamics is coming on time evolution on the state psi. Suppose the Hamiltonian is kinetic energy+potential energy and you are putting potential energy like harmonic oscillator or hydrogen atom, they are all called time independent potential energy. You know when you will get time-dependent potential energy? You can start having you know time dependent electric field on a charged particle.

Then, the potential energy will be actually time-dependent right but we are not going to consider that at least for this course. In this course, your Hamiltonian which we are going to take is always time independent. So this is a very simple thing, if the operator is independent of time, you can take all the things on one side, so this will give you a log function and then this will give you a iHt and you will have some constant, then you can solve it and get this equation.

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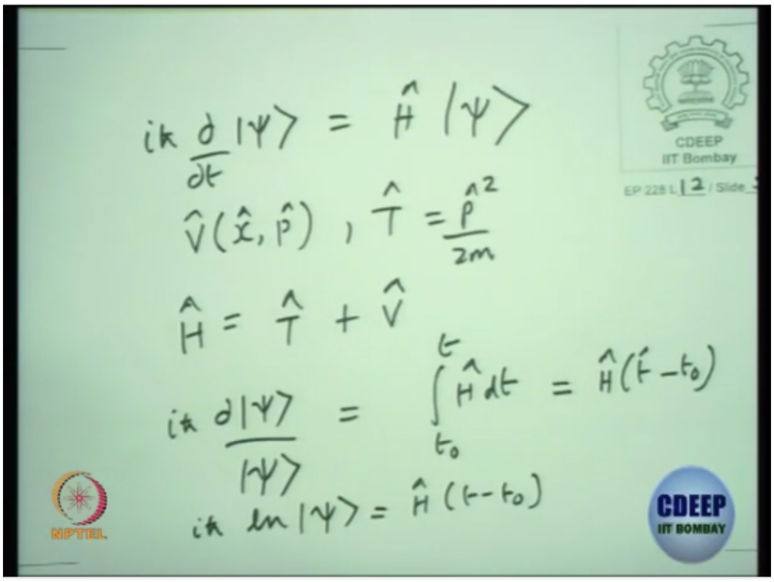

I is H operator on psi and if you take V to be only a function of x and p, V also in general is an operator and of course kinetic energy operator is P squared/2m, Hamiltonian will be T+V. So in such cases, I can write ih cross del psi/psi to be integral of H hat t dt which is independent of time we can pull it out and go from t0 to t and that will give you H t-t0. What is this left hand side?

Left hand side is log function of psi; psi h cross log psi is H hat t-t0 then take the exponential on both sides.

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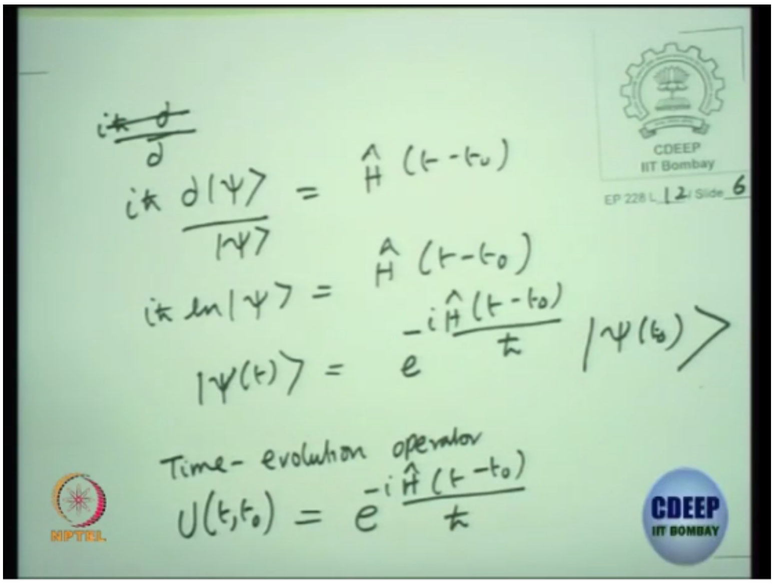

And then you will get what you have ih cross del/del sorry ih cross del psi/psi=H t-t0 so ih cross log psi is H t-t0, psi as a function of time will be e to the power of –iH t-t0/h cross times some constant and you have to make sure that at t=t0 the left hand side should match with the right hand side. Is that right? So at t=t0 this term vanishes, this is an identity operator, so psi t0 will be psi t0 and this gives you the state vector initial state vector at t0 evolves in time by this operator to give you the new state.

What was Hamilton's equations doing? Hamilton's equation was only looking at the evolution equations in the phase space but here in quantum mechanics we say that the information about the system is contained in the ket vector psi and we are interested in the time evolution of that ket vector psi and the time evolution is given by this operator and this operator is known as the time evolution operator.

So let us call that as time evolution operator. What are the properties of it? So let me call this also the time evolution operator, formerly people write it as U of t, t0. So what are the properties? U of t0, t0 is identity operator and you can also see some more other properties. What will be if you go from t0 to t this is the operator. If you go from t to t0 it becomes the inverse of the operator and you can show some of the properties.

