Quantum Mechanics-I
Prof. Dr. S. Lakshmi Bala
Department of Physics
Indian Institute of Technology, Madras

Lecture - 21
Square-Integrable Functions

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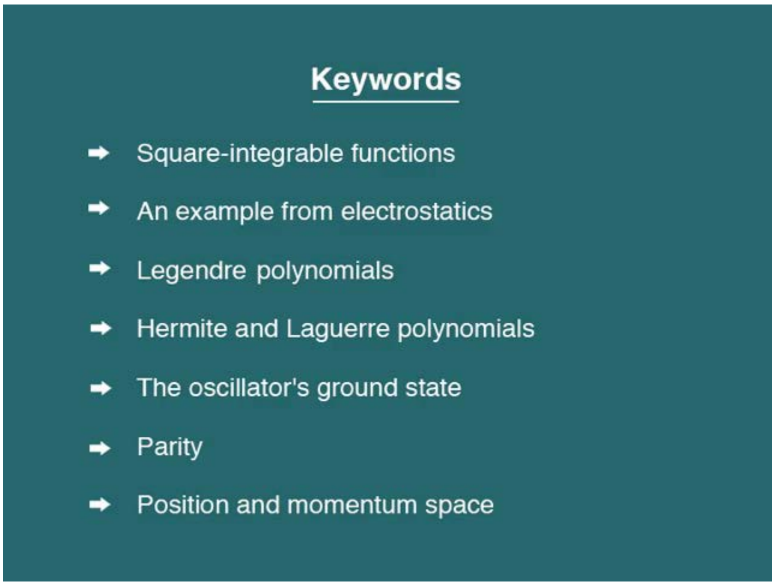

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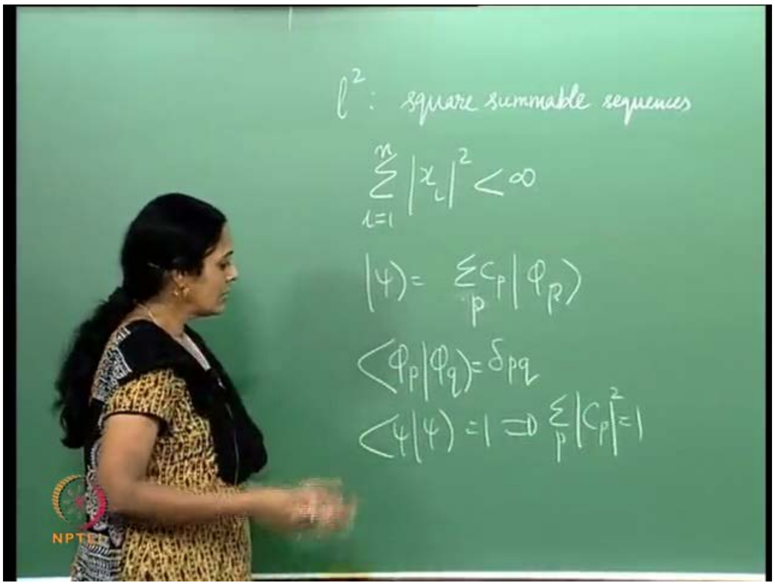

We have already discussed, l 2 the space of square summable sequences. So, I have a sequence x sub i, which satisfies i is equal to 1 to n, mod x i squared is finite. So, this is the square summable sequence and becomes relevant in the context of quantum mechanics, in fact we have been looking only at l 2 most of the time, without saying so. Because, when I expand a state psi, in terms of a basis set phi n. This n is not to be confused with that n. With coefficient C p and given that this is an orthonormal basis and that psi is normalized to 1.

It implies, that summation over p, mod C p square is 1 and therefore, certainly less than infinity. So, the probability amplitudes C p, when expanded in this manner happen to satisfy the requirements of a square summable sequence and therefore, little l 2 becomes very important in the context of understanding the framework of quantum mechanics.

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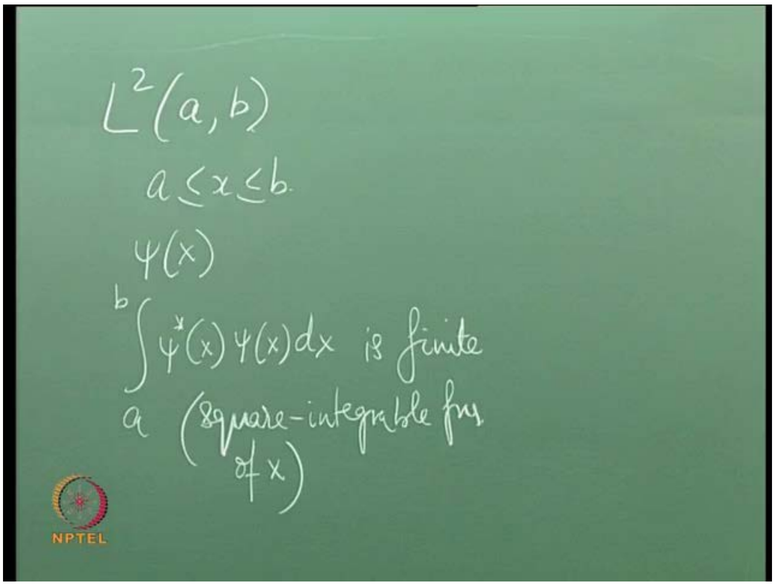

I also mentioned, another space. Which was the space of square integrable functions, defined in the region a b. These would be functions of a real variable x and if they are square integrable functions psi of x. They would satisfy psi star of x, psi of x, d x is finite. And a and b could well b minus infinity and infinity respectively. So, this is kind of direct extrapolation of a square summable sequence. These are squared integrable functions of x. So, today I will talk about certain aspects of square integrable functions of x, in other words we will be discussing, the space L 2, of a,b.

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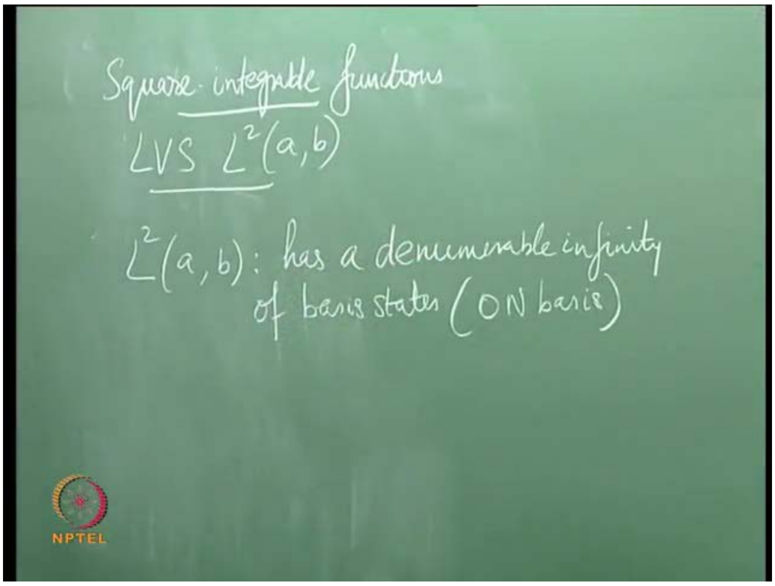

So, square integrable functions. The linear vector space, is L 2 of a, b. So, this is what we will talk about today. L 2 of a, b is an example of a separable Hilbert space. So, that means that the space L 2 of a, b has a denumerable infinity, or a countable infinity, of basis states and this could be an orthonormal basis. You can always make it an orthonormal basis. Since, it is the space of functions, clearly the basis states are functions of x and any state any arbitrary state, in this linear vector space can be expanded in terms of these basis functions. So, since a and b can take various values, I would like to give certain examples of L 2 of a, b right away.

