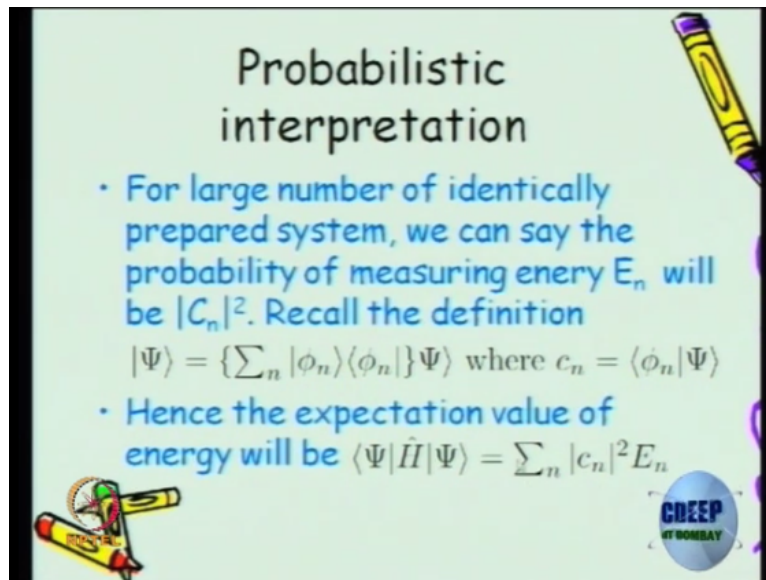


Quantum Mechanics
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Lecture - 25
Classical vs Quantum Mechanics - I

(Refer Slide Time: 00:32)



Probabilistic interpretation

- For large number of identically prepared system, we can say the probability of measuring energy E_n will be $|c_n|^2$. Recall the definition $|\Psi\rangle = \{\sum_n |\phi_n\rangle \langle \phi_n|\} \Psi$ where $c_n = \langle \phi_n|\Psi\rangle$
- Hence the expectation value of energy will be $\langle \Psi|\hat{H}|\Psi\rangle = \sum_n |c_n|^2 E_n$

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Okay so just towards the end of the last lecture, I just talked about the measurement which is probabilistic in the sense that you take a large number of identically prepared systems and then if you want to measure a specific energy E_n then the value will be mod C_n squared which is what is the probability for finding the energy E_n right, everybody is there, that is where these kind of stopped.

So recall the definition of ψ , you just insert an identity operator which is in parentheses here on the same side and then the coefficient C_n is nothing but the product of ϕ_n with ψ . Everybody with me, we did this okay. So then if you want to find the expectation value of a system prepared in the state ψ , then Hamiltonian expectation value of the energy then it will be weighted average where mod C_n squared is the probability for this energy E_n to be measured and so on.

So you sum it over and that will give you the average energy. So what have you learnt in classical mechanics?

(Refer Slide Time: 01:42)

Classical Mechanics

- Dynamical variables A, B in the phase space (position x and momentum p of the particles in the system)
- Hamiltonian $H(x,p)$ helps in finding the time evolution of x and p

$$\{A, B\} = \frac{\partial A}{\partial x} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial x} \quad \text{Poisson bracket}$$

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial x} \quad \text{Hamilton's equations}$$

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You have a phase space. Phase space is defined by position and momentum right and then you have dynamical variables which I call it as capital A, capital B which are functions of this example. Then, if you want to know the time evolution, Hamiltonian helps in finding the time evolution in classical physics. What are those equations? First you need to write the Poisson bracket of A and B which is governed by the Poisson bracket of x and p.

