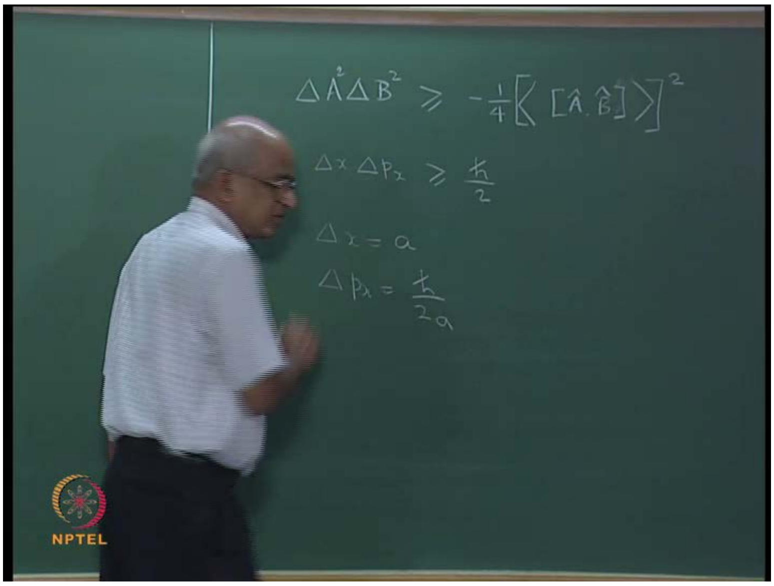
**Introductory Quantum Chemistry**
**Prof. K. L. Sebastian**
**Department of Inorganic and Physical Chemistry**
**Indian Institute of Science, Bangalore**

**Lecture - 32**
**Generalized Uncertainty Principle – Continued**

We were discussing this uncertainty principle and it is derivations. I actually demonstrated the uncertainty principle as apply to position and momentum. For example, we show that delta x into delta p x is greater than or equal to h cross by 2.

(Refer Slide Time: 00:43)



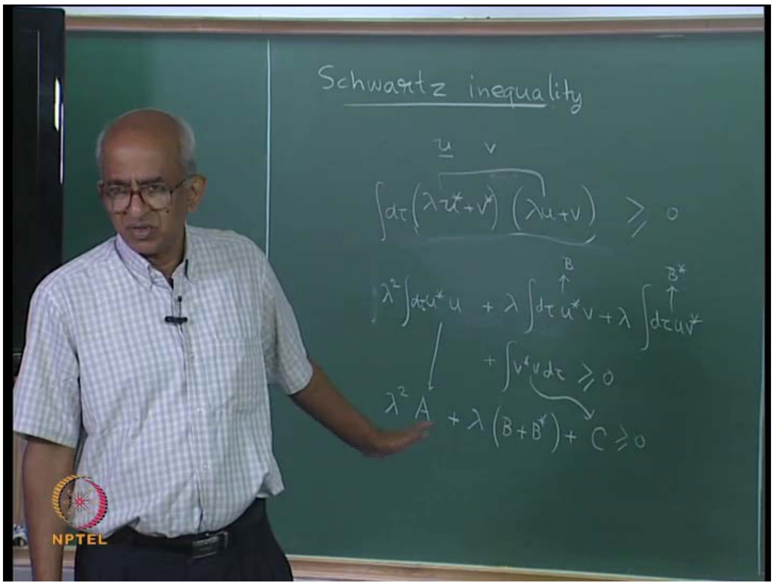

And I also told you that this is actually a special case of a generalized uncertainty principle, which says that delta A into delta B must be greater than or equal to minus 1 by 4 expectation value of the converted of A with B. So, would we will spend a little bit of time, I hope I got it right, if not anyway, I have going to derive it so, we would get it right. And in the specific case of x and p x, this actually let to their relationship that delta x into delta p x must be greater than or equal to h cross by two.

Now, this is a actually a peculiarity of a quantum mechanics, same classical mechanics it is possible for you to have a particle with a well define possessions as well as a well defined momentum. If I have this chalk piece and if I let it grow each instant. I know where it is and I also can find out what is the momentum of the particles. So, there is no uncertainty according to the classical mechanics, either in possession or momentum. You can define both at the same time to any precision that you want, but there is not what quantum mechanics is says actually if you look at this relation. This uncertainty principle what it says that, there is no state of the system in which the momentum and the possession are both well defined there is no such that.