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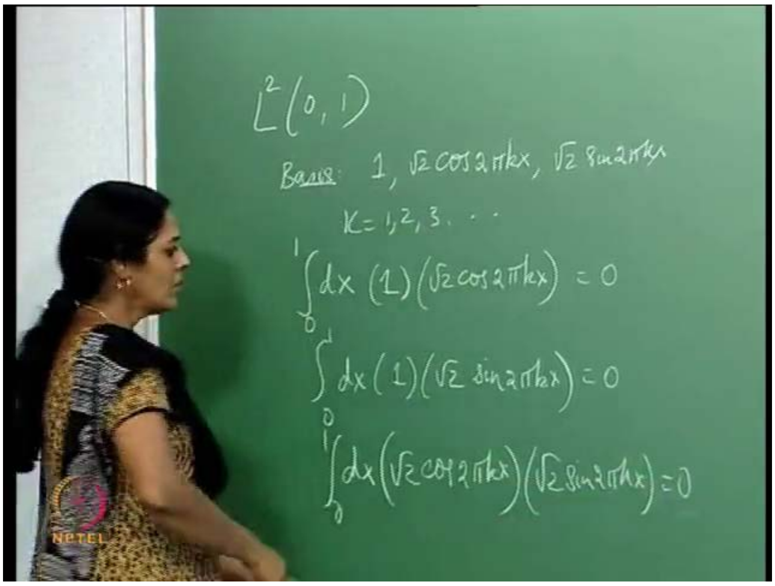

So, let us look at L 2 0, 1. Now in this space we can easily check, that the basis states, the basis vectors, are 1 root 2 cos 2 pi k x and root 2 sin 2 pi k x. The k itself takes values 1 2 3 and so one. So, I have a denumerable infinity of basis states, that is an infinity and that is another infinity because k takes various values. This is an orthonormal basis, I have taken care to normalize these basis states to 1, by putting that root 2 there and how do I see that they are orthogonal to each other? Suppose, we did integral 0 to 1 d x. Let us consider those 2 basis states root 2 cos 2 pi k x. It is trivial to check that, that is 0. Similarly, if I took these 2 basis states 1 and root 2 sin 2 pi k x. That is 0, root 2 cos 2 pi k x, for any k an integer k, positive integer k, that is also 0. So, they are orthogonal to each other.

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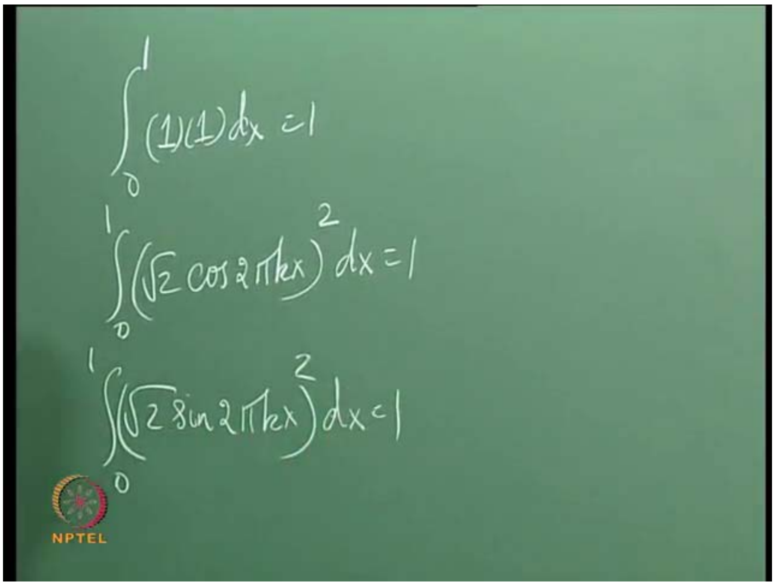

They can be normalized to 1, indeed they are normalized to 1. Because, clearly 0 to 1, of 1 times 1 d x is 1, 0 to 1, root 2 cos 2 pi k x, for a given k and so on. The root 2 is important because, it is needed to normalize this to 1. So, this is a denumerable infinity of basis states, in the linear vector space, L 2 of 0, 1. So, that is my 1st example and all functions in this space, (Refer Slide Time: 04:30) can be expanded in terms of these basis states.

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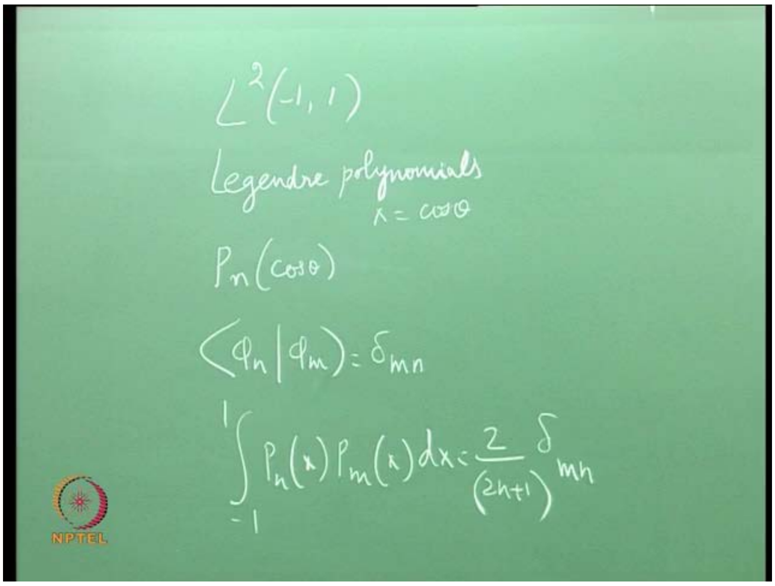

Let us look at the next example. Let us consider the space, L 2 of minus 1, 1. I did mentioned this, in an earlier lecture. The basis states could well be the Legendre polynomials, because minus 1 to 1 rings a bell. You could choose x to be cos theta, because, cos theta goes from minus 1 to 1. The Legendre polynomials could be chosen as the basis states. So, these are P n of cos theta.

So, my x is cos theta and they are certainly orthogonal to each other, in terms of the Dirac ket notation. The orthogonality property would be this, normalized to 1 and orthogonal. Let us just look at the fact, that if n is not equal to m, that is 0, there is no overlap. So, this would simply be P n of x, P m of x, d x integral over the range minus 1 to 1, is 2 by 2 n plus 1, delta m n. And I mentioned earlier, that we could write the completeness relation in this context analogously.