And those properties will tell you what is the nature of this time evolution operator and this is the Schrodinger equation which gives you the evolution of the state vector depends of the Hamiltonian of the system. If the Hamiltonian has no time dependence, then I can do this and this piece is what we call it as a time evolution operator.

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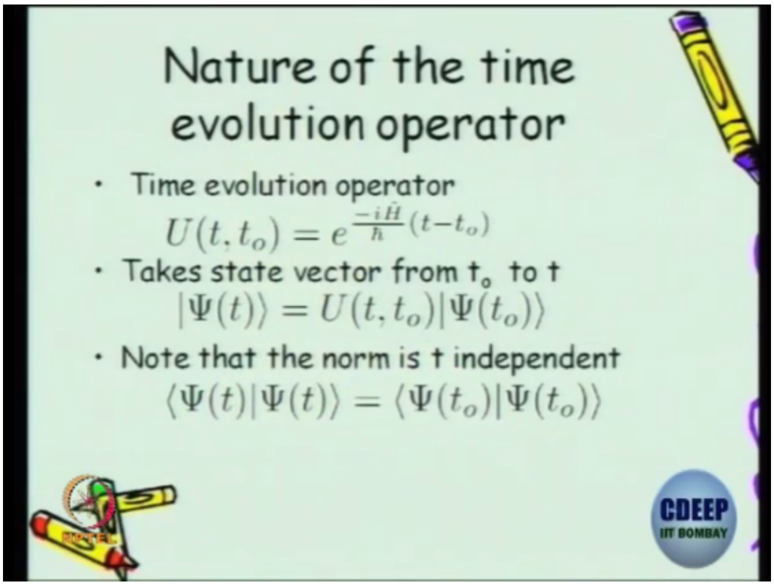

So the nature of the time evolution operator as I was saying the time evolution operator is denoted by the letter U takes a state vector from t0 to t and you can write psi of t as formally as U of t, t0 and psi of t0. Why is norm time independent? Suppose you take the states to be stationary state suppose, what happens? This evolution operator when you put on the ket, when you put it on the dual of this ket, you will put it as a U dagger right complex conjugate and transpose of the adjoint of this U operator.

Is this Hermitian? Is U=U dagger. What is Hermitian? Hamiltonian is Hermitian. Hamiltonian is the one which is Hermitian, U is not equal to U dagger but UU dagger is identity okay.

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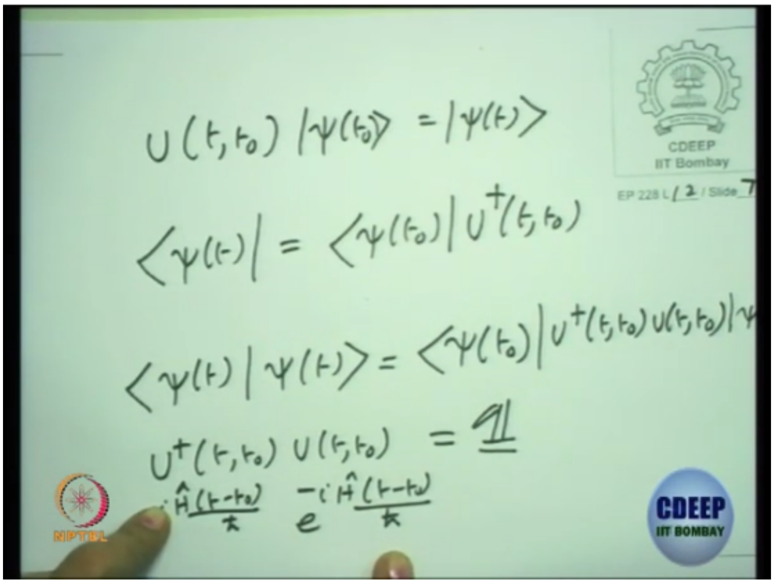

So this is the beauty that U t, t0 operating over psi of t0, we call this as psi of t, I want to write what is psi of t, I would have written this as psi of t0 U dagger of t, t0. So in a product of psi of t with psi of t is same as psi of t0 with U dagger t, t0 U of t, t0 psi of t0 right and U U dagger or U dagger U is going to be identity. Why? Because Hamiltonian is Hermitian, so e to the –iHt/h cross*e to the power of +iHt/h cross, is that right?

This one is e to the+ih t-t0/h cross, this will be e to the i is a H operator-iHt t-t0/h cross. Suppose I had an operator H here and some other operator here, I do not know what to do right.

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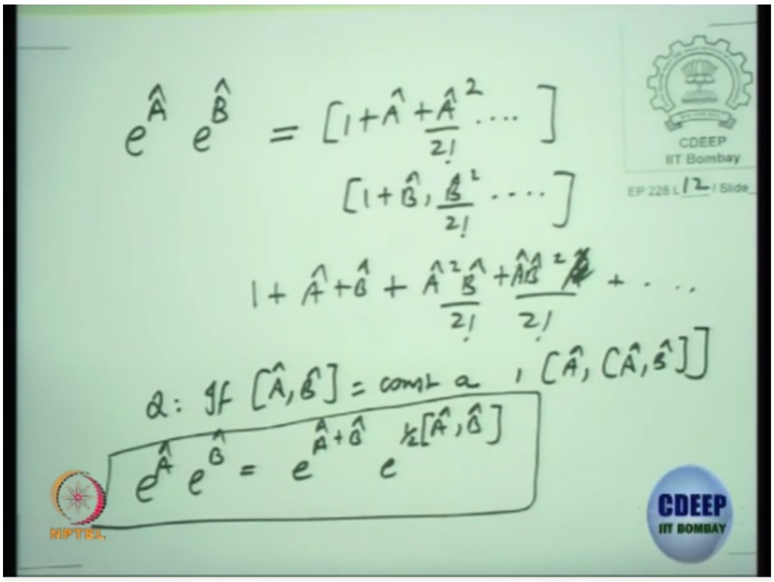