So, if you try to construct a state with a very little and uncertainty in momentum, then as we have seen previously in the previous lecture the momentum becomes very uncertain. We did derive an expression for delta x and delta p and if you look at that expression what we found was, delta x was actually when we, I am not going to write the wave functions about delta x. If it I said delta x is equal to a then I found that delta p x was actually h cross by 2 a.

So, if you try to reduce the uncertainty in possession by reducing the value of a, then uncertainty momentum increases, right. Or if you try to reduce the uncertainty in momentum by increasing the value of a, that you can do then what will happen is the wave function? That we had it actually becomes very, very broad in the possession for it uncertain. So, let us now look at the derivation of this expression. The derivation is based upon an inequality with separate us Schwartz inequality.

(Refer Slide Time: 04:01)




So, let me first tell you what this is actually? If you think of any arbitrary function u and another arbitrary function, which I shall be note as v, these are two functions. If you because, we are thinking of quantum mechanics, we can think of them as acceptable wave functions. What I will do is? I will take the first function multiplied by a parameter lambda. So, lambda into u plus v, I am going to take, lambda I will assume is a real; it is not a complex number, lambda is real, but u and v are arbitrary they may be complex.

So, what I am going to do is, you can take this function, take it is complex conjugates, I mean, make thinks simple, I mean, I was going to say, I will make it one dimensional, but it is not necessary. So, these are the functions of any number of variables u and v. So, lambda u plus v, I am going to take the function multiplied by it is own complex conjugate. And then I will multiplied by the volume element d Tau and integrate over the entire space. I am just say the parameter and because you have taking this combination in the function and multiplying it by it is own complex conjugate what will happen.

The products this is actually equivalent to calculating the magnitude of lambda u plus v and squaring it, that is what this objectives. And this I know has to be positive and therefore, if I integrated it over the entire space, what should I get? I should get a number which is definitely greater than 0. So, this has to be greater than 0, but it may so happen that, have some I was not very careful and then what might happen is that, I have taken lambda to be minus 1 suppose and u to be equal to v.

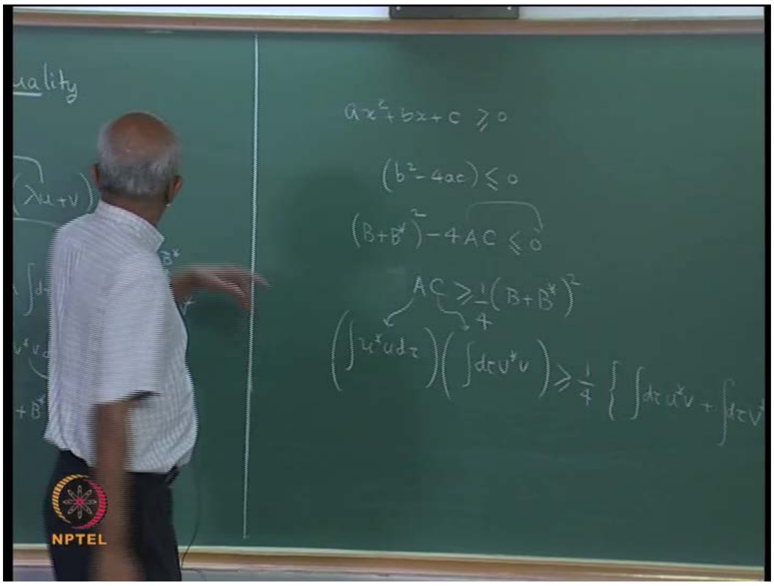
Suppose I mean by accident I choose that then what will happen this function, will came out to be 0, which case I have the possibility have in this equal to 0 and therefore, I can very confidently say that this integral has to greater than or equal to 0 right. And if that is the way it is I can expand this if you multiplied it out say lambda well this star operation you can take it inside. It is not going to affect lambda because lambda is assume to be a real. It will affect u as well as v.

