Quantum Mechanics- I

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Lecture - 6
Postulates of Quantum Mechanics – II

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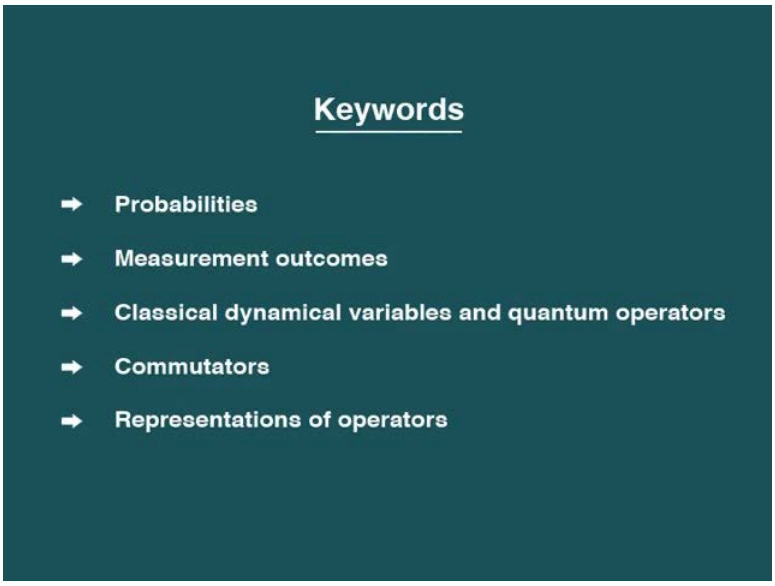

In my last lecture, I spoke about some of the postulates of quantum mechanics and today I will continue to talk about the postulates. In particular, I will concentrate on the postulate relating to expectation values basically, the outcomes of experiments.

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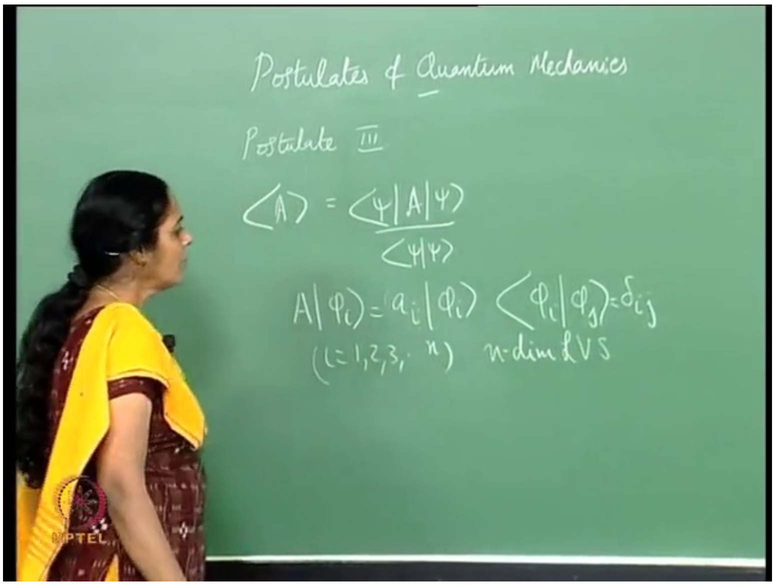

So, postulates of quantum mechanics. And, we were on the 3rd postulate last time so, postulate 3 where I had introduced the concept of the expectation value of an operator, this is the notation. This operator stands for a physical observable pertaining to the system of our choice and it is a very state dependant quantity and it is to be understood in this manner.

So, we have a basis set which is the set of Eigen states corresponding to A with Eigen values: a 1, a 2, a 3 and so on and I it takes values 1, 2, 3 to n. This is an orthonormal basis and these are real numbers, because A is a physical observable and therefore represented by a Hermitian operator, n is the dimension of the linear vector space and that is why n basis vectors which we have chosen to be an orthonormal basis set. To begin with if they were not orthogonal to each other we would use the Gram-Schmidt procedure and make it an orthonormal set.

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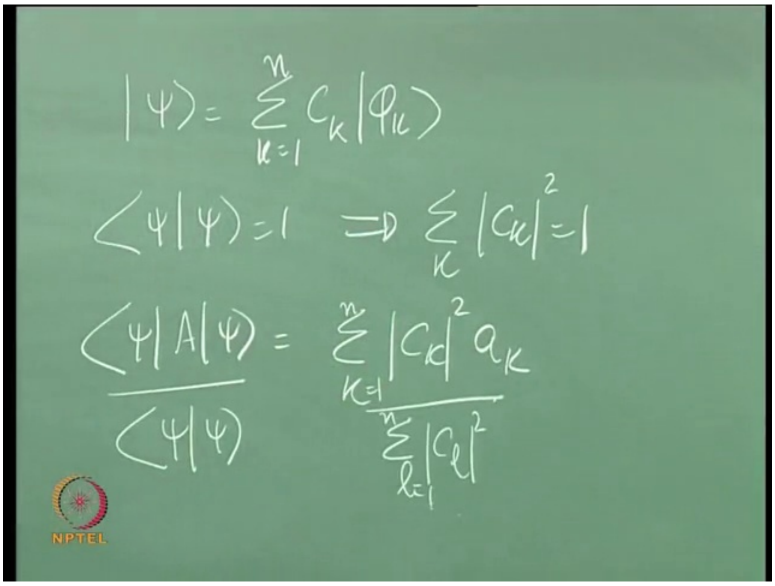

So given this, you consider any state psi which is expanded in terms of this basis set in the following manner and let us imagine that psi is normalized to 1. In that case, it is clear that summation over k mod C k square is equal to 1. In general, psi may not be normalized to unity. In any case given this psi we showed that psi a psi or summation over k mod C k squared a k and suppose, you also had this denominator which was not equal to unity this was simply summation over l mod C l square always going from 1 to n. Of course, I stopped at a point where I said that if this were normalized to unity it simply means that the denominator is 1 and we need to give an interpretation here.

It is obvious that the outcome of the experiment which is the expectation value of a is a weighted average. Because it looks like a 1 is going to be the outcome. The corresponding state of course, would be phi 1 with a probability mod C 1 square. There is a weighting coefficient mod C 1 squared. Similarly, a 2 comes with the weightage mod C 2 squared and so on. And this is what gives a probabilistic interpretation to quantum mechanics and measurement itself.

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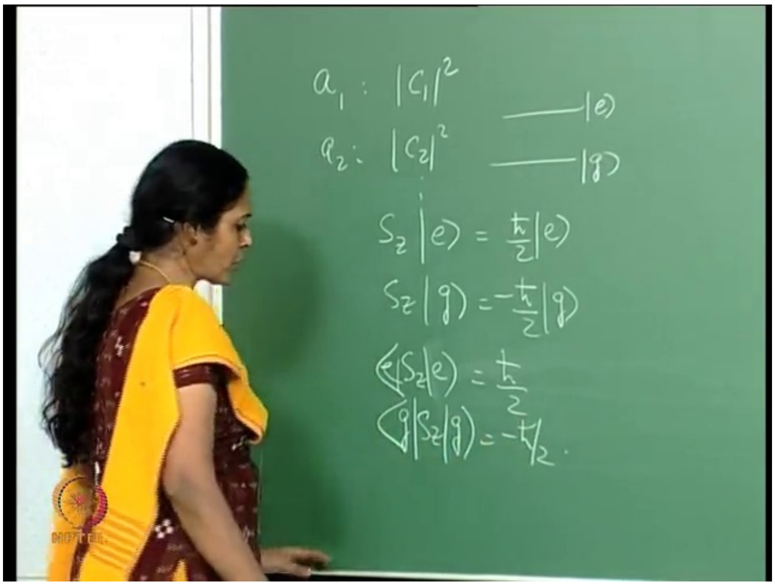

Because I would do the following thing: I would say that a 1 appears with probability mod C 1 square as the measurement outcome, a 2 with probability mod C 2 square and so on. So, let us demonstrate this with a concrete example back to the 2 level atoms. So, the Hermitian operator in consideration let us say is S z given the states g and e, we had S z when it operates on e gives me h cross by 2 e ket e and S z acting on g gives me minus h cross by 2 ket g. So, these are the basis states and I have chosen them to be Eigen states of S z. It is therefore, clear that if I have to find the average value of S z say in the state e it is simply going to be h cross by 2, because it is already an Eigen state. Similarly, if I have to find this, this average value is minus h cross by 2. The expectation value is simply the Eigen value in this case.