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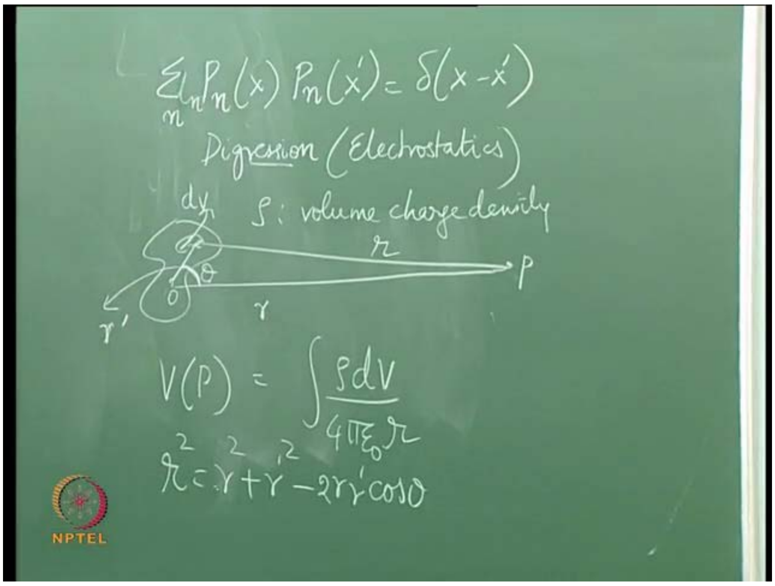

Summation over n, L sub n, P n of x, P n of x prime, is delta of x minus x prime and L sub n is 2 n plus 1 over 2. So, it forms a complete orthonormal basis. You can expand functions in this space, as linear combination of the Legendre polynomials. This is, already well known to students who have studied electrostatics. Take the example, of trying to find out the potential, far away from an static charge distribution. An arbitrary charge distribution, (Refer Slide Time: 07:02) this is a digression we recall what we learned from electrostatics. So, you have an arbitrary charge distribution, this is the origin and it is a uniform volume charge density row.

And let me take a small element here d v which is at a distance, r prime from the origin of coordinates. Now, I want to find out the potential at some point p, which is pretty far away from this arbitrary charge distribution. Let us say at a distance r from it. This distance itself is r; this is r prime, the distance from the origin to d v, which is an elementary charge distribution, an elementary volume of charges. The distance from d v to p, which is where I want to find the potential is r and p is assumed to be very far away from this distribution.

So, that to first approximation, the arbitrary charge distribution looks like a spherical object and of course, from the origin of coordinates to p the distance is r. So, it is clear that the potential at the point p, is the simply the total charge. Of course, there is a four pi epsilon 0 r. Now I do a multi pole expansion, in the sense I expand, this 1 by r, in terms of r and r prime. Now if I did that, it is clear that r squared, is r squared plus r prime squared minus 2 r, r prime cos theta, where theta is this angle that is theta this angle. Clearly I can simplify this better, when I do the following.

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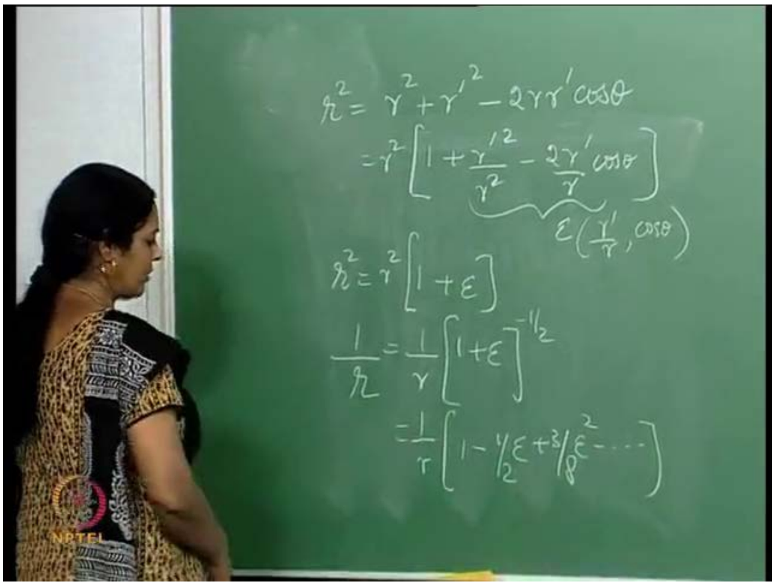

So, I have r squared, is r squared, plus r prime squared, minus 2 r, r prime cos theta. Pullout an r squared and write this as 1 plus r prime squared by r squared, minus 2 r prime by r cos theta. It is very clear that r prime is a very small distance, compared to r, (Refer Slide Time: 08:35) because p is pretty far away from the charge distribution and therefore, the expansion is done in powers of r prime by r. I could call this epsilon. Now this epsilon is a function of r prime by r and cos theta. So, I have r squared, is r squared 1 plus epsilon and therefore, I need 1 by r. (Refer Slide Time: 08:35) That is what figures in the potential V of P. So, 1 by r is 1 by r, 1 plus epsilon to the minus half and then this expansion, is in powers of epsilon, alternating positive and negative and this is what I have.

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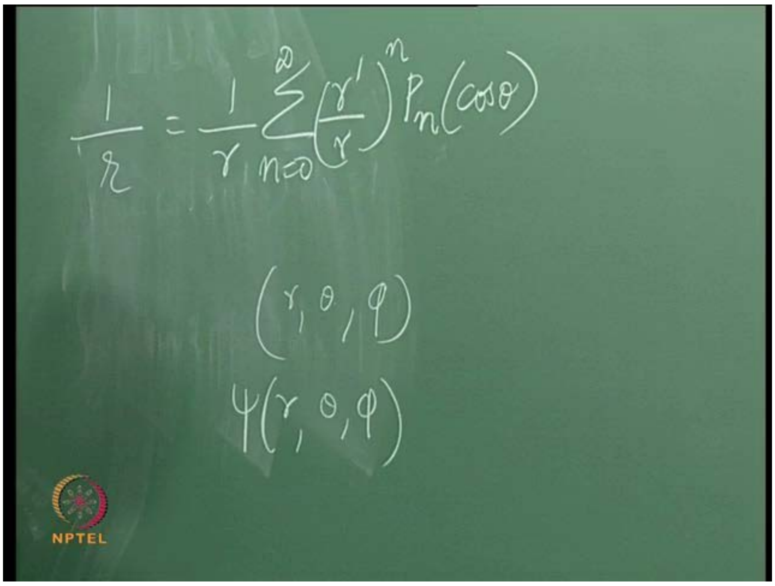

Now, I could well go back and write out epsilon and substitute for 1 by r and I find that 1 by r once I simplify this by purring in the value of the epsilon, putting in epsilon in terms of r prime by r and cos theta I find that 1 by r, (Refer Slide Time: 11:52) is this 1 by r and this series, is summation n equals 0 to infinity, r prime by r to the n, power of n, P n cos theta. So, already you see there is an example from electrostatics. Where the potential due to an arbitrary charged distribution pretty far away from the location of the charge distribution is expanded in this basis and the first term in the basis turns out to be the monopole contribution. The 2nd term is the dipole contribution, the 3rd term is the quadrupole contribution and so on.