So, I will take this star operation inside and I am going to get that. lambda is just a parameter it does not depend on the possession coordinates, it is something that you can choose anywhere it may be 1 or 2 or 3 or 3.5 some number. But interestingly whatever value you choose for lambda, the answer is guarantee to be greater than or equal to 0 that is important. So, let us multiply this out you will have the product of this two, that is going to be lambda square u star u that is 1 term right. When you multiply you are going to get that because lambda into lambda is there and then you will have the volume element d Tau and actually the integral we are locally here, but the integral I am going to put it here because lambda does not depend upon any possession coordinates is just a number just a constants.

So, therefore, this will be made first term and they will have 3 more terms. One of the next term will be lambda times integral d u sorry not d u, but d Tau u star v right, that will come when you multiply these with that and then you will have another time which is roughly of the same form lambda times integral u v star, correct. And the last term will be how much it is going to be integral v star v d Tau and this has to be greater than or equal to 0 right. Actually something very obvious and what I am going to do is I am going to say this is actually of the form lambda square into some capital a where capital a is this, plus lambda times well, I let me call this capital b.

Then if you look at this you would realize that this nothing but B star, the complex conjugate of B. The way it is this one and that one are complex conjugates. So, if I put this equal to B that equal to B star. So, here I can say lambda times B plus B star plus, this objects I am just going to denoted it temporarily by the symbol C and this has to be greater than or equal to be 0. And it does not matter, what the value of lambda is this is greater than or equal to 0.

(Refer Slide Time: 11:21)



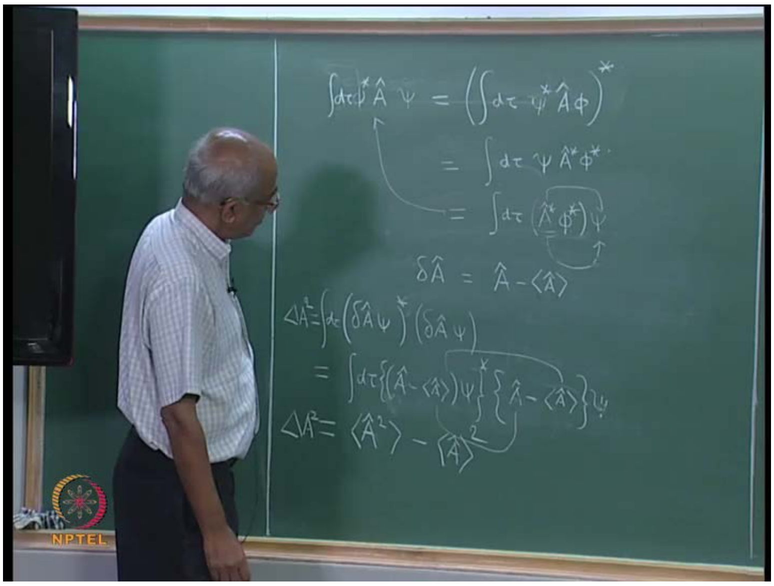

So, you can give any value either negative or positive it is guaranteed it should be greater than or equal to 0 correct. So, you look at this is a quadratic in lambda. And you have to remember whatever you study at regarding quadratics, a quadratic is greater than is guaranteed that, the quadratic is greater than or equal to 0. What does this means? This means that, this object that I hope you remember discriminates has to be negative.

You remember that I suppose it is see. If I have quadratic, quadratic like a x square plus b x plus c, if it is guaranteed that is greater than or equal to 0; that means, actually b square minus 4 a c has to be less than or equal to 0. This is something that, I shall assume you know already. And therefore, if I just applied it here what is the result that I am going to get? I am going to get b square while in this case you say this is small b is to be identified with capital B plus B star. So, capital B plus B star the whole square minus 4 times A into C has to be less than or equal to 0 right.

And that implies that, let me a write it may be revise, while I will take this to the other side; that means, for this left hand side is less than or equal to 4 A C or I will write it in this portion 4 A C must be greater than or equal to B plus B star whole square. Or if I divide by 4, I should get this, right. Straight forward, but now let me put back the definitions of and A C and B what is A? A is actually integral u star u d Tau, that is A, this is A. C is integral d Tau of v star v, that is C, is greater than or equal to 1 by 4, what are the values of B and B star well you have the definitions here.

