Quantum Mechanics
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Lecture - 16
Basis for Operators and States in LVS - II

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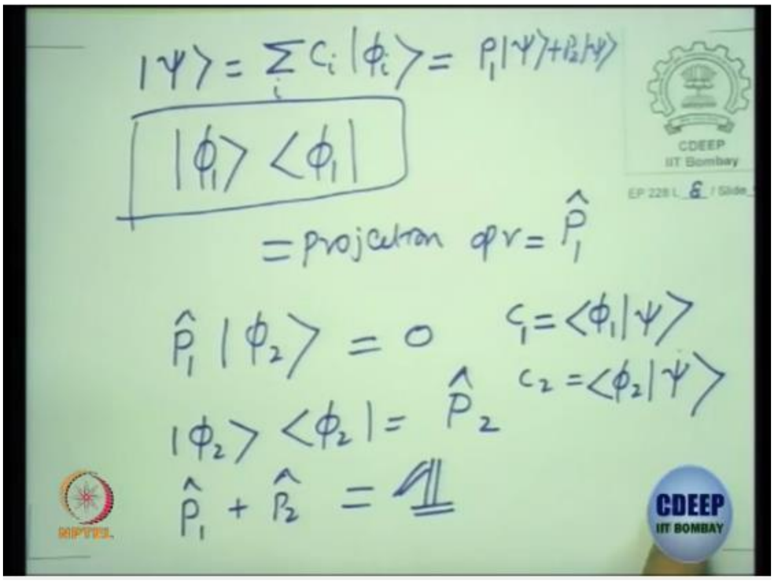

So I have tried to introduce the outer product here, which is an operator but this outer product if you see, this outer product if you see, it is the outer product of the same set. What is the property of a projection operator? Let me ask you this. What is the property of a projection operator? If you do it twice, it will be the same, any number of times you do, it is going to be same. Can we verify that here?

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Let us take $\hat{P}_1^2$, what is ? $\hat{P}_1^2$ is $\hat{P}_1$ is $|\phi_1 >< \phi_1|$ okay. You will also have a $|\phi_1 >< \phi_1|$ but what is this? We have taken an orthonormal basis so that is 1, so this is same as $< \phi_1|\phi_1 >$ that is the property of a projection operator and sometimes I do not put the hat but from now on you should know whatever we are doing when I write an outer product it is an operator.

So this is the property of the projection operator. What are its eigenvalues? Now you can give in the two-dimensional vector space, you can rewrite this as a 2 x 2 matrix right. So let us write suppose $|\phi_1 >$ is taken to be $\begin{pmatrix}1\\0\end{pmatrix}$ and $|\phi_2 >$ is taken to be $\begin{pmatrix}0\\1\end{pmatrix}$ what is $|\phi_1 >< |\phi_1|$? $\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$. What are the eigenvalues of this? 0 1 right. If the state is in that subspace, it will get projected with the same, it will be as it is.

But if it is not in the subspace, it is going to be 0, so that you can also satisfy some here $\hat{P}_1^2$-$\hat{P}_1$ can solve that equation, you can rewrite $\hat{P}_1^2$-$\hat{P}_1$ as=0 which implies $\hat{P}_1$ is either giving 0 or 1 as eigenvalues right. So this condition when I write this is a product of two operators. This condition this will either tell me that $\hat{P}_1$ is 0 or $\hat{P}_1$ is=1 that is all I am trying to say.

And it should also satisfy $\hat{P}_1^2$=$\hat{P}_1$ with these constraints these are the only possibility okay. So that is the beauty of this projection operator where this outer product $|\phi_1><|\phi_1|$ is $\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$, then the other product $|\phi_2><|\phi_2|$will be $\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$.