So, it is in this very same spirit, that in quantum mechanics. If you have a linear vector space L 2 of minus 1 1. (Refer Slide Time: 07:02) You could use P n of cos heat as the basis and functions of cos theta any arbitrary function of cos theta, can be expanded in terms of the P n cos theta. In fact it turns out the P n cos theta figures in quantum mechanics, in the study of orbital angular momentum. That is a situation, where one wants to study orbital angular momentum, obviously in physical space because, it is r cross p and that would mean using coordinates x y z or if you wish in spherical polar coordinates.

The radial coordinate r, theta and phi and then if you write, the state of the system the Eigen state of orbital angular momentum, as a function of r theta and phi. The dependence on theta can be expanded, in terms of P n cos thetas. So, that is one place, in quantum mechanics where P n cos theta comes in and we will certainly look at the problem of orbital angular momentum in subsequent lecture.

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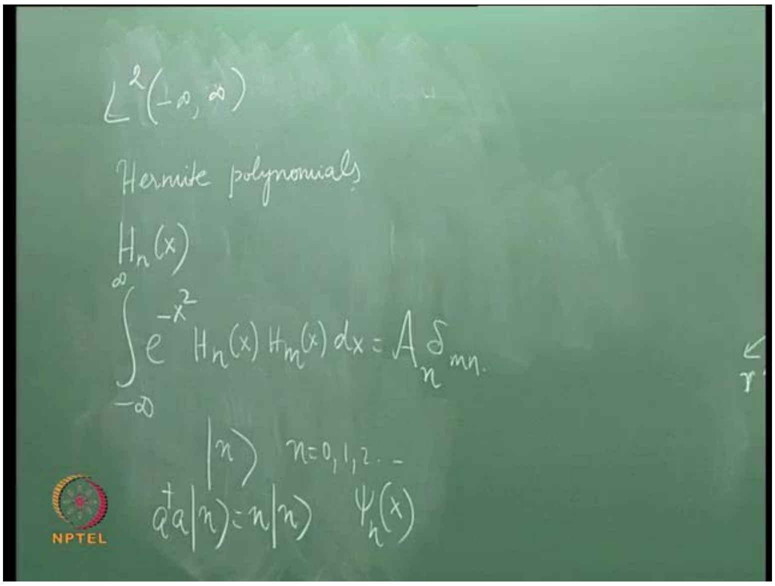

The 3rd example, that I wish to consider, for the space of square integrable functions is L 2, minus infinity infinity. I did mention this earlier. In this case one could use the Hermite polynomials. The Hermite polynomials as the basis functions, H n of x and their orthonormality property, involves a Gaussian measure, e to the minus x squared. H n of x H m of x, d x is sum A n delta m n. They form a complete basis, in L 2 minus infinity infinity. The H n's figure in quantum mechanics, in the context of the simple Harmonic oscillator, a problem which has already been studied by us, in the abstract ket notation, where we had the energy Eigen states of the oscillator, represented by n and so on.

You will recall, that these were Eigen states of the operator a dagger a. With Eigen value n and when n is 0, it represents the ground state of the oscillator, n is 1 it is a 1st excited state and so on. Equivalently, in quantum optics n is 0 would refer to the 0 photon state, n is 1 to the 1 photon state and so on. Now, if I represent this abstract ket, in function space. The relevant function space turns out to be L 2 of minus infinity infinity. And the various basis states in function space, which I would represent by psi n of x, where x is position, turns out to be essentially the Hermite polynomials. So, that is another example.

Again we will study this example. We will redo the oscillator problem, in the Schrodinger formalism. Where basically the function space becomes important and we will study the properties, of the energy Eigen states of the oscillator, in terms of the behavior of the Hermite polynomials.

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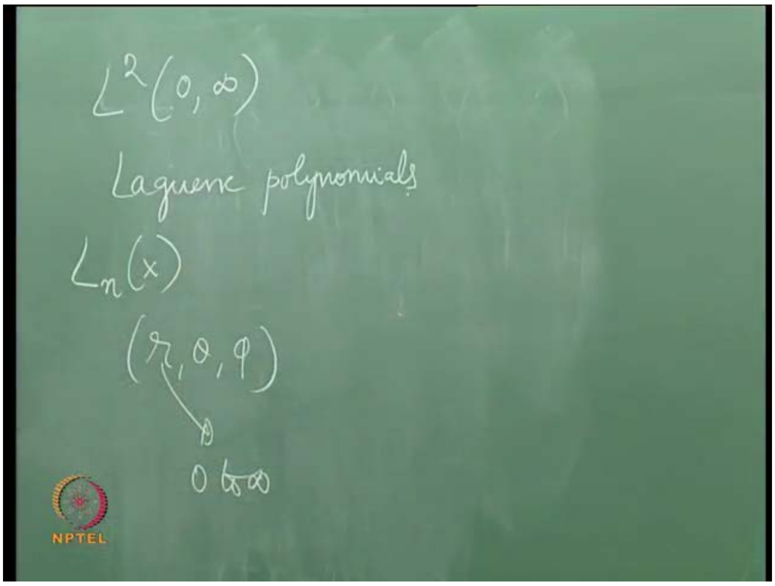

The last example that I want to point out today, is the space L 2 0, infinity of there. It is clear that the argument, in a physical context should be the modulus of a vector. And in this case we use the Laguerre polynomials as the basis states that is an example. You could use the Laguerre polynomials. L n of x and this appears in the context of the hydrogen atom problem for instance, where once more if the hydrogen atom is considered, in a 3 dimensional space.

In spherical polar coordinates, this r obviously takes value 0 to infinity and the radial wave function, or the state of the system expressed in terms of the radial coordinates, can be expanded in terms of the Laguerre polynomials, which forms an orthonormal basis, in the space L 2 0, infinity. So, these are various examples. Where function spaces are very important in particular these square integrable functions, are very important in studying various quantum mechanics problems. I want to draw attention to a very important fact in this context.

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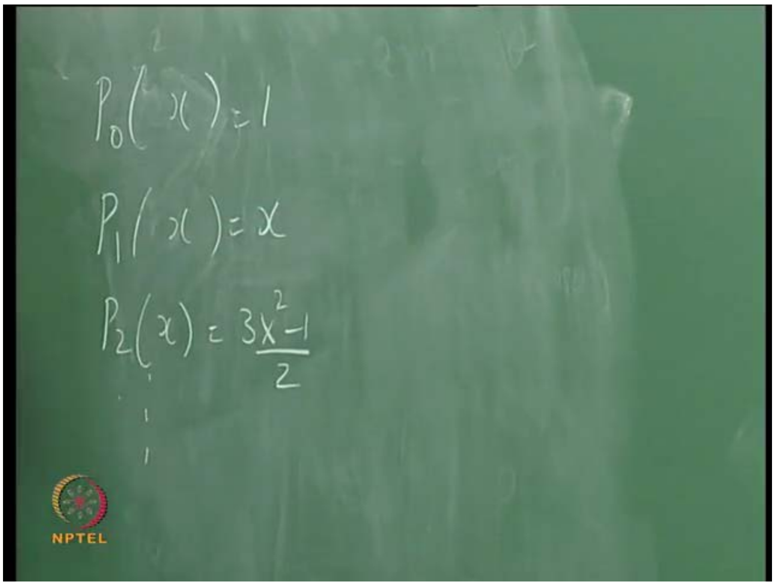

Suppose, you look at the various, Legendre polynomials for instance, so, P 0 of cos theta, is 1, P 1 of cos theta, is cos theta itself, so let me call it x. So, P 0 of x is 1. P 1 of x is x. P 2 of x is 3 x, squared minus 1 by 2 and so on. You would find, that these are odd functions of x, P 1, P 3, P 5 and so on. And P naught P 2, P 4 are even functions of x. Similarly, if you look at these are the Legendre polynomials.