So, what will happen is, integral d Tau u star v plus integral d Tau v star u, there is a square right. And this inequality is separate to as the Schwartz inequality. It is quiet useful in quantum chemistry actually. Whenever you encounter the later on it, whenever you encounter overlap integral they will exit to be you can prove inequalities regarding overlap integral that overlap integral I have not introduce. So, starting from here or using this inequality, I will be proving that inequality. And the way in this inequality is, we can actually you can compare the two and you realize that somehow what I have to have delta A square here. And how I will have to, if you compare the two I will have to have delta B square here. And then I have to see what that happens to the right hand side, and eventually the right hand side will work out to be equal to that, this is what going to happen. So, how do I mange this things is the question. Now these will take a few steps. Well let me start with this operator A. Operator A of course, we are doing quantum mechanics who operator A is Hermitian.

(Refer Slide Time: 15:44)



So, the moment using A is Hermitian, I know that, if you allowed d Tau operate upon psi multiplied it by phi star and then the volume element d Tau, answer will be equal to this expression. You allowed A to operate upon phi multiply by psi star integrate over the entire space and then take the complex conjugate right. In fact, if you took this complex conjugation inside, when you can see what is going to happen? You will get d Tau, this star and that star will be make it just psi, then you will get A star phi star right. This is what will happen if you took this star of operation inside. And that is equal to integral d Tau; see what is happening is that? I have to take A, take it is star what do you mean by taking the star, if A contains square roots of minus 1. If it contains i, then you have to replace that with minus i, A does not contain i, then you do not have to worry this, just unchanged.

So, if you like you can write this expression in a slightly different passion, you see I have this A star it is an operator remember, operating upon phi star. So, what this say is take A star allow it operate upon phi star and then multiply the result by psi and integrate over the entire space, that is what it says. But now, what I will do is, you see, I will put this A star phi star first. And then I am going to put psi but then of course, this can be confusing because A should not operate upon psi. So, therefore, I will put a bracket here to indicate that this is operating will be upon phi not on psi.

So, if you look at this expression, if you compare this two, what is if that you find? If you had a Hermitian operator and if you had an expression like this actually what you can do is? You can allow A to operate upon phi star instead of allowing A to operate upon psi, but then of course, not A itself, but a star has to be operating look at this is. This operate it can, at the moment it is operating on psi, but instead of that operate can be operating on phi star that what is saying it can be operating upon phi star.

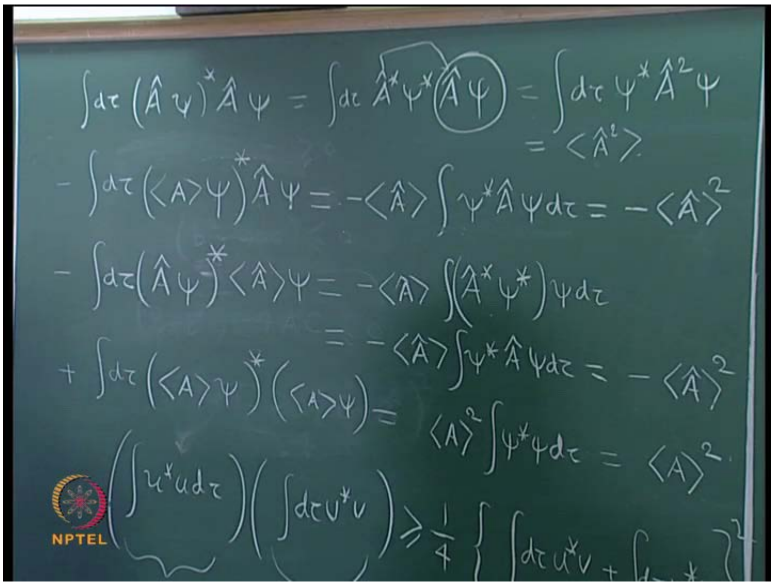
Then it is not the operator itself, but it is complex conjugate, that has to operate upon psi star you will get the same answer right. So, therefore, you can put then the other way, if I had an A star here operating upon this phi star. That A star can be transfer to A, sorry, transfer to psi, but then, when you transfer it becomes A. So, if you had an expression like this A star is operating upon phi star, but then this can be allowed, I mean it from here it can moved and allow to operate upon psi.