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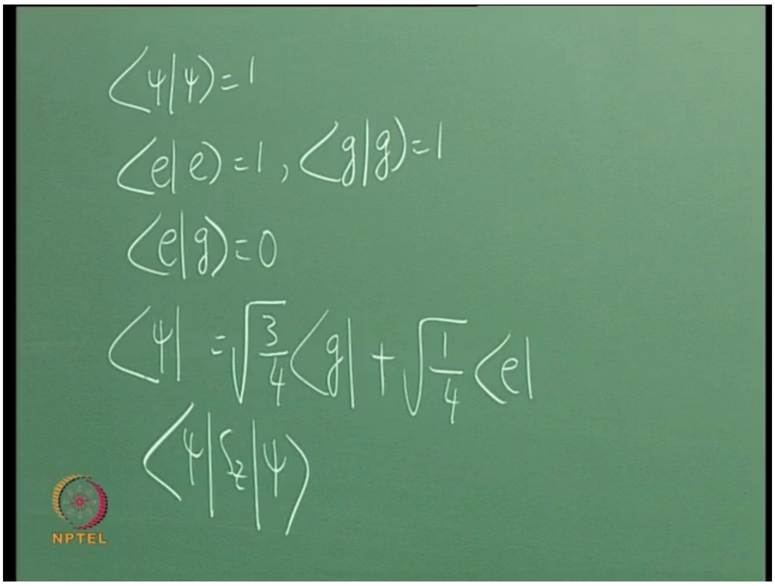

On the other hand, let me consider a state psi is root 3 by 4 ket g plus root 1 by 4 ket e. Of course, it is normalized to 1 because this inner product is 1, this inner product is also 1 and the state ket e is orthogonal to the state ket g. Bra psi correspondingly, is root 3 by 4 bra g plus root 1 by 4 bra e and now, I wish to find the expectation value of S z say in the state psi. I have not put in the denominator, because that inner product is 1 and I wish to compute this object.

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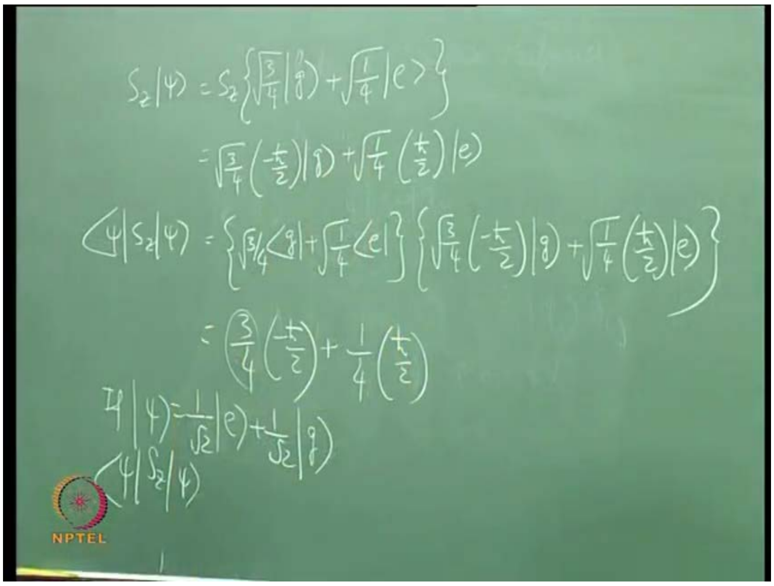

So, I would do the following: first of all I would find out the action of S z, on the state psi. Well, that is the same as S z acting on root 3 by 4 ket g plus root 1 by 4 ket e. That is root 3 by 4 minus h cross by 2 ket g plus root 1 by 4 h cross by 2 ket e. Now, I need to find out this object. Just to remind you, an operator acting on the state gives me another state in that linear vector space. So, this is simply going to be root 3 by 4 bra g plus root 1 by 4 bra e with root 3 by 4 minus h cross by 2 ket g plus root 1 by 4 h cross by 2 ket e.

It is pretty clear that this is 3 quarters minus h cross by 2 times minus h cross by 2 plus 1 quarter times h cross by 2. This is the probability with which the measurement outcome is minus h cross by 2 and this is the probability with which the measurement outcome is plus h cross by 2. In other words, I have several trials conducted because I need to look at the average value, the expectation value of S z in the prepared state psi, ket psi. And it looks like, 75 percent of the time my answer would be minus h cross by 2 the corresponding state of course, would be ket g after measurement, and 25 percent of the trails would give an answer plus h cross by 2 with the state collapsing to the excited state of the atom, that is ket e.

So, this is expectation value S z of course, I can simplify it and write it for you as minus 3 h cross by 8 plus h cross by 8 and that is equal to minus h cross by 4. It is clear, that if psi is an admixture of states with the following coefficient: 1 by root 2 in both cases. 50 percent of the time the expectation value would give me h cross by 2 as the answer and 50 percent of the time I would get minus h cross by 2 as the answer. Let us recall that the measurement is made on an ensemble; on each member of the ensemble the measurement is made once.

After the measurement the state collapses to either ket e or ket g in this case. Get to the next copy in the ensemble and make a single measurement and so on. Take the arithmetic mean of the values and that is the expectation value. One can ask the following question, we are expanding the states ket psi in terms of the basis states which are Eigen states of S z. What is the expectation value of S x?

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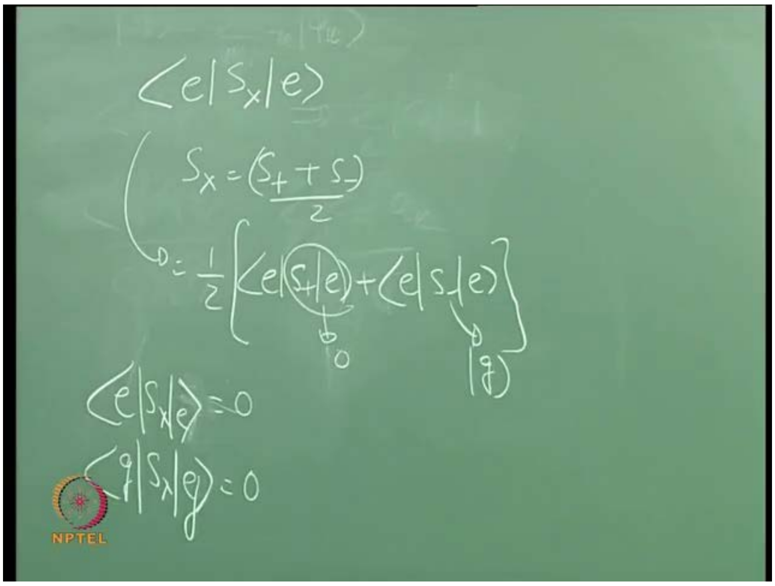

For instance, in this case let us take a simple example. Suppose, I wanted to find the expectation value of the operator S x in the state e. Well, this is simply done because S x you will recall is S plus plus S minus by 2 and therefore, this quantity is simply half e S plus e plus e S minus e. So, computing the expectation value of S x reduces to finding out these expectation values. But S plus acting on ket e simply gives me 0 and S minus acting on ket e takes it to ket g and e and g are orthogonal to each other and therefore, the expectation value e S x e is equal to 0.

Similarly, in the basis state ket g we can show that the expectation value of S x is equal to 0. Now, let us look at that superposition which I considered earlier and in a similar manner we can find out what the expectation value of S x is in the superpose state.