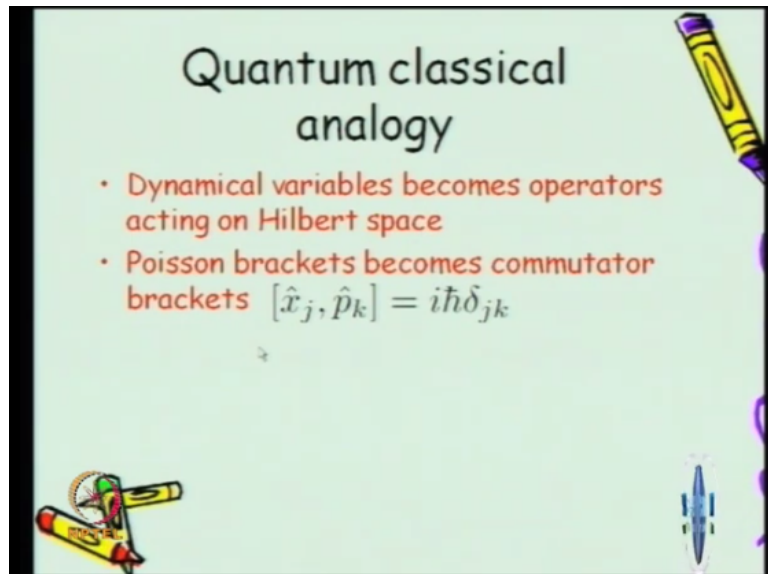
You all know Poisson bracket right okay. The definition of a Poisson bracket of two variables in a phase space defined by x and p involves these partial derivatives in this fashion. So that is the definition. If you want to find what is the Poisson bracket of x then p here, so del A/del x is 1 del B/del p is 1 del x/del p is 0 del B/del x is 0.

So it is just 1, so I am just trying to bring in some kind of a correspondence between a Poisson bracket which is learnt in classical mechanics with commutator in quantum mechanics. That is the main motivation why I am going and comparing and contrasting classical mechanics with quantum mechanics okay. So this is the formal definition of this Poisson bracket and evolution equation depends on the Hamiltonian.

And you can write $x \dot{x}$ involving the partial derivative. The Hamiltonian is also a dynamical variable which is dependent on x and p. So you will have an equation which gives you the time evolution of the position coordinate, another equation which gives you the evolution of the momentum right. What does these equations called? Hamilton's equations okay, so these two equations are classical mechanics, this one is called Poisson bracket.

And these two equations which I have written which gives you the evolution in phase space time evolution, they are called Hamilton's equation.

(Refer Slide Time: 03:59)



So now we want to see an analogy to quantum physics. So you clearly see that here the phase space time evolution is governed by some equation. We also want to write the state vector which we write in quantum mechanics to be governed by some equation that is 1 and what will be the analog of Poisson bracket when you go to quantum mechanics. So those are the questions you can ask.

And so the first thing is all the dynamical variables, example your Hamiltonian and other operators which are functions of x and p they get promoted to become operators in Hilbert space. To be more precise, you can take linear operators on Hilbert space. Poisson bracket which we had you can replace that by a commutator bracket. What is a commutator bracket?

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$$\text{Tr}[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \text{Tr}[i\hat{C}] \Rightarrow \hat{C} \text{ is traceless.}$$

$$[\hat{A}, \hat{B}]^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A}, \hat{B}] = i\hat{C}$$

$$\boxed{\text{Tr}\hat{A}\hat{B} = \text{Tr}\hat{B}\hat{A}} \rightarrow \text{valid only for finite dim LVS}$$

$$\text{Tr}[\hat{x}, \hat{p}] \neq i\hbar$$

A commutator of A, B is AB-BA okay. A and B are Hermitian operators. Let us take them to corresponding to observables, its commutator. When you do the commutator what happens? So suppose I want to find a dagger of this. Someone what is this? So B dagger sorry BA-AB. Is that right? This is nothing but minus of commutator of A with B. Something bothering us. If you have two observables which are Hermitian operators, the commutator is not a Hermitian operator right.

If you want to make it Hermitian, what do we do? Suppose I call this to be C operator then it is not Hermitian. What do I do? Yes, multiply by an i and then this dagger that i will also get in here. So i so you will get this to be again ic hat. So these are the reasons why you will have an i here because your left hand side is not going to be Hermitian. If you want to make both left hand side and right hand side to match, you put an i factor.

Why ih cross? Why do you need a h cross? By dimensional arguments, the Planck constant is the relevant one for the product of x and p which you can introduce okay. So this is one naïve way of arguing why it is postulated that the Poisson bracket goes to commutator bracket and the commutator bracket is ih cross delta j. You are done for a finite dimensional Hilbert space, is that right?