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Look at the Hermite polynomials. Hermite polynomials also, H 0 of x is 1. H 1 of x is 2 x, H 2 of x is 4 x square minus 2. Once more H 0, H 2 are even functions of x and H 1, H

3 etcetera are odd functions of x. Now if you look at the Laguerre polynomials, same thing. This is Hermite, L 0 is 1, L 1 of x is an odd function of x. So, there is an x and that just becomes, L 1of x, where x goes to minus x, it becomes 1 plus x. Let us forget this as far as x is concerned it is an odd function and L 2 of x, is x squared minus 4 x, plus 2, apart from a constant.

So, that is a quadratic n x and so on. So, it alternates even function the highest power of x is odd in the case of L 1, L 3 and so on. And the lowest power and the highest power of x in the case of L naught L 2 and so on is an even function of x the highest power is even. Now this becomes very important because, if you look at the Hermite polynomials for instance here. So, if you look at one dimensional oscillator the simple harmonic oscillator, where I have mentioned that the Hermite polynomials become important. You find that, the wave function has a definite parity.

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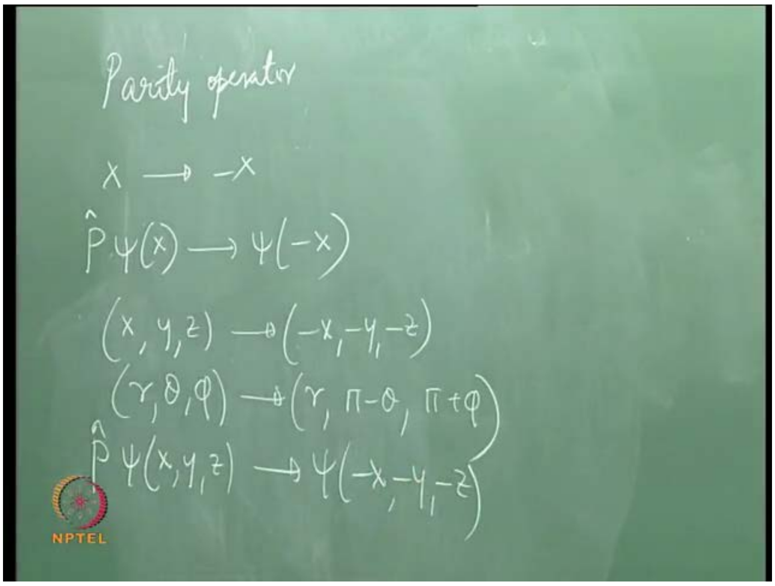

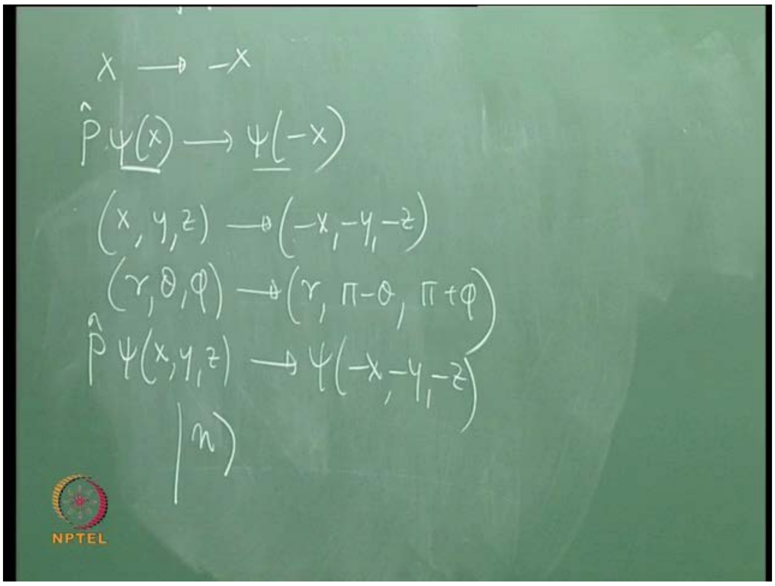

In other words, I define a parity operator, which basically takes x to minus x. That is a job of the parity operator. So, when the operator, if you wish I put a cap on it, acts on a function, in the space L 2 minus infinity infinity, which is the relevant linear vector space, for the simple harmonic oscillator. This takes it to psi of minus x. Of course, if the parity operator were to act in 3 dimensions, then it acts it takes x y z to minus x minus y minus z, equivalently takes r theta phi to r, theta goes to pi minus theta and phi goes to pi plus phi.

So, any function psi of x y z, under the action of the parity operator, becomes psi of minus x minus y minus z and so on. So, you find that the H n's which are essentially the energy Eigen states, or the Eigen basis, of the simple harmonic oscillator are definite parity states. So, from what I have said earlier one now suspects, that these states are simultaneous Eigen states of the parity operator and the Hamiltonian. And indeed that is what happens and I will comment on this later. So that the states ket n of the oscillator, which I spoke about earlier, when represented, as functions of x.

Because there is only one argument here because, it is a one dimensional oscillator, turn out to have definite parity and they are also simultaneous Eigen states of energy and the parity operator. So, the parity operator and the Hamiltonian commute in the case of the simple harmonic oscillator, a matter which will be studied in much detail in a subsequent lecture. So, now as I have already indicated, most times by x we mean position. Not always true but quite often.

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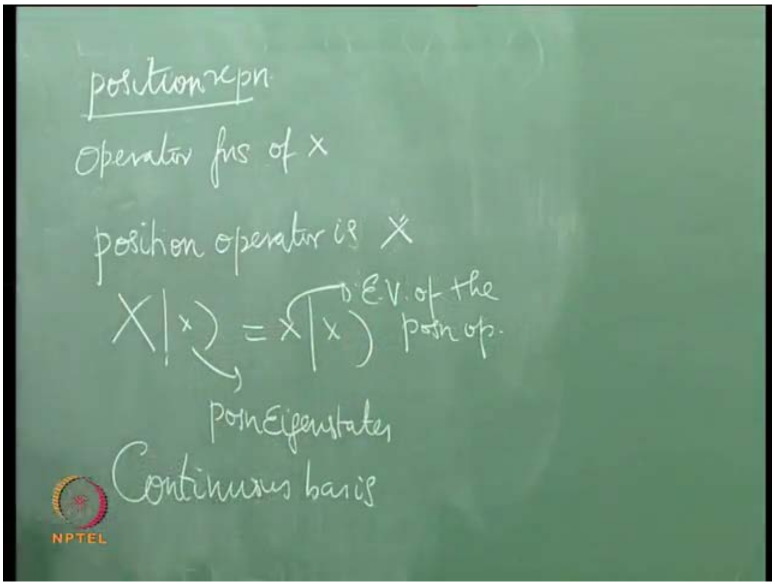

So the argument x, turns out to be relevant to position. And in the position representation, you have to define operator functions of x, which will act, on the state psi of x. Which itself is an arbitrary state, expanded in terms of the basis states that we have selected, could be the Laguerre polynomials, could be the Legendre polynomials, could be the Hermit polynomials depends on the space. The simplest operator function of x, that I can think of is x itself. There is no need to put the cap. So, in the position representation, the position operator, this is a very crucial point is x. I should use the same x. It has position Eigen states. The job of the operator is simply to pullout the position Eigen value.