Like what I am asking is suppose I have e to the A and e to the B. In classical mechanics, you would have written this as e to the A+B, can you do that here? So this one you have to meticulously write because why are we doing this, order matters, unlike in classical mechanics, you could have written AB e to the A+B, you cannot do it here, you have to be careful okay.

So lot of things will happen, so you will see there will be 1+A+B+then you will also have A squared B+B squared A and so on. So A’s will always be on the left side thank you. It is definitely not if you have got A hat squared+B hat squared+AB+BA then probably you could have written the other one as A hat+B hat the whole squared, so it is not possible right. You need to have some kind of an approximation and see what is the commutator of A with B and then maybe there is a way of writing it okay.

So these are things which you can play around and see what is happening. Question is if AB commutator is a constant then I think you can show it, let us call that constant as some number, some a or something. You can show this as e to the power of A+B times e to the power of 1/2 of commutator of A with B. Do this expansion and check this out okay? Use this assumption that the commutator of A with B is a constant.

What does that mean? This means that if I take commutator of A with A with B, what will that be? If AB commutator is a constant, it is a constant so this will be 0. So you can play around with these commutators. If something is a constant, you will be able to simplify it. In such a case, you can simplify and get something like this. I am forgetting whether it is +or- but you will figure it out okay.

So this I am not sure about the sign here, it maybe a +sign not a – sign, just check it okay. So these are things which where the classical mechanics and the quantum mechanics differs and you have to keep it in mind when you are doing your operator algebra, you should not be like a machine I know in classical mechanics that you cannot list it, you have to make sure that quantum mechanics, the concerned quantities which evaluate.

If there are products of operators which are Hermitian, you have to try and write the Hermitian combinations of the products of operators and then only do the commutation okay. So this is very important.

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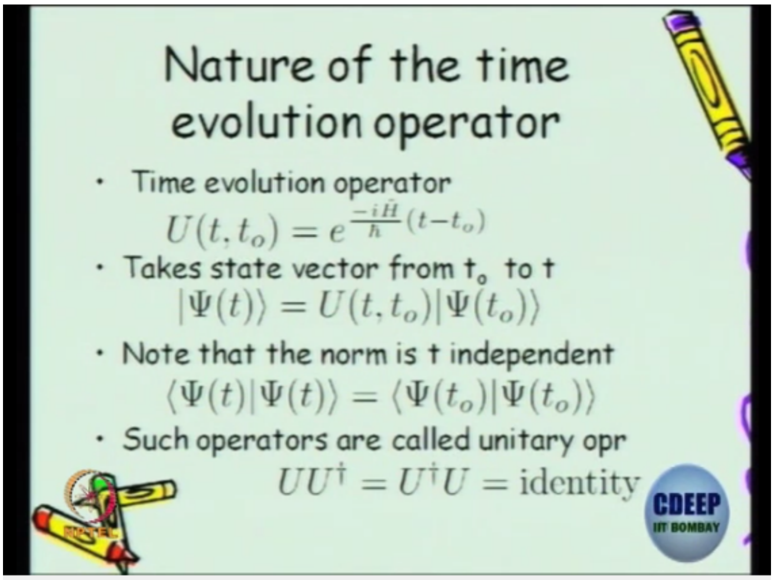

So I have already showed for you that since it is the same operators, A and B are the same operators, there you can add it up okay. If the commutator of A and B is 0 then also you can add it up. This is what I was trying to show in the previous slide right. So U U dagger is always identity and what is that property which you have all seen, these operators are called unitary operators right.

Unitary matrices are such that complex conjugated transpose multiplied by the matrix is identity.

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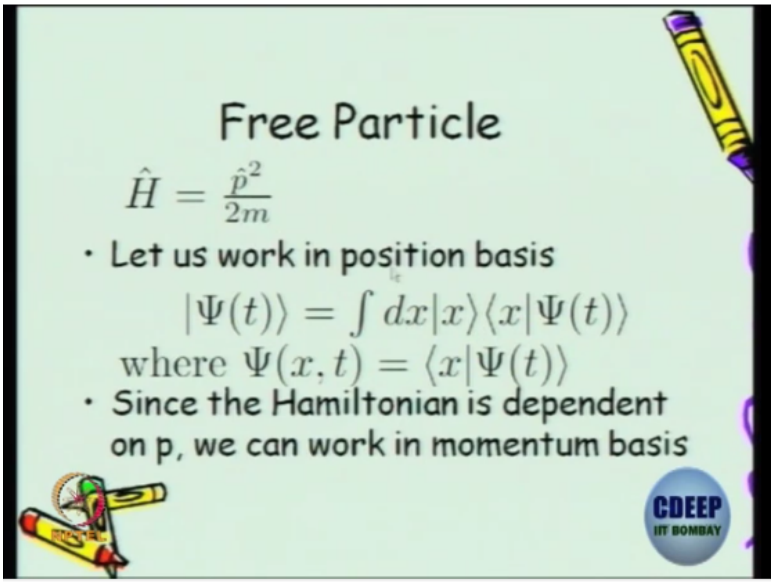