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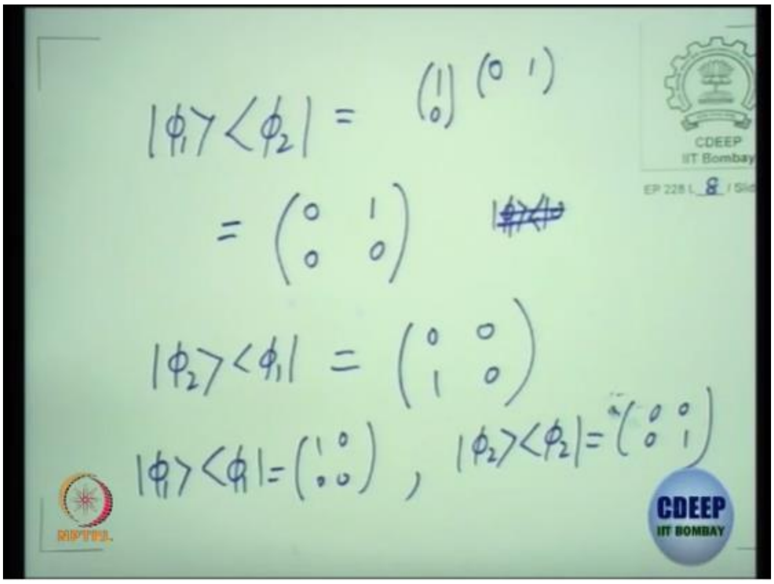

So what is $|\phi_1><|\phi_2|$? ϕ 1 ϕ 2 is not a projection operator but it is still a 2 x 2 matrix. What is that 2 x 2 matrix? Someone can help me. It is 1 0 which is a column multiplying 0 1. Is that right? Similarly, what is $|\phi_2><|\phi_1|$? $\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}$ so what am I tried to do? I have tried to show that the 4 possibilities of outer product which I can write for the 2 basis two-dimensional vector space.

They can be given the outer product can be given a 2 x 2 matrices with only one entry which is nonzero okay. So this appears like the 1 2 element which is nonzero. This appears like the 2 1 element which is nonzero and the earlier ones were the diagonal elements 1 1 was nonzero right. $|\phi_1><|\phi_1|$is $\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$ and $|\phi_2><|\phi_2|$ is $\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$. So this should kind of tell you something.

Any 2 x 2 matrix which you write can be represented in terms of this Dirac notation where you will have 4 possible basis states with $|\phi_1>$ and $|\phi_2>$ in the two-dimensional case, so let me write that.

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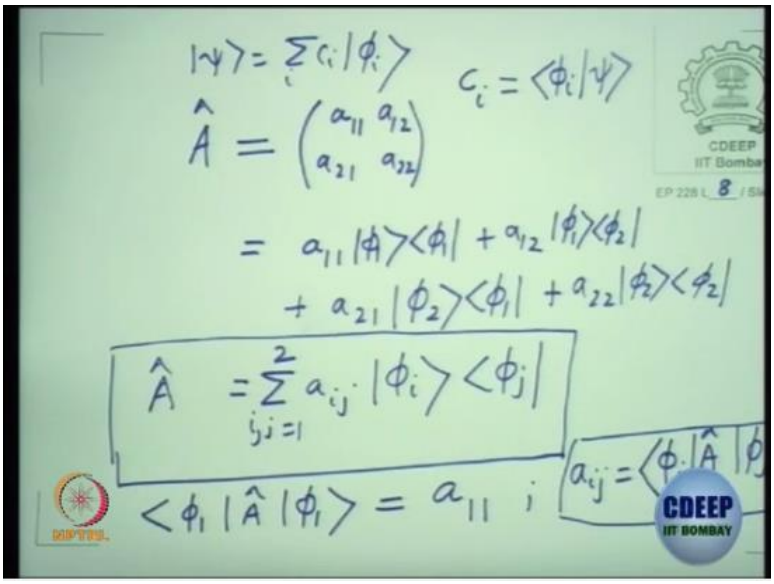

So if you take some operator $\hat{A}$, you can rewrite a representation for this in this two-dimensional vector space as some $\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$. I can also rewrite this as $a_{11}\,|\Phi_1><\Phi_1|+a_{12}\,|\Phi_1><\Phi_2| + a_{21}\,|\Phi_2><\Phi_1| + a_{22}\,|\Phi_2><\Phi_2|$. This is also correct, write this compactly as summation over i, j which is 1 to 2 $i.e\ \sum_{i=1}^{2}\ a_{ij}\,|\Phi_i><\Phi_j|$. So just like we wrote a state $|\psi>$as summation over i, $\sum_i c_i|\phi_i>$, I can write any operator.

This operator could be position operator, momentum operator, angular momentum operator, all possible. By operator I mean, anything which you see in the observable, so they can be given an operator in quantum mechanics and they can be defined just like $|\phi_i>$ or the basis for the states, outer product will be the basis for the operator. How many will be there in n-dimensional vector space? N squared basis.