The answer is going to remain unchanged provided you take not A star, but A right, this is useful. So, with this I am going to think of, let me think of an operator which, I will denote as delta A, why do I call it delta A because, I am going to say it is nothing, but A minus the expectation value is nothing wrong in that, I mean you are going to give me an operate any operative I will first calculated expectation value and I am going to subtract that expectation value. Expectation value will be a number, in fact, it will be a real number because, this is our experimental answer right. So, this object will be a real number.

So, from A, I will just remove that and then I have this operative. Now, what I am going to imagine is that, I want to calculate delta A operating upon psi multiplied by delta A operating upon psi star, volume element d Tau integrate over the entire space. Now, you may wonder why do all these things. The answer is extremely simple, this is actually nothing but I am going to claim that this is nothing but delta A square. That is what I will show, this object and that is the reason why introduce this operate otherwise there is no reason for make introduce this operator.

This operator is such that the uncertainty in A can be written as delta A operating upon psi star multiplied by delta A operating upon psi. How do I show that? Well this is actually equal to integral of d Tau A minus expectation value of A into psi, you have to take this star of that. And you have A minus expectation value of A right. So, there are actually I mean if you multiply this, I would you will realize that, there are four terms, correct. There are four terms.

(Refer Slide Time: 22:45)



Let me look at the terms. So, the first term will look like what? Integral d Tau well A operating upon psi star and A operating upon psi this is the first term. There are 4 terms; I am just writing the terms are one by one. So, this is the first term correct. It comes from this and that. I mean A operating on psi multiplied with star operations and then you A operating upon psi that is first term. And this is actually equal to integral d Tau A star operating upon on psi star multiplied by A operating upon psi right.

Straight forwards step, but then I have already told you that, if I have the A operate A star operating here, I can actually allowed this to be transfer there, in general. Because you look at what I have done here for any arbitrary psi, if I had A operating upon psi multiplied by phi star integrated over d Tau. The answer is equal to this expression and therefore, I already told you, if I had an A star here, that A star can be transfer to psi, but only thing is that in that transfer process A star becomes A that is all.

So, that is what I am going to do here, I am going to transfer this A and allow it to operate upon this part. The only thing as I have told you is that the transfer process A star becomes A and therefore, what will happen? This is nothing but integral of d Tau psi star A square psi or what is that? That is nothing but the expectation value A square that is my first term right. Then you look at the next term, if there are 4 terms, we will take the next term by which one should I take, well may be this with that, this into that, into psi and psi star of course,.

So, that will appear with a negative sign. The negative sign you are going to minus integral d Tau what are the terms, that we have expectation value of A into psi, you have to take it complex conjugate and then you will have A psi, this is one of the next term correct. And what is going to happen is expectation value of A is just in number right. If you calculate the expectation value, this is the average of a large number of measurement, it just a real number.

So, this number is not affected by the integration. So, I can take it out. So, what will happen, I will have this object right, because I have taken this expectation value outsides. So, the expectation value is come out then I have psi A operating upon psi star right. And what is this? Nothing but expectation value of A right. So, therefore, this expectation value of A into expectation value of A, I forgotten to put the negative signs it should be there. So, therefore, minus A expectation values square is what this term fine. And you look at this next term what is it actually the we have taken this into that, into that, we have taken this into that, into that, the next term will be A psi star, we again this will going to be with a negative sign.