So what do I want to do here? I want to reproduce your familiar Schrodinger equation in the wave function formalism which you did; you have done it many times from this approach where we have postulated how the time evolution of the state ket vector happens okay. So how do you go to the wave function formalism, we did this. This thing is the one which is involving the integral over the position without the product of the position states that is an identity operator.

This integral dx x with x is an identity operating on the same, so left hand side is same as right hand side because this is an identity and we had also defined how to write the wave function. Here you can also write the time-dependent wave function as the inner product of x with psi of t. Since Hamiltonian is dependent on p, we are working for a free particle. So the Hamiltonian is dependent on p, I do not know what is p squared on x.

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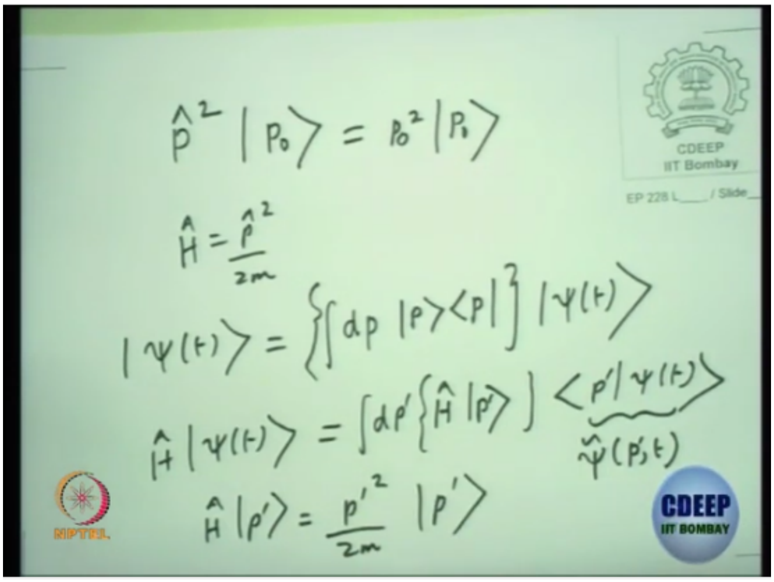

But I definitely know what is p squared on p hat squared on a p0 state will be p0 squared eigenvalue times p0 okay. Hamiltonian is p squared/2m, so we wrote the state psi of t in position space but you could have written it in the momentum space right. So that will give you the Hamiltonian when you operate H on psi of t, you can take the integral of dp outside, this will be H on p.

And what will I call the inner product of p with psi of t, so this is a Fourier transform of your wave function psi tilde of p, t. So we will call this as psi tilde of p, t and H on p for p=the p squared/2m will give you just a eigenvalue, so this is just a dummy variable, if you want you can put a p prime and then you can use the fact that H hat on p prime is p prime squared/2m on p prime.

It is an eigenvalue equation in the momentum space. If you had done it in the position space, we do not know p squared/2m on x what it is we do not know. We need to find out but here in the momentum space, it becomes very simple to write it as an eigenvalue. Since the Hamiltonian is dependent on p, it is convenient to work in momentum space basis instead of working in position space.

So convenience depends on the situation, so which basis you choose and how to go from one basis to another, all these things we did for a finite two-dimensional linear vector space, we can do it even for the infinite dimensional countable uncountable where you can define how to go from one to the other or you can directly take an identity operator the momentum basis because the Hamiltonian states will be eigenstates of the momentum basis.

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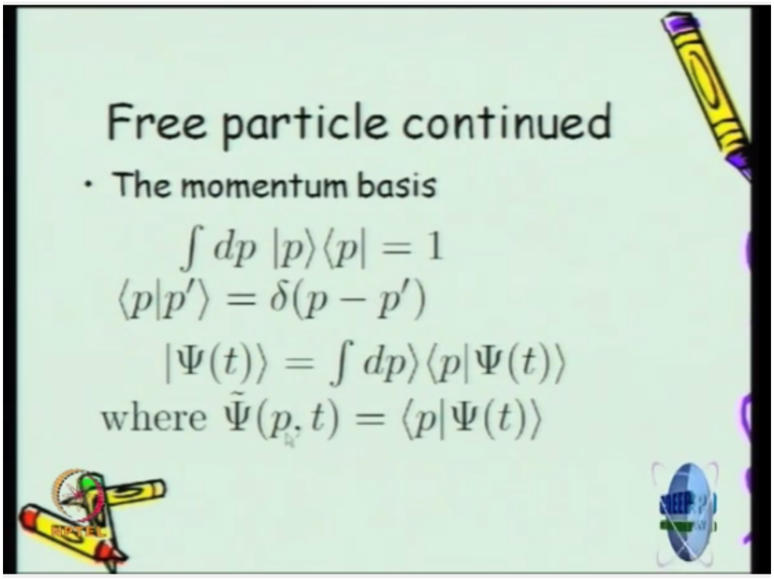

What is the momentum basis? The same like your position basis. I am doing it in one dimension. So this is an identity operator and because it is a continuum inner product of p with p prime should be a Dirac delta function and we can write the arbitrary psi of t as dp there should be a p sorry there is a dp and then p outer product okay and psi tilde as I said is this inner product of the state psi with p which we call it as is to make contact later with the Fourier transform, we call it as a psi tilde.