But, unlike the earlier examples we spoke about. Now we have moved to a more complicated situation, where x is a continuous real variable, which takes values in the range a to b and therefore, the position basis, or the Eigen basis of the position operator happens to be a continuous basis. Since, it is a continuous basis we cannot imagine that it can be represented as a column vector with discrete entries, nor can be imagined that the operator, the position operator can be represented by a matrix, which has got distinct rows and columns. In fact the rows become continuous the columns become continuous and that is why we call it an operator. Cannot do better than that, this is the position operator and in the position representation, the operator itself can be represented by x.

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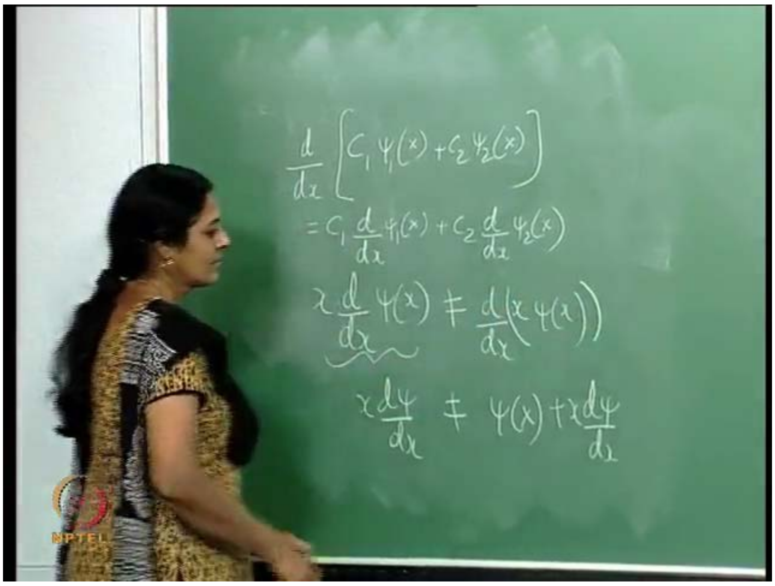

There are other linear operators, in this position space. An example would be d by d x. Clearly this is a linear operator, because if it acts on say C 1 psi 1 of x, plus C 2 psi 2 of x. Where psi 1 of x and psi 2 of x are functions in the space and C 1 and C 2 are constants. That is just d by d x psi 1 of x, plus C 2 d by d x psi 2 of x. So it is a linear operator and this operator becomes important, to begin with operators need not commute with each other. Because, if we look at x d by d x, acting on psi of x. Since they are linear operators first d by d x acts on psi of x and then x acts on psi of x.

Now an important point to remember is that operators do not commute and so, if I found the action of x d by d x, on the functions psi of x. That is not the same as d by d x, x psi of x, because this is simply x d psi by d x whereas, this is psi of x, plus x d psi by d x. That bracket that makes a crucial difference and therefore, operators in general do not commute. But, this relation, that I have seen here, this example, tells me something.

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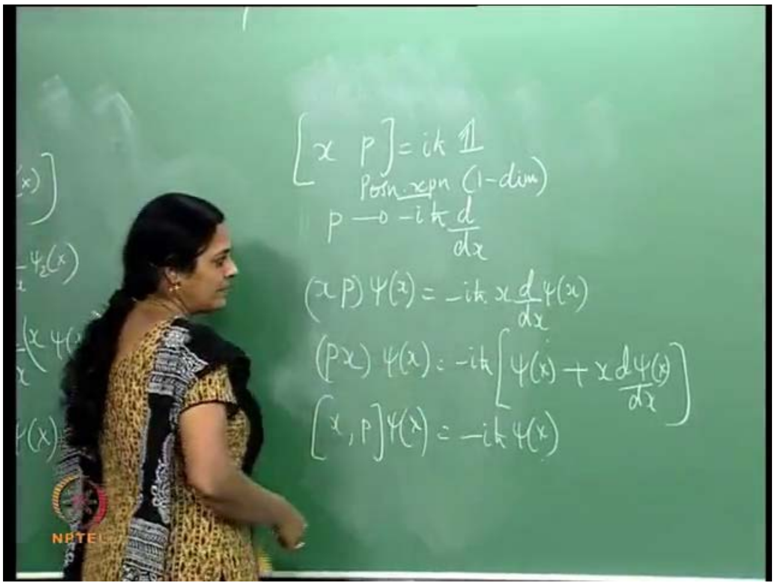

We know that the position and momentum operators, do not commute and in one dimension x p is i h cross identity. And therefore, p can well be represented in the position representation, as minus i h cross, d by d x and I am doing one dimensions. There is only one variable x. So if we check now, x p acting on psi of x, is minus i h cross x d by d x, psi of x, p x acting on psi of x, is minus i by i h cross, psi of x, plus x d psi of x by d x. And therefore, the commutator of x with p, acting on an arbitrary state psi of x, gives me i h cross, psi of x or x p is equal to i h cross. So, in the position representation, the momentum operator has to be represented as an operator function of x and it is written as minus i h cross d by d x.

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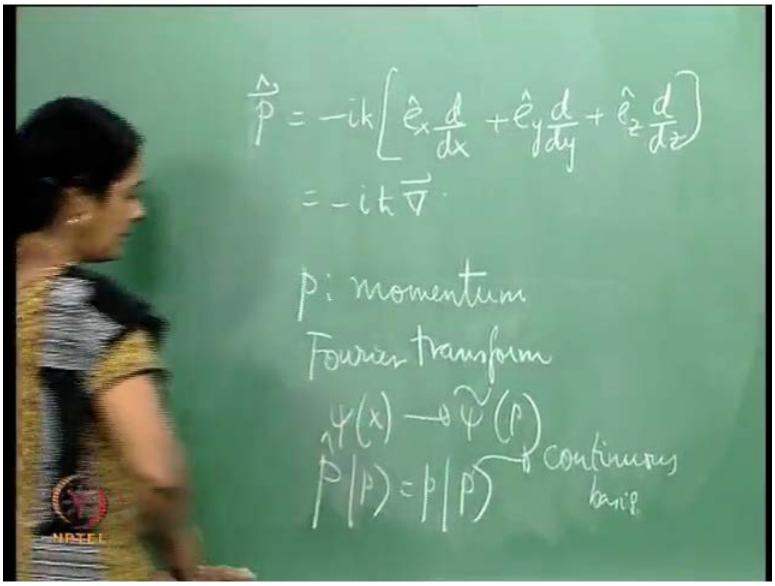

In 3 dimensions one deals with x y and z and therefore, the momentum operator, if you wish I will put a hat there, is minus i h cross e sub x d by d x, plus e sub y d by d y, plus e sub z d by d z, or minus i h cross dell. This is in three dimensions and this is the manner in which we represent the momentum operator, in the position basis in the position representation. Now similarly, I could think of working with states in the momentum space. What I mean is, I could think of the argument as momentum, I certainly know how to go from functions of position to functions of momentum through the Fourier transform, by which psi of x goes to psi tilde of p, which is a state in the momentum space.