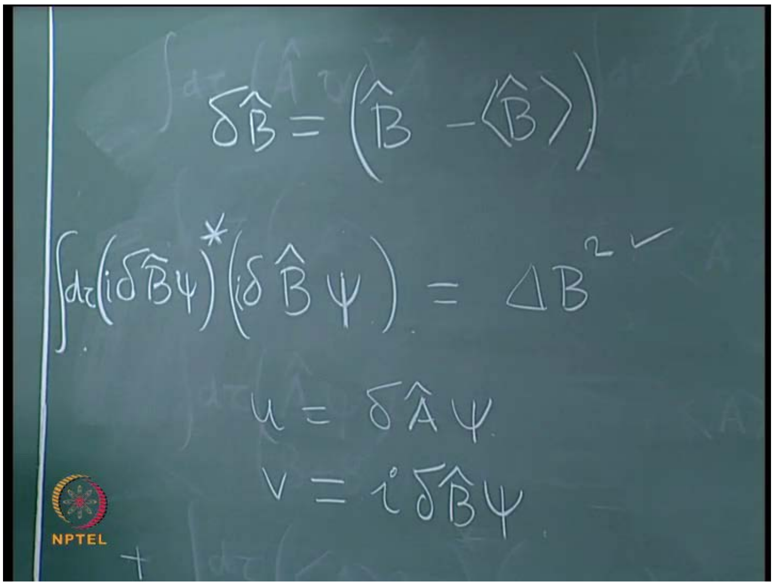
So, this is the next term right, I hope I got things right A operating upon psi correct. I take it from here and this A multiplied by psi is the term that I take and so, this is what it is and what is this actually A I can take out. So, minus expectation value of A integral A star psi star take the complex conjugate of this. So, I will get A star psi star multiplied by psi d Tau fine. And just as previously I can transfer this A star to that psi. So, if I transfer that what is that I am going to get minus A integral psi star A psi d Tau and what is this. This is nothing but expectation value of A and therefore, what is A to get another minus A square. And what is the last term? Last term is obtained from this into that right. So, that is actually quite simple might because, we have the product of two negatives sign it is actually plus.

So, what will happen is, I will have d Tau A psi star multiplied by expectation value of A into psi that is it. That is the last term, but there you know that the A is a real number. So, therefore, star does not affect it, this is the real number. So, this and that together they may be taken out. So, I will get A expectation value of A square multiplied by integral psi star psi, but we are assuming that psi is a function that is normalized and therefore, this integral is 1 and therefore, what happens the final answer that I get is expectation value of A square.

So, interesting we have four terms, the first term is actually nothing but the expectation value of A square. The second two terms are actually identical right, you get the same answer for the second two terms and to the last term is A square. So, if you added the four terms together, what is the answer that I had to get? I can write it here. If I added the four terms what do you get? You get expectation value of A square minus expectation value of A square that is all, correct.

Because there were two with the negative sign, two expectation value of A square with negative signs and to one with the positive sign and therefore the net result is this. And therefore, what is it I mean, whatever I want it to show, I have achieved in what sense. I claimed that delta A square if I define it to be like this it is nothing, but our previous definition. This is something this is the way; we define the delta A square in the previous lecture.

(Refer Slide Time: 31:43)



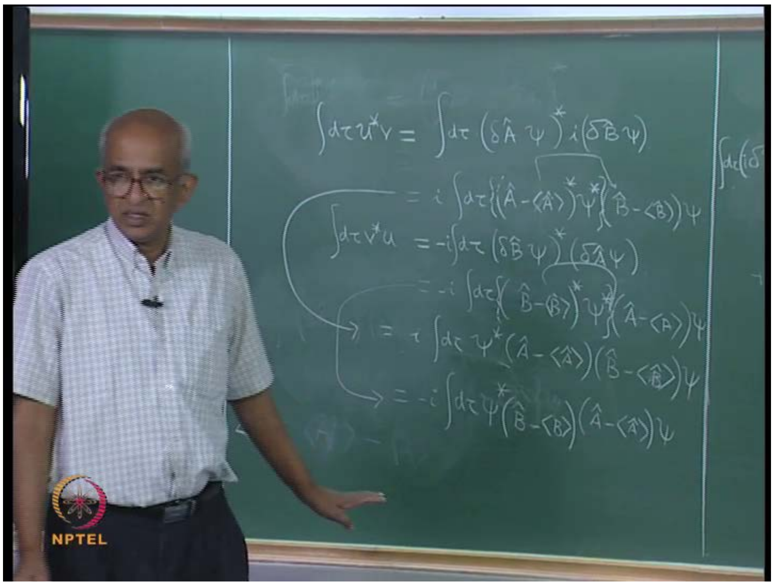

So, if that is the way it is, suppose I take the operator B and I am going to define something which will be B minus expectation value of B correct and I will say that I have delta B which is define to be this right. And if this delta B operates upon psi and delta B operates upon psi ones more you take it complex conjugate integrate over the entire space. What will happen? The answer will be actually equal to delta B square the uncertainty in B correct. And square of the uncertainty in B right, if you agree with that, then I am going to make a slight modification by introducing an i here.