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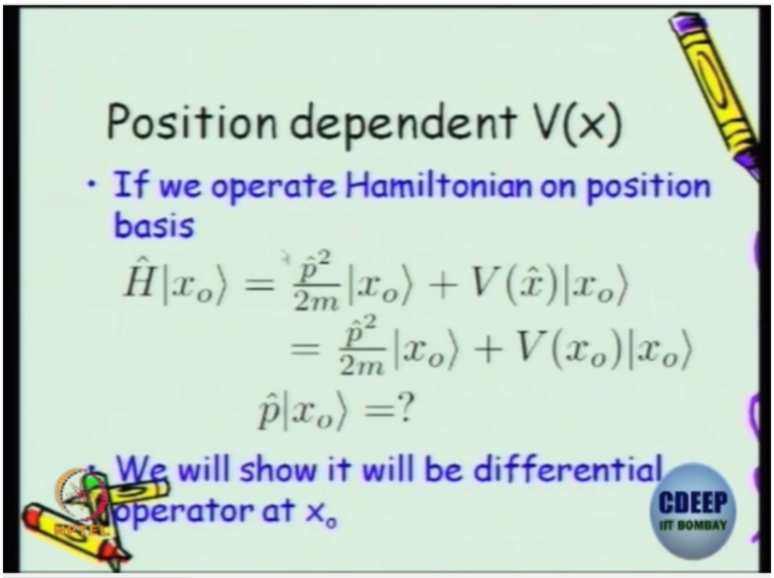

If you operate Hamiltonian on position basis, suppose we have potential energies which are dependent only on position which is what we see in the harmonic oscillator and we operate it on a position basis state. Let us take in x0 state and this becomes we do not know what is p hat operator on x0 but we definitely know that V which depends on a position operator will pull out the eigenvalue which is again a function.

The same functional form will be there. This also you have tried in one of the tutorial sheet right. If the eigenvalue equation of x operator on x0 is x0 times x0 any function of x operator will give you the same functional form of x0. Recall, so I have just written. So p with x0, the question is still remaining, what is p with x0? There are various ways in which you can proceed. You can insert an identity operator of the momentum space.

Take the inner product of the momentum with position, all these things we can start doing and figure it out how the p operator will be done. So that is what we are going to do now.

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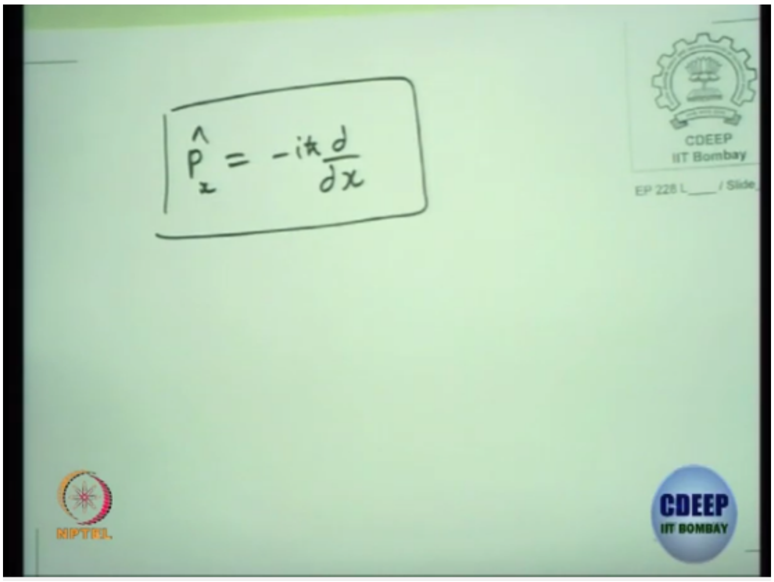

So we essentially show you have all read that the p operator is dx operator. We are going to prove this. We want to derive. We want to derive that the px operator can be written as in the position basis as a differential operator with these right signs for the ih cross. So let us go over the proof and why do you want to do that? Why do we want to do that? It is because we have to evaluate this piece.

If we write a differential operator representation here, it would have given me del squared/del x squared with a -h cross squared, where are we heading, we are going to head to the familiar Schrodinger equation. We want to see that but for that we need to found formally we should be able to say what this is in a systematic fashion rather than just taking the postulate as –ih cross Dirac delta function.