And from here can we extract what is let say what is a_{11}? If you want to find what is a_{11}, how will I go about it? So let us do that. So let us take $\langle\phi_1|\hat{A}|\Phi_1\rangle$. If you do this, what do we get? This left hand side angular braket the bra will only give nonzero with which two terms only with the first term and the second term. Third term will be 0 by the orthonormal property right.

The $|\phi_1>$ if I operate, $\langle\phi_1|\Phi_2\rangle$ is 0. Similarly, $\langle\phi_2|\Phi_1\rangle$ is 0, so these two terms will be 0 by putting the braket, the bra vector $<\phi_1|$ if I put on both sides; this is going to be 0, these two terms. If I put the ket $|\phi_1>$ after that, that will operate on this state and it will what happens to this term, $|\phi_1>$ will be 0. So what do we get from here? The only nonzero element will turn out to be a_{11} okay.

So what have I tried to present here is that if you have an abstract operator and an abstract basis states, you can find the components of this abstract operator just like c_i when I wanted to find, c_i was $\langle\phi_i|\psi\rangle$. In the context of operators, if you want to find these coefficients a_{ij}, you have to take $\left\langle\phi_i|\hat{A}|\phi_j\right\rangle$, that is it, any operator, Hamiltonian operator you could write and so on.

The operators also has a basis, the basis are these outer product of this. This is vectors so that be n squared basis and you can write any arbitrary operator as a linear combinations of these outer product spaces.

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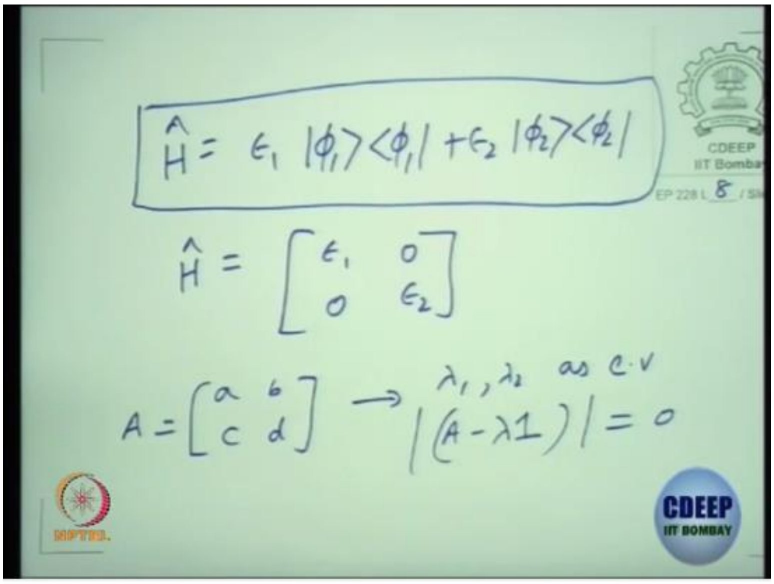

Suppose I give you that Hamiltonian is given to be $\varepsilon_1|\phi_1><\phi_1| + \varepsilon_2|\phi_2><\phi_2|$ suppose I give you this, what does this mean? These two are like the projection operators, there are no cross terms. So this will be the matrix representation for this can be written as a diagonal matrix with the off diagonal terms b and c. So you need to be able to read given any operators in this notation.

What actually it mean if you put it as a matrix operator, matrix representation, we should be able to read from there, whether it is diagonal, whether it is off diagonal but once you put it in this notation finding the eigenvalues and eigenvectors you have already done right in your math course. Any 2 x 2 matrix if I give you $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, how do you find the eigenvalues? So $A - \lambda I$, determinant of that=0.

You can find the eigenvalues from that right. So you have to give you lambda 1 and lambda 2 as eigenvalues just given by this matrix is A, A-λ I determinant of that, that has to be 0, then you solve this and you find what is the two eigenvalues and once you know the eigenvalues you know how to find eigenvectors. This is a compact Dirac notation for a diagonal operator.

But whatever I write there for a finite dimensional vector space, you can try to rewrite it in matrices and you can work with what you know from your matrices. So what are the eigenvalues of this operator if I ask you, it is very trivial. Epsilon 1 and epsilon 2 are the eigenvalues and the basis states are $|\phi_1 >$ and $|\phi_2 >$ which is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ on $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. So this can be a trick question asking you find the eigenvalues and eigenvectors, there is nothing to work out.