If I had put an i either, what is going to happen? I am going to get, I am going to take it is stars. So, it will come out and it is going to be minus i, I have to neutralize that I cannot just have a minus i. So, I will put another i here. So, that everything combine together will give me a plus point. So, I have not done anything. So, therefore, this also is valid right. I mean this are the simple mathematical manipulations. The reason for doing this is not obvious at this moment, but you will get that answer, which is what we want any way.

So, what I am going to do now is this is my, this is correct and now, I have this Schwartz inequality. This is valid for any u and v, what I will do? I will say that u is going to be delta A operating upon psi right. This is valid for any u and v or let me say, u is delta A operating upon psi. And what is v, I will say is i times delta B operating upon psi, I can always do that, because this Schwartz inequality is valid for any arbitrary u and v. So, I am perfectly justified choosing, whatever you can chose your own u and v, it has to be valid because this is the general inequality that is valid. So, if you did that what will happen they, if you use that then we have attend whatever we wanted to attend because, what we want this is equal to? This should be equal to delta A square that is what we wanted.

So, if we use yet u to be that, then this will actually be equal to delta A square and what will this be? If we made this choice, this will be equal to delta B square. Uncertainty in A square and uncertainty in B square and now, with this choice what will happen to this part is the question and we will work that out it is not a difficult calculation, fairly simple if you work it out powerfully, I will get that answer. So, let me do that. So, if you chose u to be this and v to be equal to that, what will happen to integral d Tau u star v?

(Refer Slide Time: 36:03)



What will that be, it will be actually equal to integral d Tau, u is how much delta A psi star into v. v is i into delta B psi correct. So, you can take that I outside, that go to get i then integral d Tau, you are going to have A minus expectation value of A psi. You have to take the complex conjugate. So, star will comes here then you will have to let it stay here. Because I am taking the complex conjugate then, delta B will be B minus expectation value of B into psi. And what will be integral, what is the other integral v star u right.

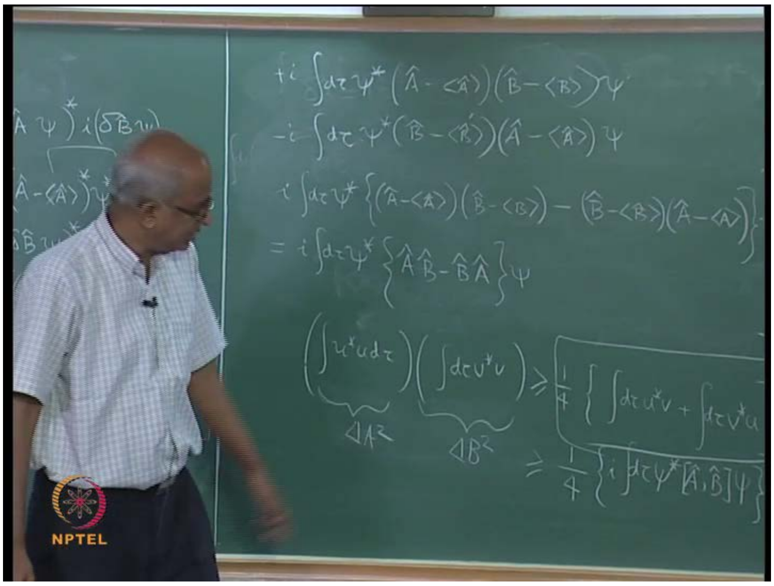
So, you are going to get integral d Tau v star u and that be equal to integral d Tau v star. v star will give me a negative sign there will be minus i because u, this is v. It took the star, it going to give me a minus i delta B. delta B operating upon what, psi then you have to take this star then you have to have delta A operating upon psi, it actually will be equal to minus i integral d Tau B minus B expectation value, you have to take this star of the whole thing, psi star A minus expectation value of A psi. Now what happen if I add these two things up? Correct.

I have to add these two things up. So, if I added these two things up, what is the answer that, I am going to get is the question, but before I add the two up I want to do something more I just want to see this is. This whole thing is an operator and A is a Hermitian operator, this we said just a number right. So, what I can do is, I can actually transfer and allow them to operate upon this I from here, I can allow them to transfer to here and operate and all that what we have to do is when I transfer I have to take the complex conjugate of that. So, let me do that as a intermediate step there. So, here what is going to happen is, this is going to be equal to i times integral d Tau, you transfer it to the allow to operate the upon that. So, I shall get psi star A minus expectation value of A there is already a star, but when you transfer you will put one more star.