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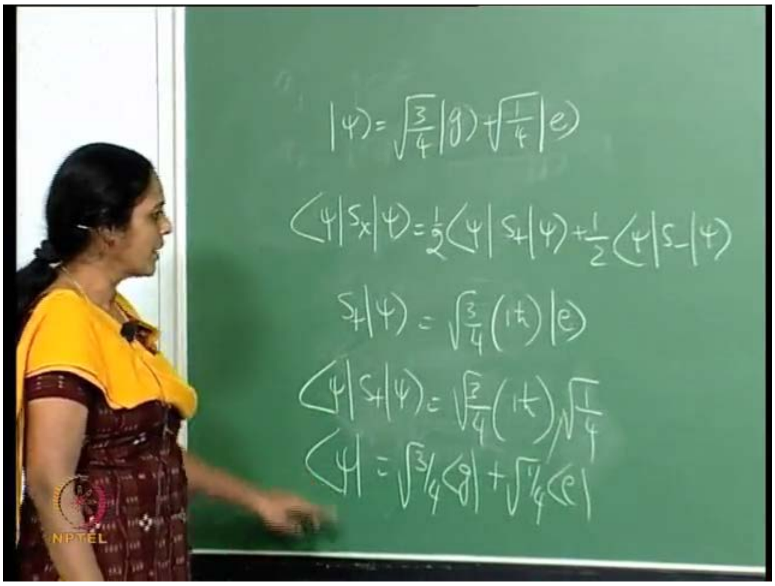

So, once more I write psi as root 3 by 4 ket g plus root 1 by 4 ket e and I wish to find the expectation value of S x in this state. So, that amounts to finding out this object. So, S plus acting on psi to begin with, when S plus acts on ket g it gives me ket e with coefficient 1 h cross and when S plus acts on ket e it simply destroys the state. Therefore, psi S plus psi is root 3 by 4 1 h cross times a root 3 by 4 from this part, times a root 1 by 4, because this part of psi would contribute to the expectation value. Recall that, Bra psi is root 3 by 4 bra g plus root1 by 4 bra e. So, what contributes would really be this combination which gives me root 3 by 4, root1 by 4 times 1 h cross.

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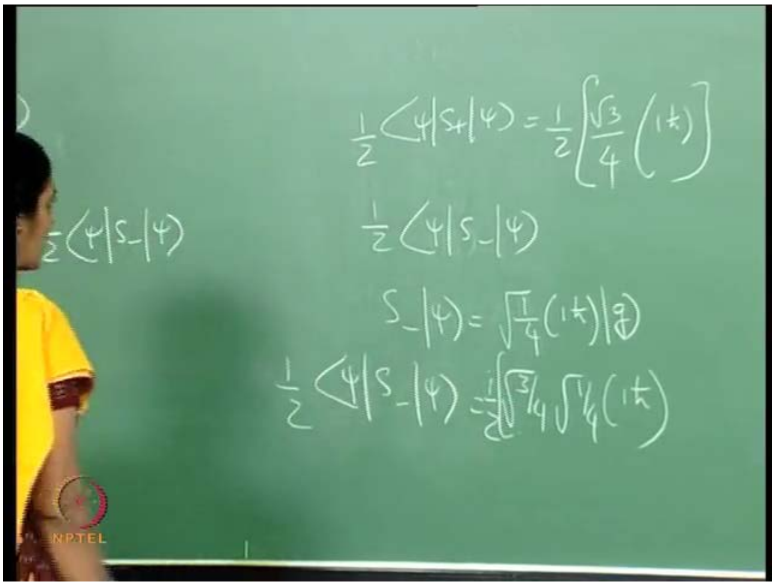

And therefore, I simply have psi S plus psi. I need to take a half out here. Half psi S plus psi is half root of 3 by 4 1 h cross. I want to write this separately to show what the measurement value is going to be, what the outcome is going to be. (Refer Slide Time: 11:54) Now, we look at the other part which is half psi S minus psi. Now, S minus acting on psi, S minus annihilates g, it acts on e and brings it down to g with the coefficient 1 h cross, so psi S minus psi. (Refer Slide Time: 11:54) This is bra psi and therefore, I am going to have a root 3 by 4 root 1 by 4 1 h cross. Of course, if I want to do half of this that simply tells me that, I have an answer which is half of that object. (Refer Slide Time: 11:54) I believe here psi S plus psi as a root 3 by 4 times a root 1 by 4 so, I should put that down.

So, that is what I have. (Refer Slide Time: 11:54) I have psi S plus psi and psi S minus psi with the factor of half. The two of them can be added together to give me the expectation value of S x in the state psi.

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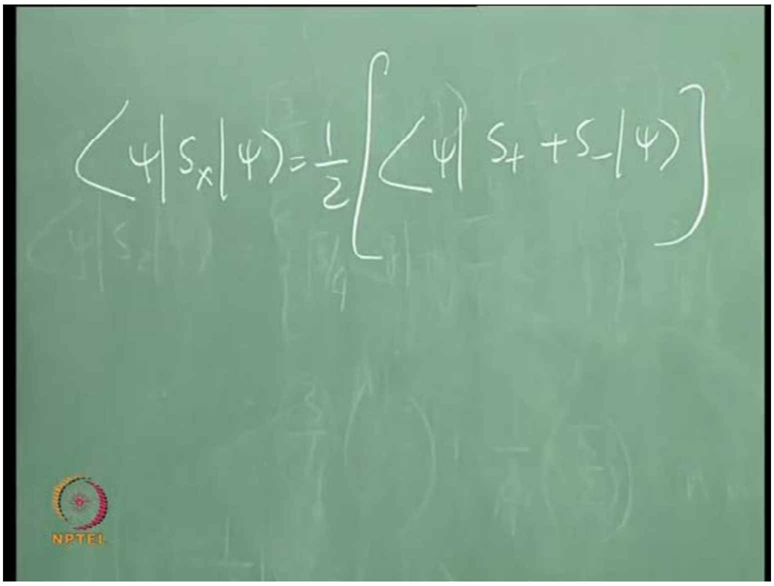

I get the value 1 h cross with the probability, this object and I get the value 1 h cross again from ket g with a probability this value. So, I can add them both up and I just write this as whatever, I have got from S plus minus S minus psi. So, this is the way the expectation value of S x is found in a state which is not an Eigen state of S x or S z, but which is expanded as a superposition of Eigen ket s of S z. So much for expectation values of operators.

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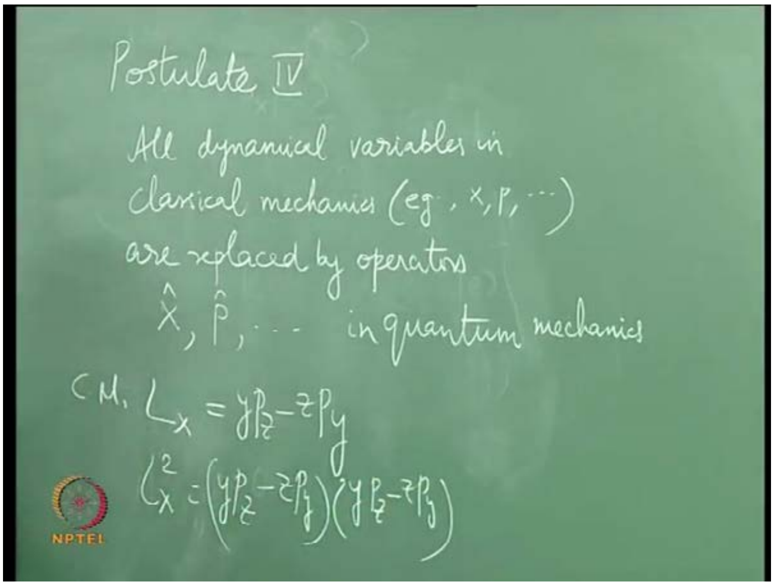

The next postulate is about how exactly you go from classical physics to quantum physics and the postulates say the following. So, this is postulate 4. It says all dynamical variables in classical physics; let us say in classical mechanics. Example: position, momentum, angular momentums and so on, are replaced by operators and in normal standard notation an operator comes with a cap like that, in quantum physics. I have not used this cap in all my lectures till now to denote operators.