But if I give you an off diagonal matrix, you need to do a little bit work because once I have this off diagonal matrix; it is no longer you have to find out what is the eigenvectors and the matrices okay. So let me just try to okay.

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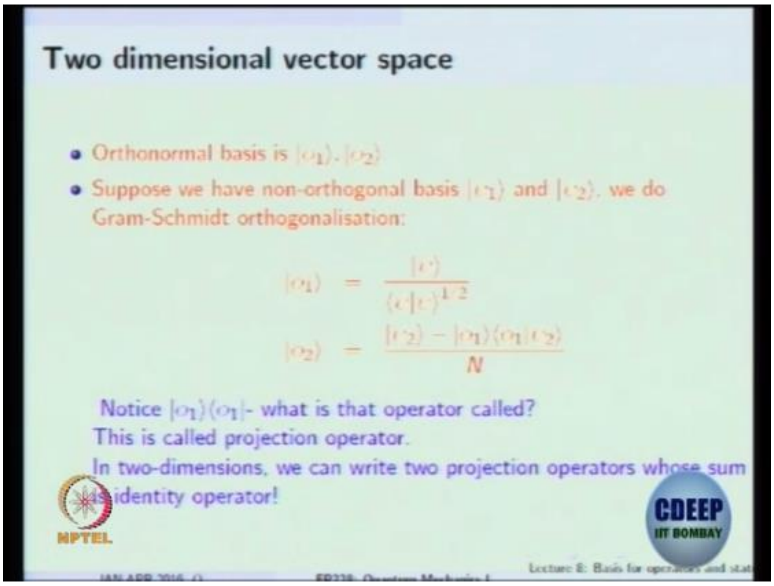

So this is what I went through just know that you have $|\phi_1 >$ and $|\phi_2 >$ which is orthonormal basis and psi 1 $|\psi_1 >$ and $|\psi_2 >$ which is non-orthogonal and you can do a Gram-Schmidt orthogonalization and in the process you see a $|\phi_1 > < \phi_1|$ which is nothing but this outer product is nothing but a projection operator projecting to a subspace $|\phi_1 >$ and you subtract that out and then what you get is the state which can be the orthogonal basis to the $|\phi_1 >$ and this is what we called it as a projection operator.

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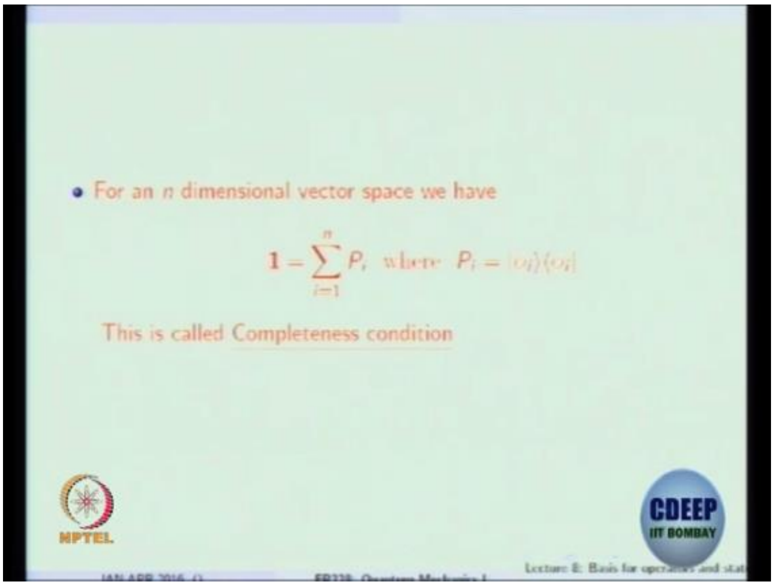

And in two dimensions, we can write two projection operators whose sum is an identity operator okay. So for an n dimensional vector space, you could write projection operators n of them and the sum of those projection operators will be turning out to be 1. If it is not 1, what does it mean? Suppose it is not 1 (()) (15:08) so you have not spanned the whole space and you have not found the complete set of basis states right.