Obviously operators acting on psi tilde of p, should be functions of p and even as we represented the position operator by just x, in the position representation, the momentum operator acting on the momentum basis. Simply picks out the momentum Eigen value and this is a continuous basis again. You will recall, that p changes continuously, it is a continuous variable it is a real variable and the momentum operator, in the momentum representation could be well represented by p itself.

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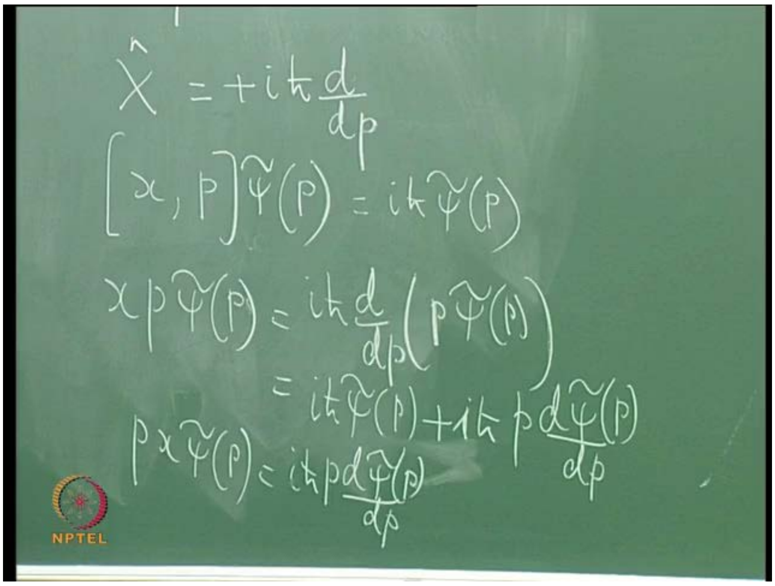

These are conjugate representations, in the sense that I can go from 1 basis, the position basis to the momentum basis, by a Fourier transform. So in the momentum representation, momentum itself is given by the label p. The momentum operator and I need to write the position operator, in terms of p, as an operator function of p. We can easily check that the position operator in a momentum basis is plus i h cross d by d p. Let us work out the commutator, x p acting on psi tilde of p, is expected to give i h cross psi tilde of p Because, it is like the identity operator acting on psi tilde of p, apart from i and h cross.

So, we can check that out. So, where we are looking at functions of momentum as the states in the linear vector space. This amounts to writing i h cross d by d p, acting on p psi tilde of p and that has 2 terms, i h cross psi tilde of p, plus p i h cross, p d psi tilde of p by d p. This is as far as x p is concerned. Now, p x psi tilde of p, is i h cross p d psi tilde of p by d p and therefore, between the two of them, the commutation relation is satisfied. This term cancels with that leaving behind i h cross psi tilde of p. So, in the momentum representation, which is another important representation that means, I would like to expand the states and write the operators, as functions of momentum and the states are expanded in terms of the momentum basis functions, psi tilde of p for instance.

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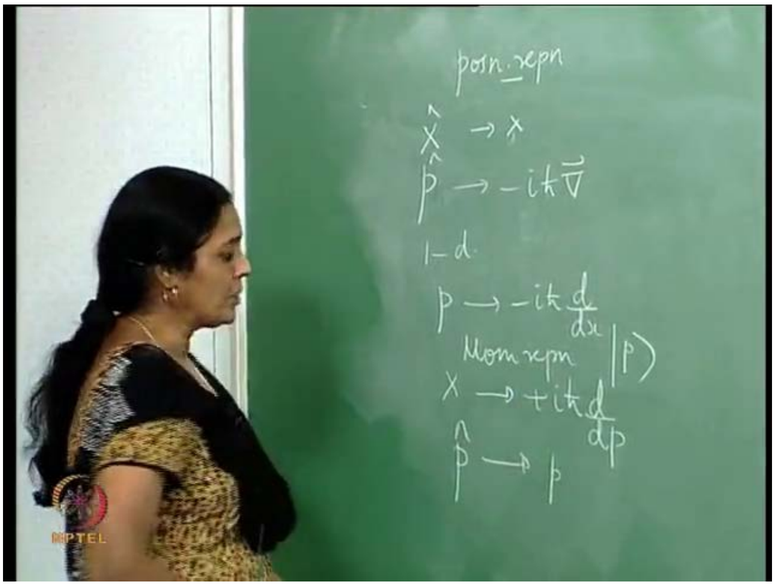

I find, that in the position representation, momentum is represented, by minus i h cross del. And this is in the position representation, where x itself is x and p is minus i h cross del. This is in the position representation. So, in 1 dimension p is simply minus i h cross d by d x and in the momentum representation, where my basis states are a continuous basis labeled by the momentum values p. These are Eigen states of the momentum operator, x is represented by plus i h cross, d by d p and p itself is simply the momentum value p. These are conjugate representations.

We may choose to work in the position representation, or in the momentum representation, if necessary. When we talk about systems in space, like a hydrogen atom and its coordinates, (Refer Slide Time: 29:52) or harmonic oscillator, at a certain point in space, or moving in space. We need to work with functions of x, where x represents the space variable and so on.

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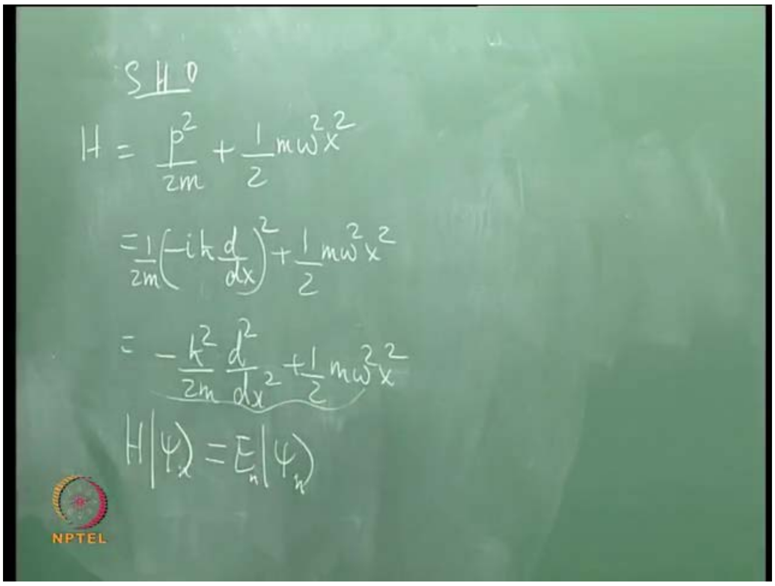

Now finally, I want to go to the harmonic oscillator problem and illustrate a certain point, The Hamiltonian of the oscillator, 1 dimensional oscillator, the simple harmonic oscillator. Is p squared by 2 m plus half m omega squared x squared. Written in the position representation this would be minus i h cross, d by d x the whole squared, 1 by 2 m multiplies that, plus half m omega squared x squared. Which is the same as minus h cross squared by 2 m, d 2 by d x squared, plus half m omega squared x squared and if we are looking out for position energy Eigen states, H psi n is E n psi n. Certainly H has to be written in this fashion and psi n has to be written as functions of position. The n takes values 0 to infinity because, it is a denumerable infinite basis set and the psi itself has to be written as a function of position.