One starts off by writing operators with a hat there and then, when one is pretty clear about: what is the operator? And what is the Eigen value? And what is the state? You could think in terms of dropping these hats and simply replacing x operator by x without the hat and realizing that it is an operator. Having said that, care must be exercised in the manner in which we replace dynamical variables by operators. For instance, you consider the x component of the orbital angular momentum. In classical mechanics, this is simply y P z minus z P y where, P z and P y are components of the linear momentum P and I have written these in Cartesian coordinates.

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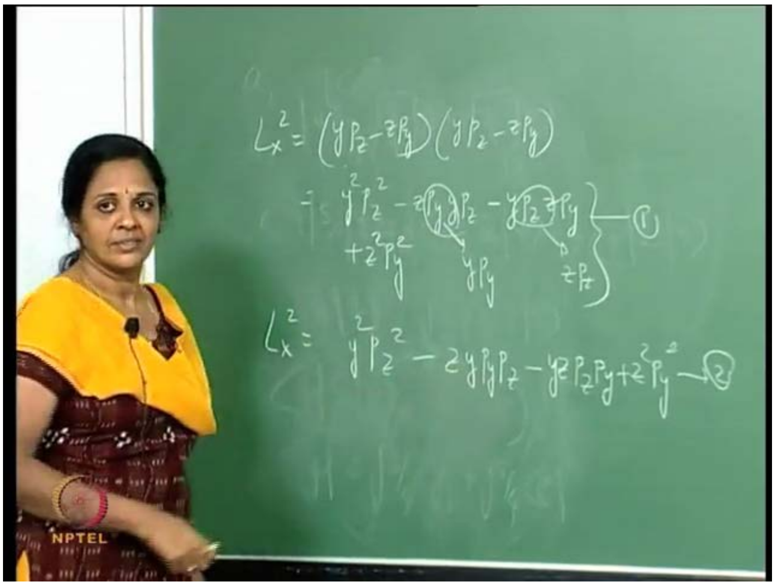

So, L x squared would be y P z minus z P y times y P z minus z P y and what would that be? These are numbers in classical mechanics and therefore, L x squared we can expand this as: y squared, P z squared minus z P y y P z minus y P z z P y plus z squared P y squared. We need not worry about the order in which these things are written for instance, this could well be written as y P y and this could well be written as z P z. But in quantum physics these are operators and as you are aware by now, operators are represented by matrices which in general do not commute with each other.

And therefore, one has to exercise care in the manner in which this is written. I cannot for instance, write this as y squared P z squared plus minus z y P y P z minus y z P z P y plus z squared P y squared. This is one way of writing this expression and this is a 2nd way of writing it. They are equivalent as far as classical mechanics is concerned, but here I should be careful because I have interchanged the order and in general P sub y and y where, P sub y is the canonical momentum corresponding to y. They do not commute in general with each other and therefore, one has to retain the order as such. So, the manner in which this is to be expanded is y P z y P z, minus z P y y P z, minus y p z z p y, plus z P y, z P y. So, that is the manner in which one retains the order of operators without changing them. Of course, when it comes to operators like spin, there are no classical analogues to worry about and again the operators should be ordered based on the commutation relations between the operators.

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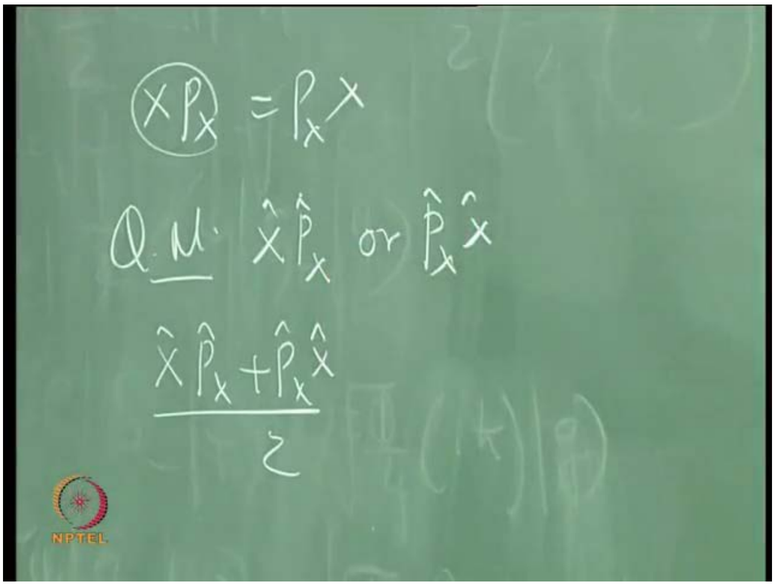

We could be thinking in terms of an operator like this; say this operator, in classical physics I can have an object X P x. In classical physics that is the same X P x X, but if I go to quantum mechanics should I write operator X, operator P x or operator P x, operator X. How do I replace X P x? I should careful and the replacement would be like this.

So, you take this combination divide it by 2 and treat that, as the operator corresponding to the classical object X P x. This is a very important point and care must be exercised because we are now dealing with matrices or non commuting operators in general. Finally, there is a postulate which I will call postulate 5 which really tells us something very important. It tells us how to go from the Poisson bracket in classical mechanics to the commutator bracket in quantum mechanics and that is how you go from one to the other.

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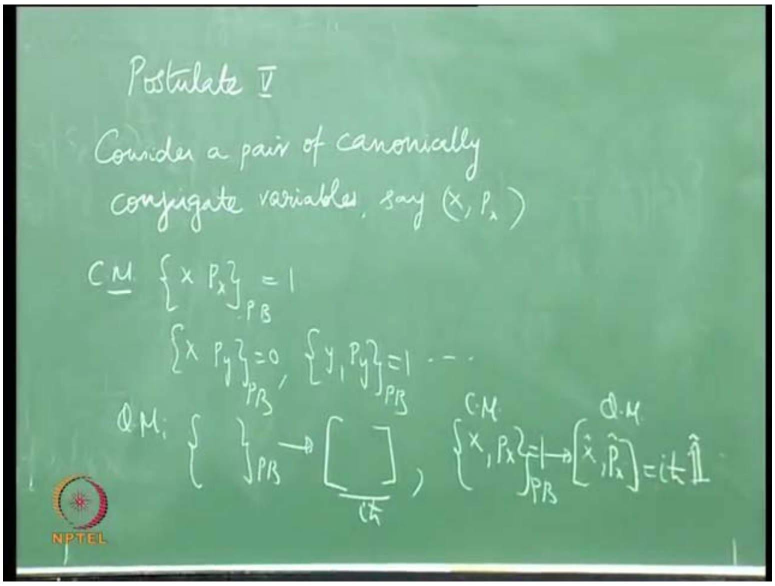

So, there is postulate 5. Consider, a pair of canonically conjugate variables say X P x. In classical mechanics, you have a Poisson bracket structure, by this I mean the Poisson bracket of x with p x that is 1. Of course, X with P y is equal to 0, y with p y Poisson bracket is equal to 1 and so on. The replacement is as follows: in quantum mechanics, the Poisson bracket is replaced by the commutator bracket divided by i h cross. In general that is how one goes from classical physics to quantum physics. And the Poisson bracket between pairs of canonically conjugate variables is replaced by the commutator bracket which is equal to i h cross.

So, X P x commutator is i h cross. I go from this commutator to the Poisson bracket through this operation the commutator divided by i h cross. So, when I go to classical physics from here I get X P x is equal to 1. So basically, X P x is equal to 1 gets replaced by X P x commutator is i h cross in quantum mechanics and this is classical mechanics. Now, this is a very important statement. First of all one understands that x is an operator so, if you wish we could put a hat here and a hat there. The commutator of two operators cannot be a number.

So, basically we mean that there is an identity operator there. To give matrix representations there is an identity matrix which means you put 1 on the diagonal and zero everywhere else and X and P X are also matrices and they do not commute in general. The same goes for y with P y z with P z, angle and angular momentum and so on. So, pairs of canonically conjugate variables which have this Poisson bracket structure would simply go to the commutator equal to i h cross times the identity.