Suppose you are in x y z and I give you only P_1 and P_2 and I say that there is only $|\phi_1 >$ and $|\phi_2 >$ and if it is not equal to 1, you know that it is not spanning the whole space, you have to have one more, then this not a complete basis set. You have to give for a three-dimensional R_3; I have to give you $\hat{\imath}$ $\hat{\jmath}$ and $\hat{k}$. If I just give you $\hat{\imath}$ and $\hat{\jmath}$, it is not complete. You all agree?

So this condition which we write, this condition that the sum of all the projection operators of a given basis set being identity is what is called as a completeness condition okay. This is the completeness condition and we need this without which we cannot work, we cannot make promise, a basis set if I say it is a basis set, it has to satisfy this criterion.

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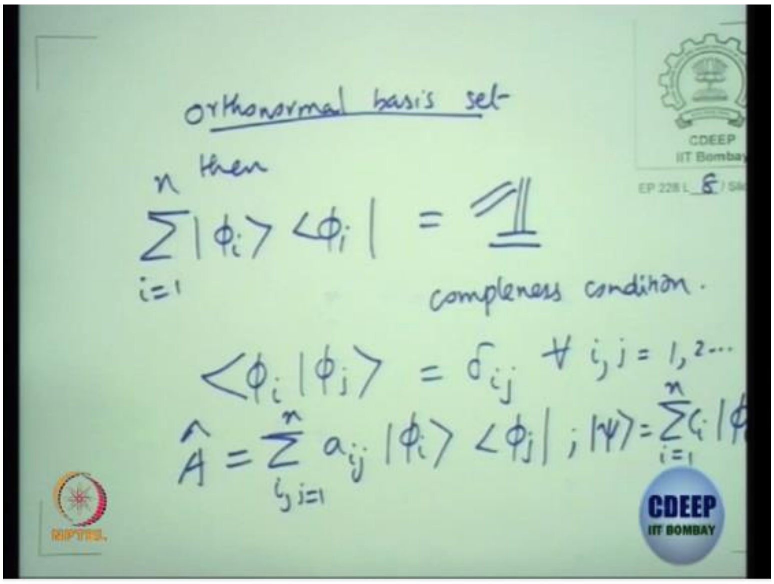

So if I say orthonormal basis set then $|\phi_i><\phi_i|$ summation over i from 1 to n has to be an identity operator. This is a if I call this by definition a basis set, then this has to be satisfied, this is called completeness condition and you have to also once you say it is orthonormal basis, it is understood that this is δ_{ij} for all i, j which is 1 to n what else. Any arbitrary operator will be rewritable as $\sum_{ii} a_i |\phi_i><\phi_j|$.

And any arbitrary state ψ can be written as this takes care basis set includes the span and the completeness condition and this criteria. Is this clear? Playing around between Dirac notation and your familiar matrices in a 2 x 2 two-dimensional vector space and 2 x 2 matrices. If you are clear about this, you can do any 3 x 3 n x n. What happens to functions of operators?

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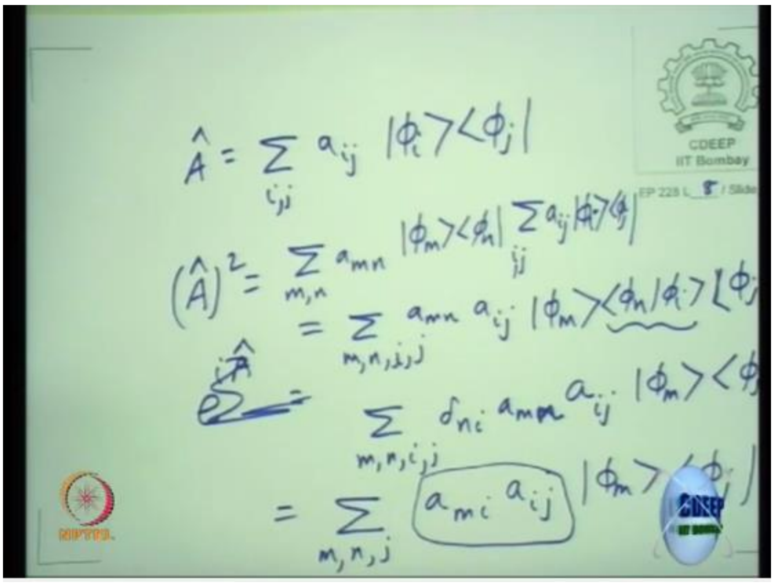

Suppose I write an operator $\hat{A}$ as $\sum_{ij} a_{ij} |\phi_i >< \Phi_j|$, what happens to functions of operators? Suppose I want to do this, that is one question and then you can extrapolate it to $e^{i\hat{A}}$ what it is, $\hat{A}^2$ is repeating this, you can put two different indices and do this right. $\hat{A}^2$ will be $\sum_{mn} a_{mn} |\phi_m >< \Phi_n| \sum_{ij} a_{ij} |\phi_i >< \Phi_j|$.