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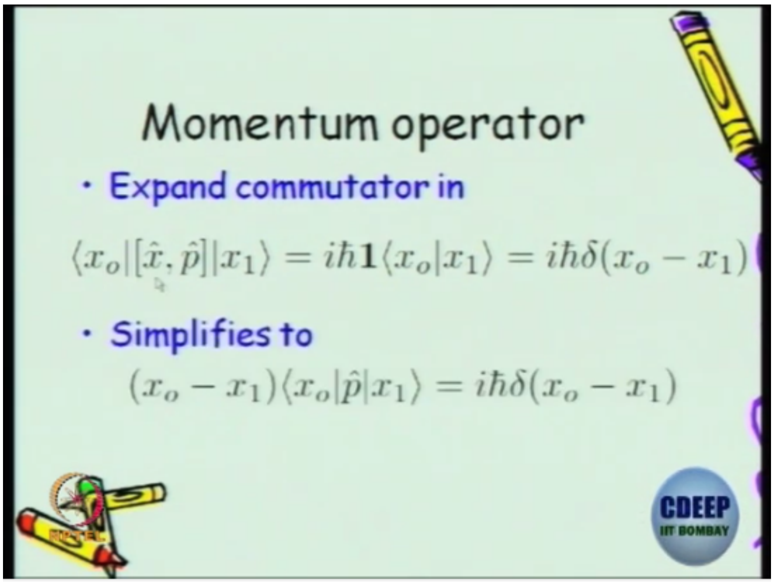

So momentum operator let us do some trick. So take two positions x1, and x2, x0 and in between the operator is a commutator of xp. What is this? Commutator of xp is ih cross identity operator. Identity operator will not do anything to the states; you can pull it out and write an inner product x0 with x1. What is inner product of x0 with x1? That is your Dirac delta function that is a definition of your position basis.

So ih cross Dirac delta function, this commutator xp you expand first, if you expand the commutator, it is xp operator-px operator. So depending on the order either the x will operate on x0 or x will operate on x1. Is that right?

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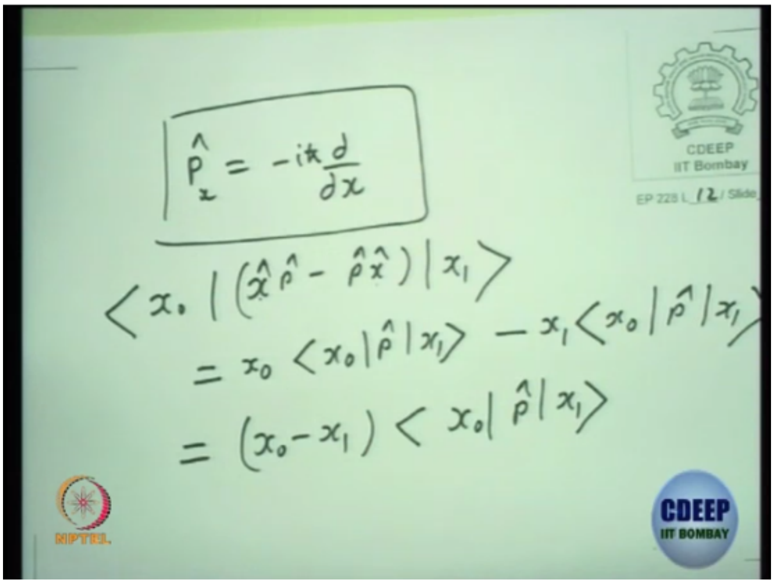

What is this value going to be? This is going to be x on x0 is x0 that is an eigenvalue right with x0 p operator x1-this x with x1 will be -x1 x0 p operator x1. This extreme left hits the x0; extreme right operator hits the x1, so the second term already has a –sign. So this is what you will get. Simplify this. It is x0-x1 matrix element of p operator in the position basis. Steps clear to you?

So this is the result we have to use for the commutator and let us look at the simplified equation here.

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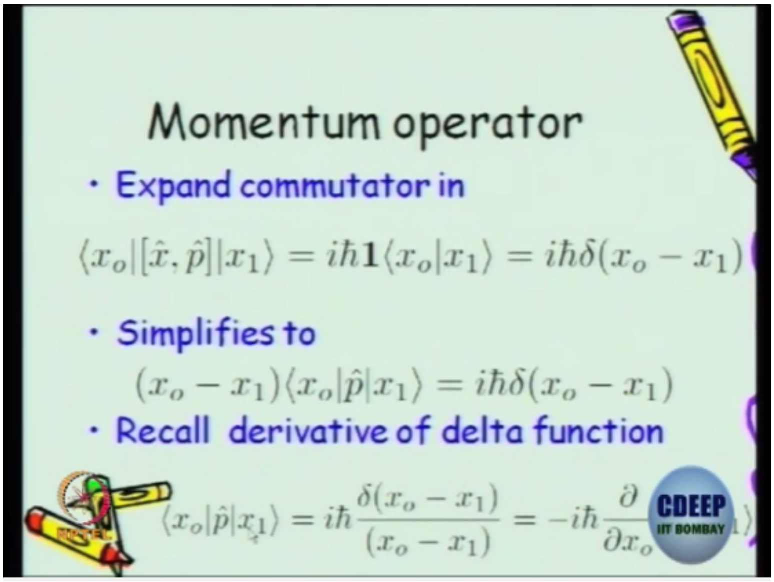

The commutator will be simplified as x0-x1 times the matrix element of the momentum operator will be x0 and x1 and the right hand side is nothing but your Dirac delta function. From here if you take x0 and x1 to be really close, it is like 1/x0-x1 delta function. What is that 1/x0-x1 times the delta function? We have to check. It will be a derivative of a Dirac delta function.