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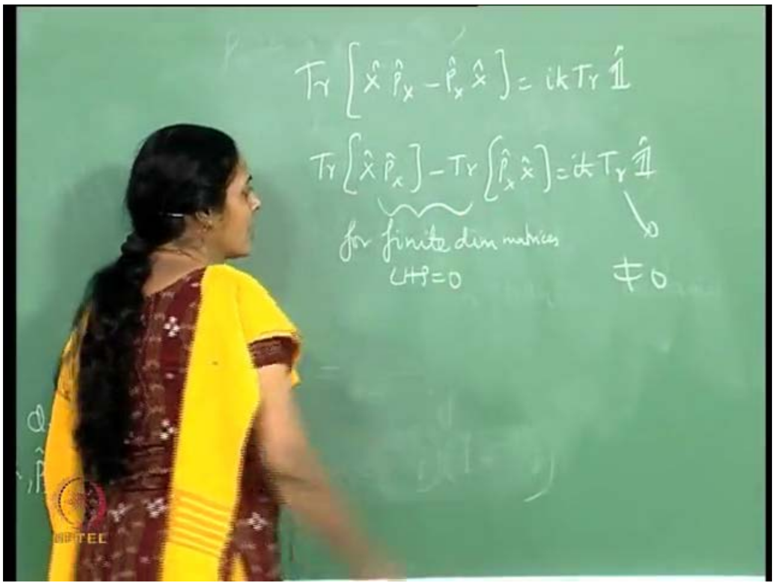

Now, some very interesting things can be seen right away. If these matrices where finite dimensional matrices suppose, I took the trace on both sides, these are operators. If these are finite dimensional matrices, we know that this is the same as saying trace of X P x minus trace of P x x is equal to i h cross trace of the identity. And since trace is invariant under cyclic permutation, for finite dimensional matrices the left hand side is 0.

Now, the right hand side is definitely non zero because the trace is the sum of the diagonal elements and the diagonal elements are one each. So, when you add up that is non zero. It is pretty clear therefore, right here that the only way out of this problem is to realise that X P x and so on are infinite dimensional matrices. And in infinite dimensions the trace invariance of the trace under cyclic permutations does not hold good. In general does not hold good.

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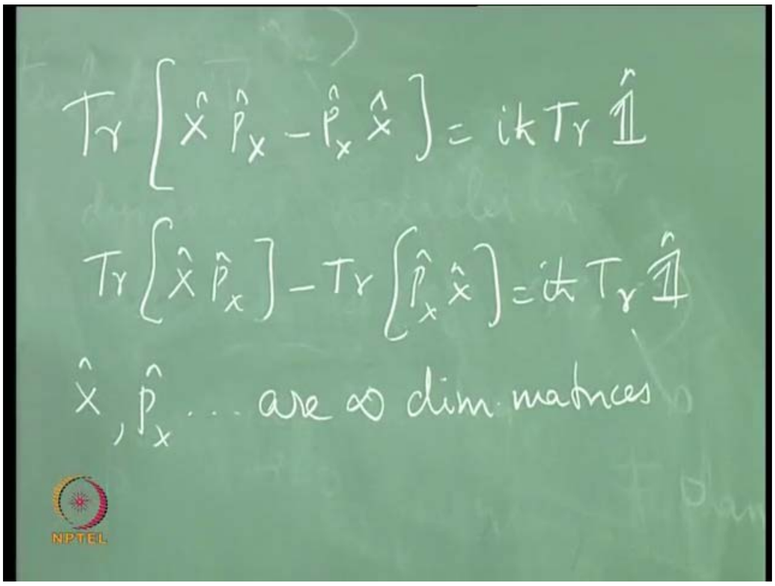

So, here is a very simple way of realising that X P x etcetera are infinite dimensional matrices. That is if I give matrix representation to these operators, they would be infinite dimensional.

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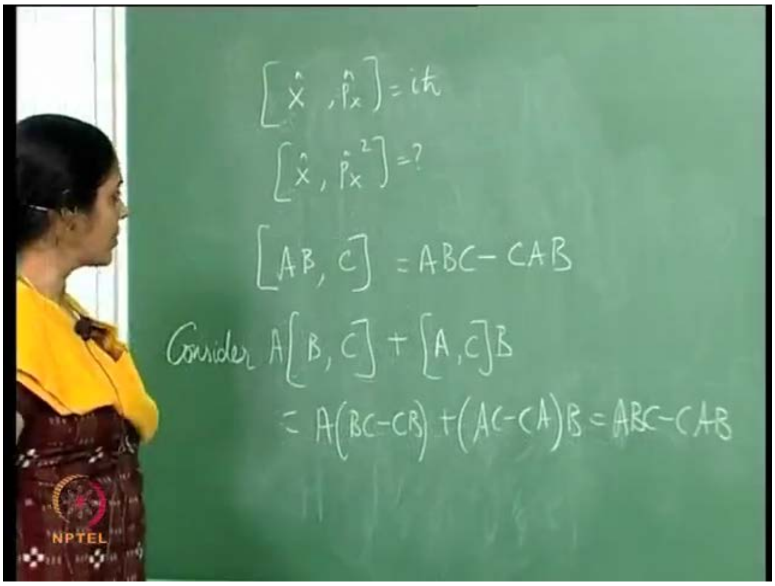

Further, I can find out commutators of X with P x squared and so on and if I did that, I see some interesting things. Given that X P x commutator is i h cross I am not writing the identity there, but it is there. What is the commutator of X with P x square? It is good in general to realise the A B C rule for commutators suppose, I have the product A B, A B being matrices the commutator with C. This is the same as A B C minus C A B. Consider this object, the commutator of B with C pre multiplied with A plus commutator of A with C post multiplied with B. Now, this is simply A times B C minus C B plus A C minus C A times B. This term minus A C B cancels with plus A C B and I am left with A B C minus C A B.

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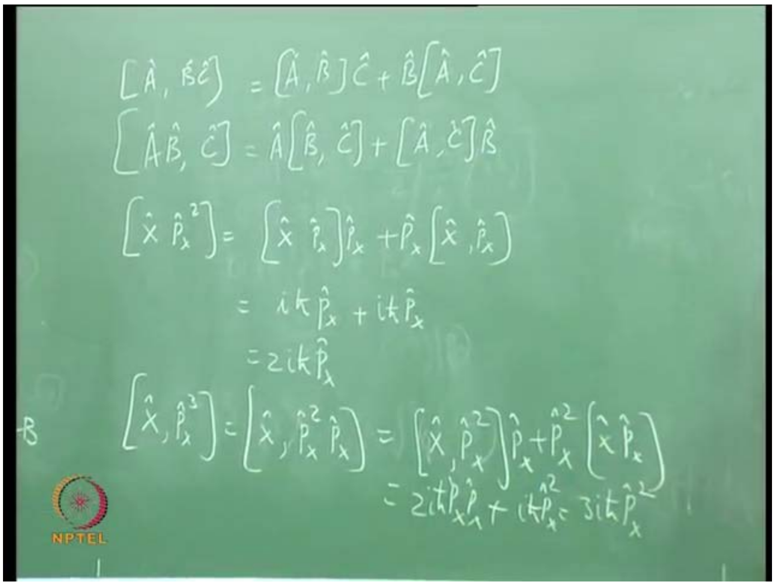

I have explicitly demonstrated by doing this. I have explicitly demonstrated by doing this. But if I have to find the commutator of A B C that is the same as this object, all these being operators. Normally, called the A B C rule and very useful for most calculations. In particular I am going to use it here. So now, X with P x squared by this rule is X with P x times P x plus this object. Well, I could have done the same thing and you could have checked that A B C, which is what I am using here is A B with C plus B A C.

All of them come with hats, they are all operators. So, that is what I have done here. These P x and C is also P x. This simplifies by that postulate phi to i h cross P x plus i h cross being a number I can pull that out and that multiplies P x which is 2 i h cross P x. Now, what is the commutator of X with P x cubed? Well I can always write it as the commutator of X with P x squared P x. I use the A B C rule that say this is B and that is C and therefore, I am going to have X P x squared with P x plus P x squared X P x which is 2 i h cross p x times p x plus i h cross p x squared which is 3 i h cross P x squared and so on.