And then what do you have to do? These are numbers ϕ and $|\phi_i >$ will be, what will that be? Summation over m, n, i, j, take it out, summations take all the scalars out then what do we have? $|\phi_m >$ then $< \phi_n|\ |\phi_i >\ < \phi_j|$. What is this? So you will have summation over $\sum_{m,n,i,j} a_{mn} a_{ij} |\phi_m >< \Phi_n|\ \ |\phi_i >< \Phi_j|$. So wherever m is there I can replace it by i and 1 summation of i is gone.

Yeah, so this thing you can write it as $\hat{A}^2$ the mjth element right. So you can actually see that if this is a then this becomes a function of $\hat{A}^2$, function of that operator, this coefficients. So this is what we are trying to see. So you can try and do this for a general. So just to tell you what is Hermitian, what have you learnt about Hermitian operator in your first course?

An operator operating on $\hat{A}\psi(x)$ if it gives you $a\,\psi(x)$ then you say is a eigenvalue. For Hermitian operator what is the requirement?

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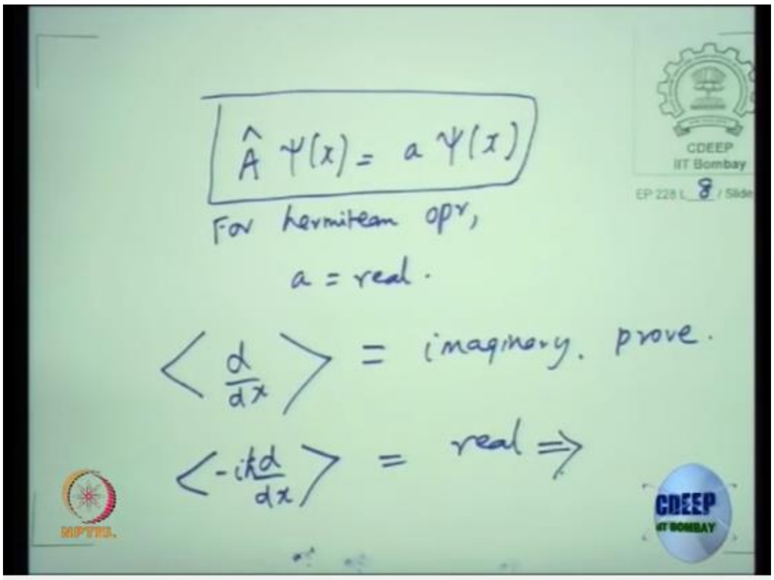

This is an eigenvalue equation; A is the eigenvalue. If you want to call A to B, A the capital $\hat{A}$ operator to be a Hermitian operator then A has to be real. When you do an expectation value of d/dx operator, what happens? You can show this to be imaginary. Have you tried this in your particle in a box? Please do this. Particle in a box, take the particle in the first excited state or a ground state or any state, find what is expectation value of d/dx?

Please do this. That is why d/dx is not a, it is giving me expectation values which are imaginary which is not an observable quantity. So that is why we do this i d/dx because with dimensional things you have a h cross also with a negative sign. This will be real; this I am sure you would have done it in one of the assignment problems. Expectation value of $\frac{\partial}{\partial x}$ is imaginary, have you done this or no?

If you have not done it, please do it. It is not difficult. Please try and prove that that the expectation value of $\frac{\partial}{\partial x}$ operator for a particle in a box. If you try to do this, it is imaginary whereas $i\,\hbar\frac{\partial}{\partial x}$ is going to be real. So all if you want to call an observable, the expectation value of the operator should be real. So d/dx operator expectation value is not real, it is imaginary.

So for you the momentum operator is $-i\,\hbar\frac{\partial}{\partial x}$ because that expectation value will be real. So this is something which if you know, then we can go to this. I will do this on Wednesday after you come back from your break and then the hermiticity condition okay. Let me stop here.