What is the derivative of a Dirac delta function? Delta of x0-x1/x0-x1 is nothing but a derivative of a Dirac delta function. So what have we shown here, from here the matrix element of the momentum operator in the position basis is nothing but –ih cross del/del x0 or x0 x1. So this is what we are showing. So now from here what is the meaning of this left hand side to the extreme right hand side?

The momentum operator can be given a dress in the position basis, representation in the position spaces as a differential operator. So I can put this momentum operator as –ih cross del/del x operator and the del/del x operator when it gives x0, it will give you del/del x0, is that clear? So this is all we are trying to say.

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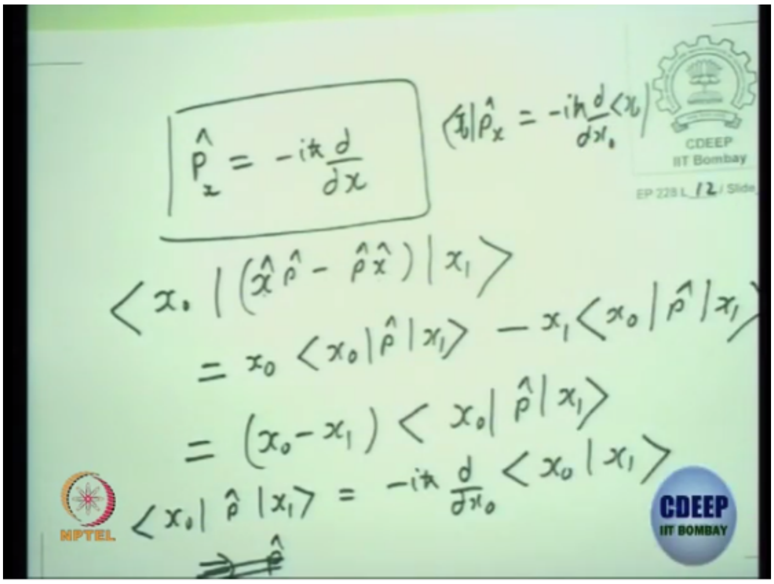

So this implies momentum operator, it implies this top equation, momentum operator is –ih cross del/del x and if this operator px operates on x0 then it will give you –ih cross del/del x0.

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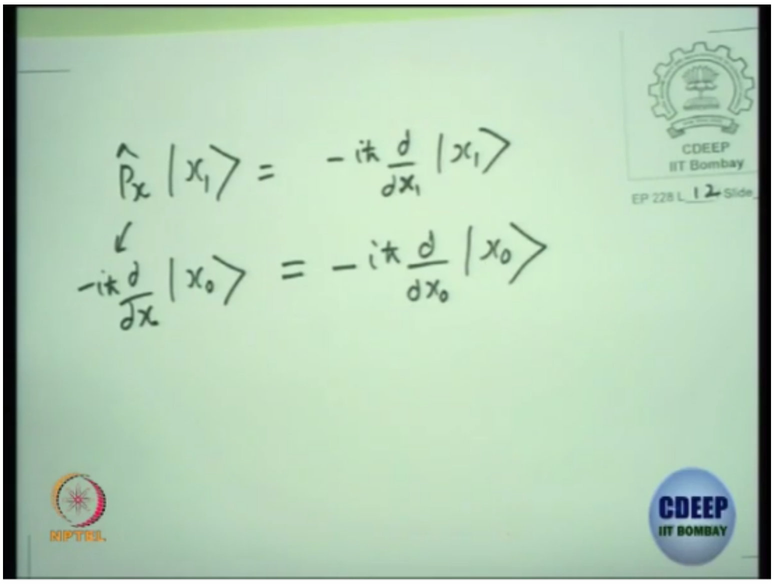

What will that be? Now this is an eigenvalue. Eigenvalue is a differential operator here; it is a differential operator of the space. It picks the x1, differential operator at x=x1 okay whereas the side I could write it as –ih cross del/del x as an operator when it hits on like x0, it will give me –ih cross. So we have given a position representation for the momentum operator which is a differential operator.

Similarly, can you give a momentum representation for the position operator, can use the same arguments and do it instead of x0 x1 p0 and p1.