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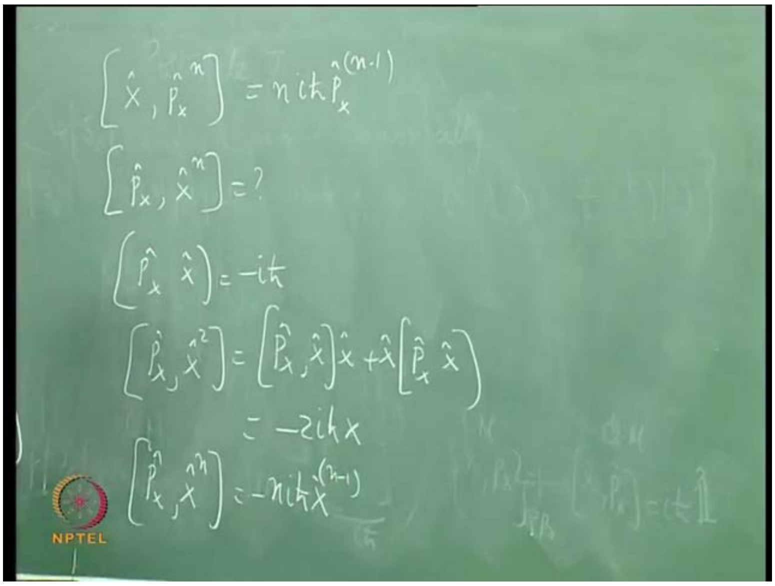

So by induction it is clear that the following relation holds. The commutator of X the P x to the power of n where n is some positive integer is n i h cross P x to the n minus 1. This is one of the things that I have come across now. I am going to see another result soon suppose, I found out P x with X to the power of n, where n is a positive integer. I would do the same thing. I would say that P x with X is minus i h cross; it is easy to check that the commutator of A with B is minus the commutator of B with A.

Of course, there is an identity here. P x with x squared by the A B C rule is this object; that gives me a minus 2 i h cross X and so on. And finally, I could have P x with x two the power of n i minus n i h cross x to the power of n minus 1.

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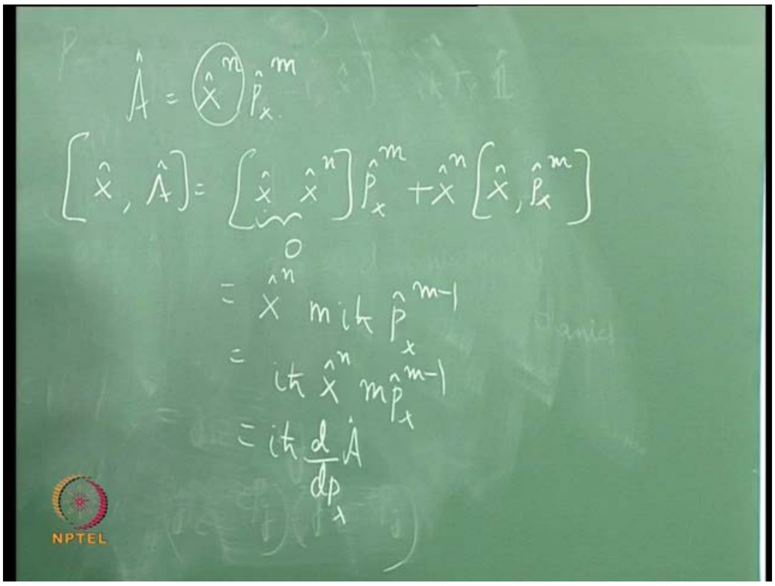

Now suppose, I consider an operator which is a function of X and P. Consider an operator A which let us say is X to the power of n, P x to the power of m and suppose, I wish to find the commutator of X with A. Well, by the A B C rule I could call this B that C and this A. This is the same as the commutator of X with X to the power of n P x to the power of n plus X to the power of n, commutator of X with P x to the power of m.

This is 0 because X commutes with itself. (Refer Slide Time: 32:56) So, the 1st term drops out and I just have X to the power of n and I already have this result I put that in there and I just have m i h cross P x to the power of m minus 1, which can well be written as, i h cross X to the power of n, m P x to the power of m minus 1. Which is the same as i h cross d by d P x of A, because A hat P x to the m and that brought down the m and gave me a P x to the power of m minus 1. You will notice, that I have removed the hat from the operator P, but that is because I am now thinking in terms of the momentum space where the operator P is simply the variable p times identity and therefore, the differentiation d by d p makes sense.

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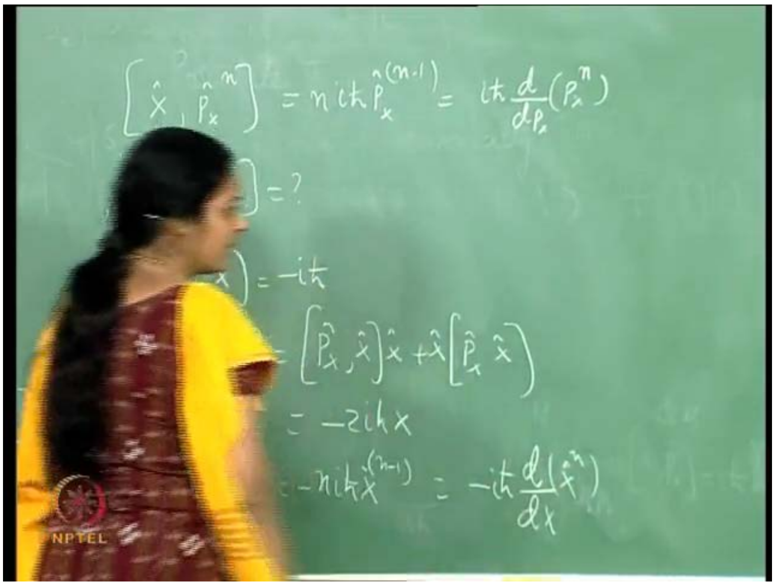

If I go back here I could well argue that this is the same as i h cross d by d P x of P x to the n. And if I look at this commutator this is the same as minus i h cross d by d x of X to the power of n. Once again, analogous to what I did in the case of the momentum operator. Here, I have removed the hat from X that is because in a function space, which is the coordinate space I could talk about the operator X as simply the real variable X times identity. And in this case, the differentiation as I have put it here makes sense. I will discuss these spaces in a later lecture.

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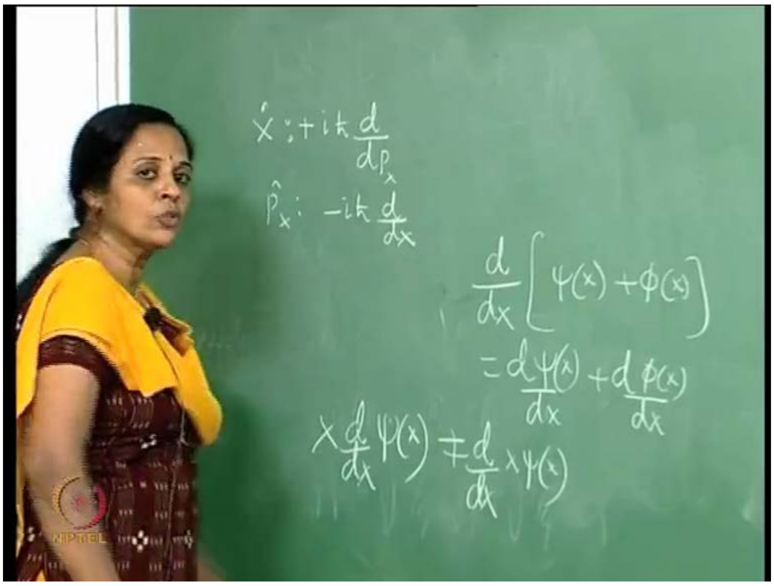

From all this, it strikes me that I might be able to make this very important identification that if I have to write X in terms of p, the identification would be that X can be written as plus i h cross d by d P x and P x can be written as minus i h cross d by d x. In other words, I can give a differential operator representation for the position operator and the momentum operator. I have already told you that this in matrices would be infinite dimensional matrices and here are differential operator representations. Clearly, they will have to act on functions.