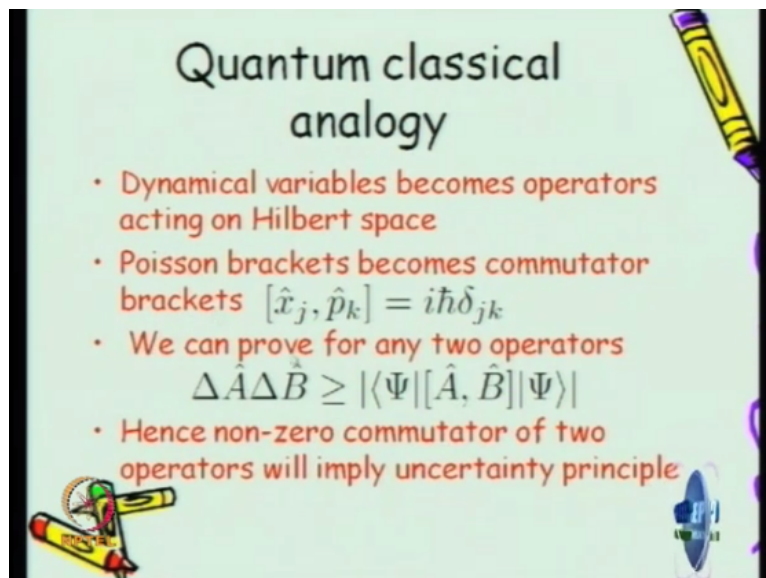
You proved this for a finite dimensional vector but if you have a commutator of A with B as i times c and what happens? So c in fact here is an identity operator right. So if you take x operator with p operator, let us do one-dimensional that will be ih cross identity operator. In

general, it could be an infinite dimensional space. If I take the trace on both sides, what will the left hand side be? Left hand side is 0 by this property. Is that correct?

Then, what is the problem, tell me? Is this allowed? This contradicts; left hand side is not equal to right hand side right. So which means this identity is valid only for finite dimensional linear vector space that is the only way you can try and say that this is in the infinite dimensional vector space you cannot have this. In general, if you have an AB commutated as ic, you have to impose what, even in the finite dimensional Hilbert space if this side is 0, this should be traceless matrices okay right.

If I want this, take trace, if this is 0, this implies c is traceless in finite dimensional Hilbert space but in infinite dimensional Hilbert space, this property cannot be satisfied because you cannot give a matrix representation even though we can write a Dirac bracket notation, you cannot write a matrix representation to argue the trace AB is=trace BA in an infinite dimensional Hilbert space, so that is just.

(Refer Slide Time: 09:48)



Quantum classical analogy

- Dynamical variables becomes operators acting on Hilbert space
- Poisson brackets becomes commutator brackets $[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$
- We can prove for any two operators
$$\Delta\hat{A}\Delta\hat{B} \geq |\langle\Psi|[\hat{A}, \hat{B}]|\Psi\rangle|$$
- Hence non-zero commutator of two operators will imply uncertainty principle

There is also something else we could prove; delta A is your standard deviation of an operator A. What is a formal definition? We saw this in one of the lectures. What is delta A?

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$$\Delta \hat{A} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

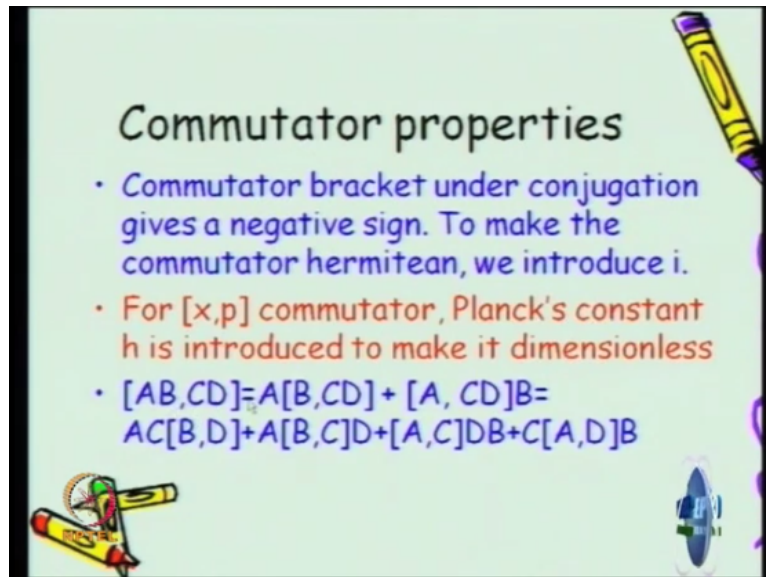
It is the expectation value of A squared - expectation value of A the whole squared and then you take the square root. So for some dynamical variable of some operator, the standard deviation is given this way. Product of two, this is what we call it as an uncertainty, standard deviation is what we call it as an uncertainty the observable corresponding to the operator A, time is uncertainty in B can be proven that this is going to satisfy.