So, double star means you get the same number original number back. So, get A minus expectation value of A into B minus expectation value of B into operating upon psi. That is what happen to this term and if you put at this term kind of thing with this. What will happen? You will get minus i integral d Tau right. You take this you are going to transfer this to the other side there is already a star when you transfer you will take one more star and therefore, what will happen? The star operations you see back the original the due to star and back the original, but then what will happen you will get psi star. This is going to be transfer and it is going operate upon here.

So, you are going to get, this you are going to transfer you see this was original operating upon psi star, but instead of operating upon psi star, you will transfer it and you will allowed it operate upon that. And while to be actually very, very clear, I should put a bracket here, because this operator was operating only upon this part. And this operator again is operating only here.

(Refer Slide Time: 43:37)



So, therefore, when you transfer it. It is going from here answer getting operated on that points. So, that is what happens. So, then if you added these two up, which are the once I should add up these two things. You will see something interesting happening, you will see that if I added these two up and I am to going get an i integral d Tau psi star. This is your first term correct, I have just written the first term and I have to write the second term, unfortunately there is no space.

So may be what I will do is, I will write the whole thing up here. I will write this term once more. The first term is actually plus i integral d Tau psi star. This term let me remove this; this term is going to be psi star A minus expectation value of A into B minus expectation value of B operating upon psi that is the first term. And the second term is actually with negative sign integral d Tau psi star B minus expectation value of B into A minus expectation value of A. So, these are the two terms. If you just added the two up I would see that the i is common, until i there are severally things others commons, let me take it d Tau psi star and then you will have this products A minus expectation value of A into B minus expectation value of B minus I am combining the two terms.

So, this is what results, right. I have not done anything great, I mean I have just simplified things. And then they, if you look at this expression, what is that you are going to get? You will get it i times integral d Tau psi star to multiply things, you are going to get A into B from here and from there you are going to get B into A is not in the same order. You see A into B minus B into A is what you will get? And then you should remember that these things are numbers as for us numbers for concern, you can put them in any order you like. They are not operators and therefore, you for example, will get minus A expectation value of A into B and you will get the similar kind of term from here.

What is that I said minus expectation value of A into B correct and from here, you are going to get minus expectation value of A into B, but with the positive sign. So, they will cancel each other similarly all the other terms you can just expand you will see that all the other terms except these two terms will cancel each other and therefore, what happens you get this as the answer. So, we have evaluated this part what is the answer? The answer is that and therefore, if I just substitute it that to the right hand side what I am going to get? I am going to get 1 by 4 i times integral d Tau psi star, what is this actually? It is the A B minus B A and this is the thing that we have been referring to us the commutater of A and B. So, therefore, you get A commutator B, this is just chotta notation right. And then I have to put psi here and close the bracket.

So, this is the object that I have written, but I remember, I have A square here. So, therefore, we have evaluated the right hand side. The right hand side evaluates to be this on the left hand side, this is delta A square this is delta B square. So, sees the delta A square into delta B square has to be greater than or equal to be this object, that is what it says, but there is i sitting inside and you have to take square of that. So, when you take the square of that you can remove this i and say that there should be a negative sign, correct. And if I remember correctly we had actually or I had actually demonstrated this by taking A to B x and B to B x that I did yesterday and you should realize that. This is a very general thing what does it say, it says that give me any two operators in quantum mechanics, give me any two operators and it does not matter what the state of the system is.

It does not matter it can be any state of the system this inequality has to be valid and this is extremely general right. Extremely general, if you apply it to possession and momentum you will get what is refer to as the Heisenberg's uncertainty principle. So, this is generalize the uncertain relation, this was not derived by Heisenberg, or somebody else. As Heisenberg derive delta x into delta p x is greater than equal to h cross by 2, but this generalized uncertain relationship was derived later and it is valid for any A and B. That is the perfect time for me to stop for today; thank you I shall continue I mean we will use this in the next lecture.

Thank you for listening.