It automatically tells us that in an example like this we are dealing first of all with an infinite dimensional linear vector space. Not only that we are dealing with the space where there are differential operators and therefore, when they act on states the states should be in a function space. This brings us, to a point where we need to understand linear vector spaces, which are actually function spaces, functions of some real variable x and those are the states. And the operators could be differential operators which act on those functions. The differential operator clearly acts linearly, because if I have d by d x acting on some function psi of X plus some other function phi of x. It simply does the following: it gives me d psi of X by d x plus d phi of X by d x and so on.

It is equally clear, that the action of X d by d x on a function psi of x is not at all the same as the action of d by d x X on psi of X, because this is simply X d psi by d x whereas, that gives me a psi of X plus X d psi by d x. So, these do not commute with each other in terms of operations X d by d x does not work the same way as d by d x of X,

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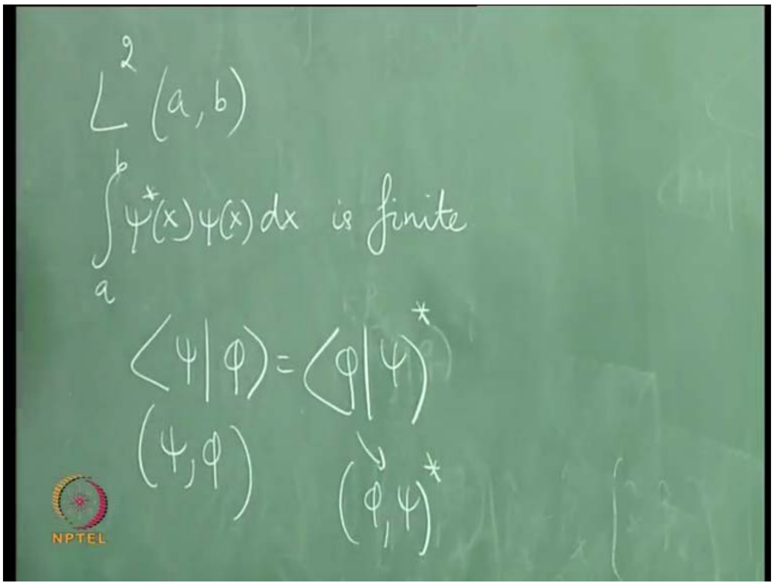

But before we go on to understanding function spaces in particular, we would be interested in the space of all square integrable functions which I did mention in one of my earlier lectures. The space is L 2 which is the space of all square integrable functions and there is a range a to b could be minus infinity to infinity. And these functions satisfy is finite and X is a real variable.

A space like this is an infinite dimensional space. It is an infinite dimensional linear vector space on which an inner product structure is defined. Just you recall the inner product in general of psi with phi is the same as phi psi star. Sometimes, you use the notation psi, phi I have used the Dirac notation. So, this is the same as phi, psi star. The inner product is in general a complex number. Further, the following properties hold for an inner product.

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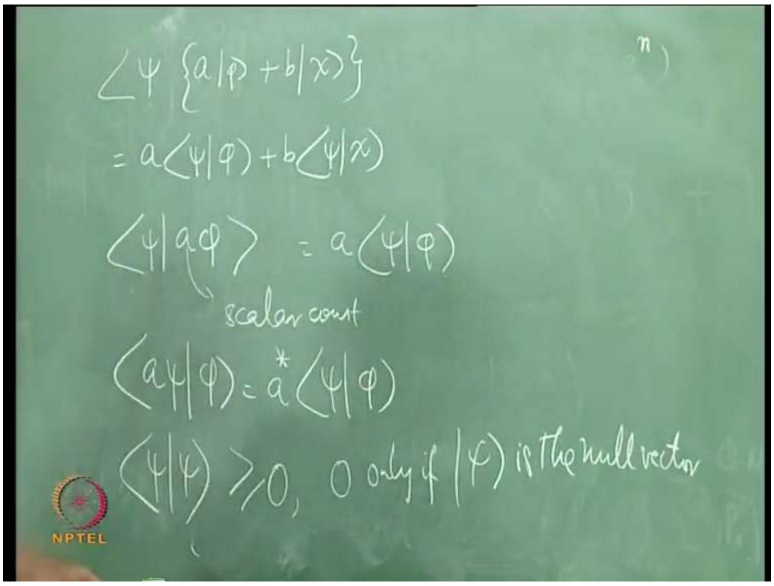

The inner product of psi with a phi plus b chi where phi and chi and psi are states, this a is psi phi plus b psi chi. In fact, we have used this all the time when we discussed 2 level atoms and 3 level atoms. Of course, the inner product of psi with a state a phi where a is a scalar constant is simply a psi phi. Of course, it follows that a psi with phi is a star psi phi and the inner product of psi with itself is greater than or equal to 0, 0 only if psi is the null vector. So, these are the properties that we did come across in our discussion earlier, but I have merely listed them out here for convenience.

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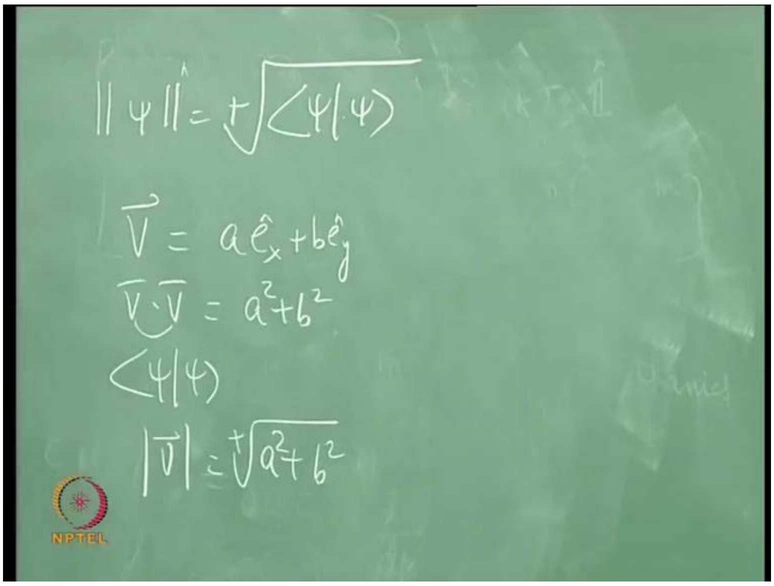

We will be dealing with infinite dimensional spaces where inner product structure is defined and we would also need the concept of a norm or the length of a vector. So, norm psi is the positive square root of psi with itself. This is simply an extrapolation of what we already know. Suppose, I have a vector a e x plus b e y in 2 dimensions where e x and e y are unit vectors. Then v dot v is simply a squared plus b squared and this is the analogue of psi psi and therefore, the length of V is the positive square root of a squared plus b squared and that is the analogue of the norm. So, we have this inner product structure and we are dealing with an infinite dimensional function space in the context of the commutator of X with P x.

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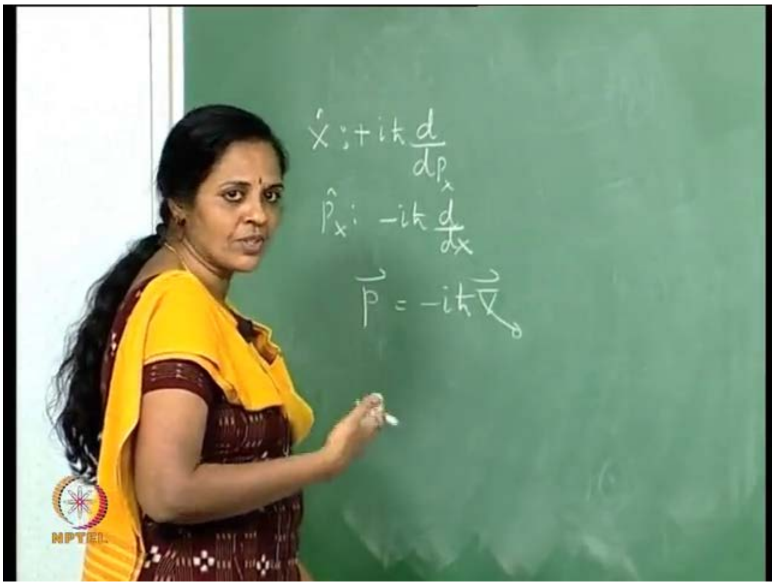

But, before we proceed given this particular identification that in terms of P x, X can be written as a differential operator plus i h cross d by d P x and P x is minus i h cross d by d x. It is clear that a straight forward extension tells me that the momentum operator P would be simply minus i h cross del where del is d by d x unit vector e x plus d by d y unit vector e y plus d by d z unit vector e z and this is in 3 dimensions.