It is going to be related to the commutator bracket. The commutator was 0, then what does it mean? What does Heisenberg's uncertainty principle tell you? You always write $\Delta A \Delta B$ is greater than or equal to \hbar cross by 2 or something right. What does that mean? $\Delta x \Delta p$ when you write, you say that if you can precisely look for the position which is Δx . Your Δp will be very large right.

So this is what is you cannot simultaneously measure x and p . If the commutator of A and B is 0, then $\Delta A \Delta B$ is 0. So you can simultaneously measure both of them with precision if the commutator is 0. So xp commutator is what? xp commutator is nonzero okay. So because xp commutator is nonzero, you do not have, you have an uncertainty principle which is your familiar Heisenberg's uncertainty principle.

In general, if two operators are commuting that is this one is 0 then you can show that those two can be simultaneously measured, is that clear? There is no uncertainty that measuring 1 will not give you precise value for other one. This we will prove in one of the tutorials okay. So hence nonzero commutator of two operators will imply uncertainty principle and we can say one is precisely measurable, the other one may not be precisely measurable.

(Refer Slide Time: 12:44)



Commutator properties

- Commutator bracket under conjugation gives a negative sign. To make the commutator hermitean, we introduce i .
- For $[x,p]$ commutator, Planck's constant \hbar is introduced to make it dimensionless
- $[AB,CD] = A[B,CD] + [A,CD]B = AC[B,D] + A[B,C]D + [A,C]DB + C[A,D]B$

So these are some things which you can play around. This I already said. If you take the conjugate and transpose of two operators, so what we showed that the commutator of A, B is same as negative of commutator of A, B dagger right. So it is not Hermitian, to make it Hermitian we introduced an i . For xp commutator, you need a dimensionless constant.

xp commutator whatever is the dimension you have to introduce Planck constant, so that the both sides dimensions are matched and some of the interesting properties of the commutators which one of the things which you should remember if you remember when I was saying the properties of operators on the linear vector space, linear operators the order matters. You cannot say whether I call AB and BA are one in the same.

AB is different from BA in general. When will it be same? When the commutator of A with B is 0, then the order will not matter or you can measure this for that in whichever order right. So you need to keep track that you cannot violate the order, so if AB, CD is the order I first do the expansion of this side. I take the A out and B commutator with CD and then this one I keep the A .

But since this one should be order is AB , the B should come this side. B cannot be here which you can do in your classical mechanics but in quantum mechanics the A will be to the left, B will be to the right okay and what else can we do, we can further do the CD also the same way. So CD also if you do it what happens? C comes to the left and D goes to the right okay, so it will become AC with B and D .

And you can also write A with BC commutator at D this side. These are the two terms which you will get from this term and similarly the other two terms you will get from. One way in which you could do is you can expand this as ABCD- CDAB right.

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The image shows a handwritten derivation on a green background. At the top, the standard deviation of an operator \hat{A} is given as $\Delta \hat{A} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$. Below this, the commutator of two products of operators is derived: $[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\hat{B}\hat{C}\hat{D} - \hat{C}\hat{D}\hat{A}\hat{B}$. This is then expanded using the identity $[AB, C] = A[B, C] + [A, C]B$. The derivation shows: $[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}[\hat{B}, \hat{C}\hat{D}] + [\hat{A}, \hat{C}\hat{D}]\hat{B}$. Further expansion yields: $= \hat{A}\hat{C}[\hat{B}, \hat{D}] + \hat{A}[\hat{B}, \hat{C}]\hat{D} + [\hat{A}, \hat{C}]\hat{D}\hat{B} + \hat{C}[\hat{A}, \hat{D}]\hat{B}$. The slide includes logos for CDEEP IIT Bombay and NPTEL.

You could do that and you can also verify that I can write this as A times B with CD+A times CD sorry A times CD and then put the B here right this one. and you can explicitly write this further as AC times BD. This term will allow one more term, which is A with BC times D. Similarly, this term will be A with C DB+A with D B where will the C go, in the left. This is clear, is the pattern clear to you?