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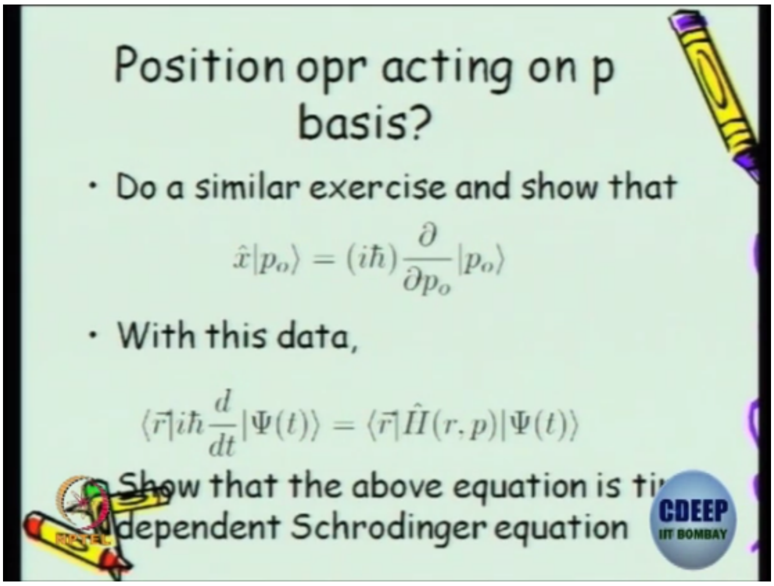

Redo the same exercise for the matrix element of the position operator in the momentum basis and show that it will have one +sign ih cross, that is also seen because if you do a commutator bracket there will be a (()) (29:43) and please show that x on p0 is ih cross del/del p0 of so that tells us that. So do a similar exercise for the position operator on p0 and verify whether this is satisfied.

What I did for the momentum operator now redo it for the position operator and convince yourself that it is again a differential operator, differential operator it was a momentum coordinates. In general, you could write for any stage psi of t. So earlier we had x0 and x1, x1 can be replaced by any arbitrary state psi, it does not really matter and you can show that the differential operator p if you take the del/del x operator, it can hit the left ket and give you a del/del x0 times is what is this, position space wave function at x0 t.

So I have given you a couple of pieces here and there and now with this data, what is the next step, take the time evolution operator or the equation which dictates the time evolution of a ket psi which is H on psi and take the projection onto a specific position in any 3 dimensions or 1 dimension, in 3 dimension you take an r vector and you can write this. Now this is the exercise for you.

H operator is p squared/2m+V of r let us take and p squared/2m can be replaced as –ih cross del squared/2m. So let us redo this and then.

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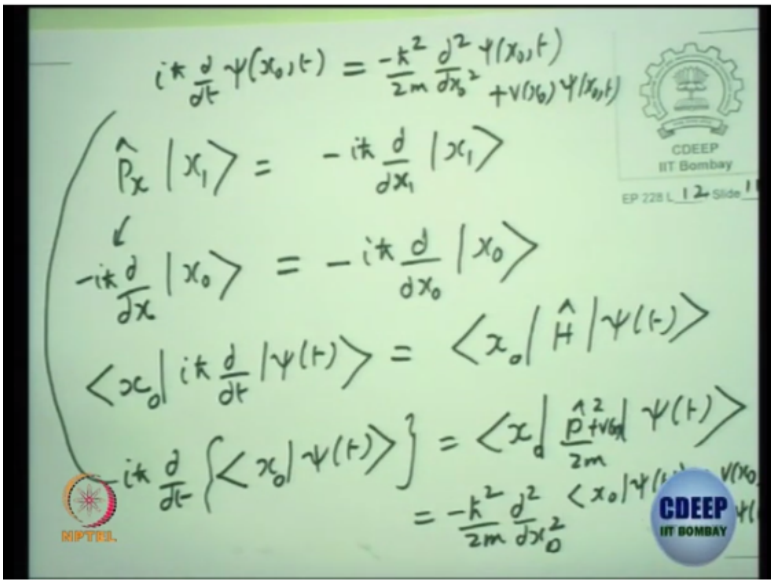

So let me do it in one dimension, let us come back to. So this piece is your time evolution equation and you take the projection to a specific x. I can still take the del/del t operator outside, it does not matter and say x of psi t, it is the same because del/del t will only hit the psi of t; x is not dependent on time. Similarly, here it will be x if suppose we had it to be a free particle p squared/2m on psi of t suppose.

We will also do V of x later. If you want let us write the V of x also, what is wrong. The p has a position representation which is –ih cross del/del x in one dimension. So you can rewrite this as –h cross squared/2m del squared/del x squared more precisely maybe I can take an x0 here, just to make it more dramatic with x0 psi of t+this term V of x. V of x will give you V of x0 will be a number multiplying x0 with psi of t.

So what is this x0 with psi of t? That is a wave function. So this equation I can write it as ih cross del/del t psi of x0, t=what about this –h cross squared/2m del squared/del x0 squared psi of x0 t+V of x0 psi of x0, t. What is this? This is your familiar Schrodinger equation in the wave function formalism. I have postulated an equation for evolution of the state vectors.

I try to systematically write my momentum operator using a position representation which became a differential operator and then the equation which we get for the wave function is exactly your time dependent Schrodinger equation. So this is what I am trying to say here that you can do it even in 3 dimensions and you can show that it is nothing but your time dependent Schrodinger equation.

So del squared/del x0 squared will become a del squared operator Laplace. A lot of things which I said today which involve for you connections between classical and quantum mechanics and then I went into the evolution equation, I gave you an evolution operator which is unitary and then we slowly studied what should be the position representation for the momentum operator.

And I asked you to find what is the momentum representation for the position operator and then I said you can using these data you can actually reproduce your wave function Schrodinger equation the time dependent Schrodinger equation. So I will stop here.