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Given, this identification without worrying too much about the Hilbert space structure or the linear vector space structure right now I want to illustrate a very important property. Consider, 3 dimensional space where I have the Cartesian axis (x, y, z) and suppose I rotated about the z axis by an angle theta taking x to x prime and y to y prime. We know that, x prime is xcos theta plus y sin theta and y prime is minus x sin theta plus y cos theta and z prime is the same as z.

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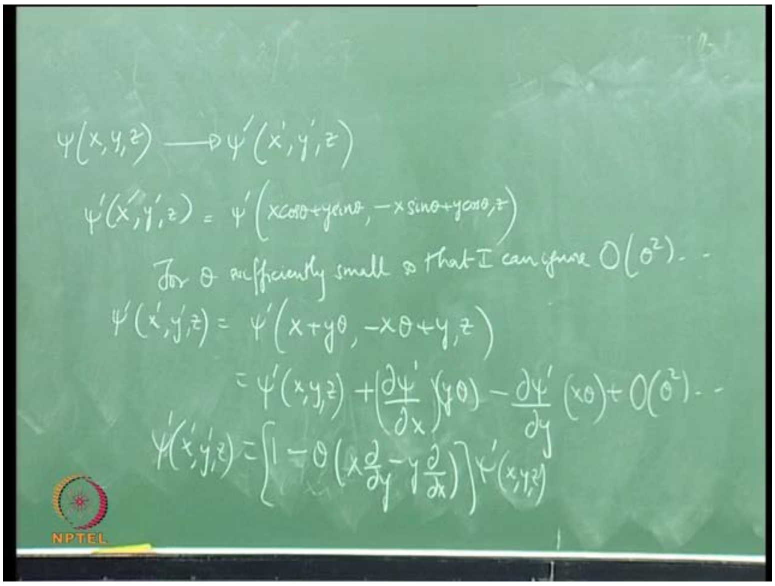

What happens to a function of x, y and z? So, I consider psi of x, y, z obviously, it goes to a function psi prime which is a function of x prime y prime and z prime, but z prime is the same as z. Now, psi prime of x prime, y prime, z prime is the same as psi prime of x cos theta plus y sin theta, minus x sin theta plus y cos theta, z. For theta small I can just retain the 1st order in theta in a Taylor expansion. For theta sufficiently small so that I can ignore order theta squared and so on.

This is the same as psi prime of x plus y theta minus x theta plus y and z. I could make a Taylor series expansion and that is just going to be psi prime of x, y, z plus delta psi prime by delta x times y theta minus delta psi prime by delta y times x theta plus order theta squared terms and higher order terms, which I ignore. Then I can write this as let us say 1 minus theta times x delta by delta y minus y delta by delta x psi prime of x, y, z. If I retain the next term, the term that is proportional to theta squared I will find that I am going to get the next term in the exponential series here.

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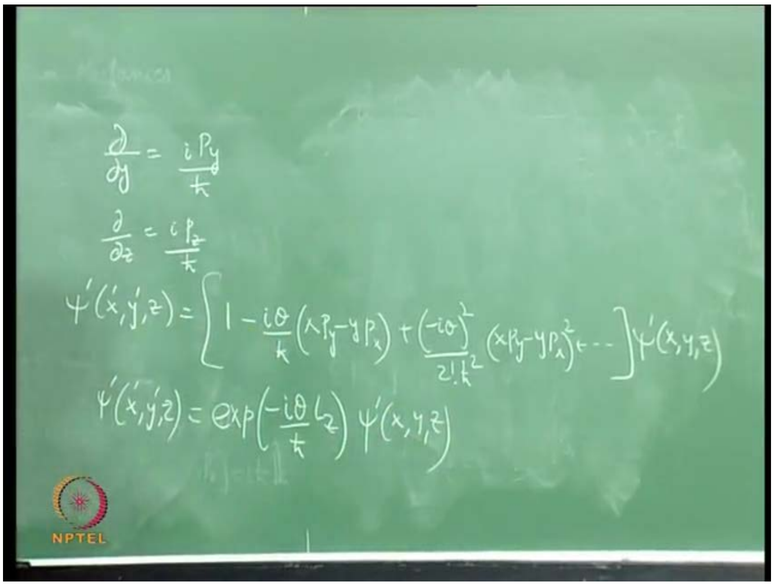

You consider, this term delta by delta y in terms of what is written here (Refer Slide Time: 44:24) is simply i P y by h cross. Similarly, delta by delta z is i P z by h cross and therefore, I have psi prime of x prime, y prime, z is 1 minus i theta by h cross x P y minus y P x plus if I worked out the next order I would get this. A word of caution as I stated earlier one should remember that, x P y minus y P x the whole squared when expanded I should retain the order of operators properly.

But this just acts on psi prime of x, y, z telling me that psi prime of x prime, y prime, z is exponential of minus i theta by h cross L z psi prime of x, y, z. This is a very important result. First of all this should strike a bell; it should remind you of the manner in which the spin matrices behaved. This theta is like the group parameter, L z is the generator of the transformation about the z axis. In this case, orbital angular momentum is a generator of space rotations.

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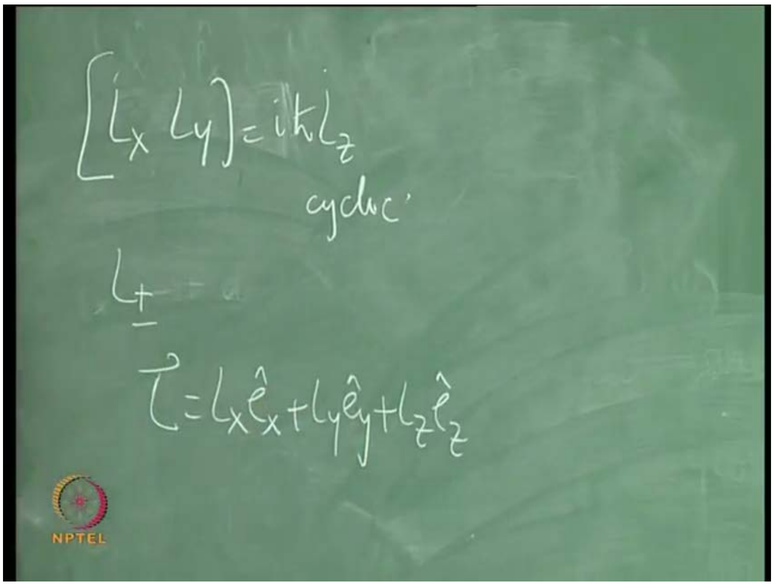

Simply, in analogy with what I had said earlier about the spin matrices L x, L y and L z are the generators of and an s u 2 transformation, but this time in physical space and the commutator L x L y is i h cross L z cyclic. These are operators you could put the hat there. I could introduce L plus and L minus as before and I have a vector L which, is L x e x plus L y e y plus L z e z which behaves under this transformation in the same manner in which the coordinates x, y and z behave. So, here is another example of the s u 2 groups. So, spin is simply like orbital angular momentum except that it is in an internal space and this is in physical space.

And, I have just demonstrated to you that, once this identification of p, the vector p or the operator p as the minus i h cross operator del. Once that identification is complete it is pretty clear from what I have done that angular momentum is the generator of space rotations and this is the angular momentum algebra. So, we have really handled two examples of the s u 2 algebra: one is the orbital angular momentum algebra and the other is spin. But, orbital angular momentum would be in an infinite dimensional linear vector space. I will stop here and in my next lecture I will talk about simultaneous measurements and what happens to expectation values under simultaneous measurements of objects which do not commute with each other operators which do not commute with each other.