This is the way to play around with the commutator brackets when you have products of operators okay. Suppose I give you x squared commutator with p squared, how will you do that? x square commutator with p square.

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$$\begin{aligned}
 [\hat{x}^2, \hat{p}^2] &= \hat{x}[\hat{x}, \hat{p}^2] + [\hat{x}, \hat{p}^2]\hat{x} \\
 &= \hat{x}[\hat{x}, \hat{p}]\hat{p} + \hat{x}\hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p}\hat{x} + \hat{p}[\hat{x}, \hat{p}]\hat{x} \\
 &= (2\hat{x}\hat{p} + 2\hat{p}\hat{x})i\hbar \\
 (\hat{x}\hat{p} + \hat{p}\hat{x})^\dagger &= (\hat{p}\hat{x} + \hat{x}\hat{p})
 \end{aligned}$$

There is one more thing you can use here x with x where there is no order right. You can use that fact here. The commutator of x with x is 0. Say this is not AB ; it is not two different operators, the same operators. How will you write this? We can write this as x with x squared + x with p squared x and then what do we do? So that is x hat with x p hat with p hat + x hat p hat x hat p hat x hat with p hat okay.

That is the first term, the second term will be x with p hat with p hat x hat + p hat x hat p hat x hat. Now you use x p to be $i\hbar$ cross right. I am doing it in one dimension. What is the simplification finally? Twice x p and then twice x p with this one will be p x hat twice p x $i\hbar$ cross that is it. So something which you see here the beauty what is happening? This x p with p x should have the property that it is Hermitian right.

That day I was telling you that the order matters and whenever I have to write a Hermitian operator, so this if you have taken A with B as C , the C should be same as C dagger help and you can verify that if you take this operator, two factor anyway will let us not worry. If you take x p with p x and take the dagger of it, it will be same as this will become p x + x p which is same.

And we did not do anything. We just used the commutative property and we see that it always comes as a symmetric combination which I was trying to insist last time that in quantum mechanics because the order matters and you have a dot product of two operators, you first write that as a $AB+BA$ remember and I said that is what is the Hermitian combination.

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$$[\hat{x}^2, \hat{p}^2] = 2i\hbar(\hat{x}\hat{p} + \hat{p}\hat{x})$$

$$\downarrow$$
 Hermitian

$$\hat{A} \cdot \hat{B} \xrightarrow{\text{quantum}} \frac{\hat{A} \cdot \hat{B} + \hat{B} \cdot \hat{A}}{2}$$

$$\text{classical}$$

$$(\hat{A} \cdot \hat{B})^\dagger = \hat{B} \cdot \hat{A}$$

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If you had a cross product of two operators, so we find $x^2 + p^2$ to be $2i\hbar(xp + px)$, this is Hermitian. So I am just trying to say that if you have $A \cdot B$ as operators even in three dimension, you have to it is not same as $B \cdot A$ which you are familiar in your classical physics. This when you go to quantum physics, this is classical, quantum you have to make it Hermitian which means $A \cdot B + B \cdot A / 2$.




Is this Hermitian? If you just took $A \cdot B$ is it Hermitian? Not Hermitian right because $A \cdot B$ dagger is $B \cdot A$. A is Hermitian and B is Hermitian but $A \cdot B$ is not Hermitian. It goes to a new operator whereas this one $A \cdot B$ goes to $B \cdot A$ and $B \cdot A$ goes to $A \cdot B$ that is a Hermitian. That comes naturally in the commutative brackets, I did not do anything. Using the properties of commutator, I end up getting combination of $xp + px$ naturally.

I did not get just xp okay. So the order really matters and you have to be careful with the ordering.

(Refer Slide Time: 22:55)

Commutator properties

- Commutator bracket under conjugation gives a negative sign. To make the commutator hermitean, we introduce i .
- For $[x,p]$ commutator, Planck's constant \hbar is introduced to make it dimensionless
- $[AB,CD]=A[B,CD]+[A,CD]B=AC[B,D]+A[B,C]D+[A,C]DB+C[A,D]B$



So just to flash that slide, so the last where the ordering is done is the one which will help us to find the commutators of any products of operators. Let me stop here.