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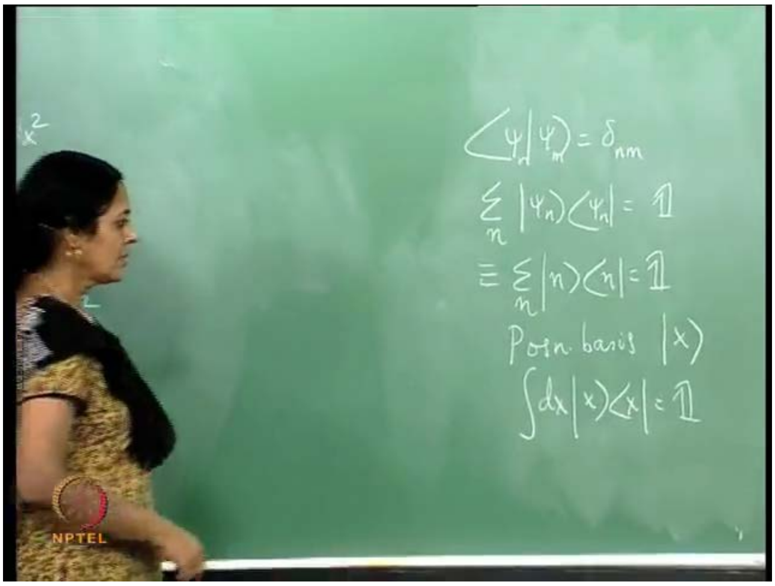

So, that brings us to a very important point. How do you represent psi of x? In terms of the Dirac notation, using the Dirac notation? Suppose you have an orthonormal basis and suppose the basis is also complete. So, I write psi n psi m is delta n m and suppose the basis is also complete. In short form I would have written this earlier, as n n is identity. Look at the position basis, the position basis is a continuous basis denoted by x, the label x takes continuous values. Then certainly this completeness relation translates to integral d x, x x is identity.

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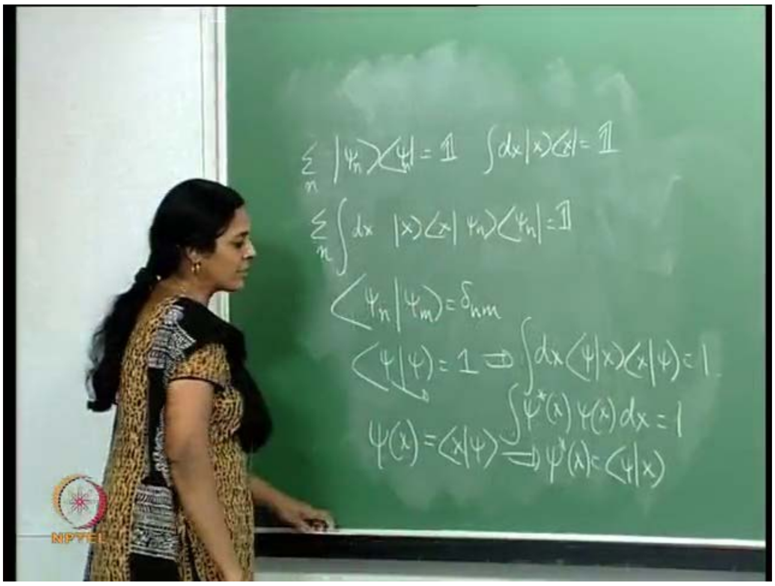

And therefore, if I were to talk about a function of x, in the abstract notation, I could have well written, psi psi, summation over n psi n, psi n, is identity. I can introduce a complete set of states, I would like to write psi in the position basis and therefore, I could do an integral d x, x x psi n, psi n equals identity. Because, this was any way identity and this would also be identity. I want to now write, psi n, psi m is delta n m, for the same value of n and m, I have psi psi equals 1, which shows that it is normalized to 1. I can do the following thing; I can write this as, integral d x, introducing a complete set of states.

I have simply introduced integral d x, this operator x x, because that object was 1. Recall that integral d x, x x is identity. But, i know the following, this is to be understood as psi star psi, psi star of x psi of x d x, integral over x is 1. It is simply 1, not the identity operator is 1. Therefore, I write psi of x as the object x psi. In other words, I have written the state psi, in the position representation, this implies that psi star of x is psi x, I use bra psi ket x for psi star of x. So, by just introducing a complete set of states, I have understood what the notation is, in terms of the Dirac notation.

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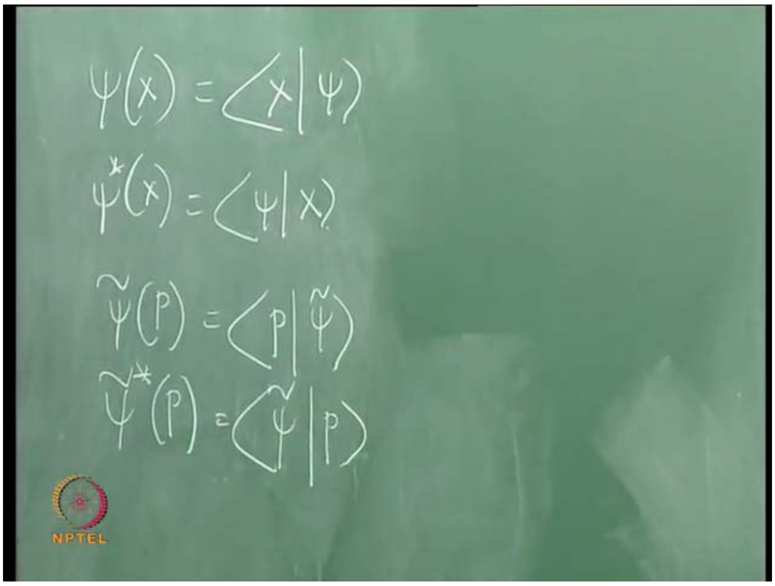

Psi of x, which is a function of x, is x psi. Psi star of x is therefore, psi x. Similarly, if I were looking at the momentum representation, psi tilde of p is p psi, psi star tilde of p which is the complex conjugate, is p psi tilde, psi tilde p. So, this is the way we represent functions or as functions of position or as functions of momentum. This is a very crucial input and now if you return to the harmonic oscillator.

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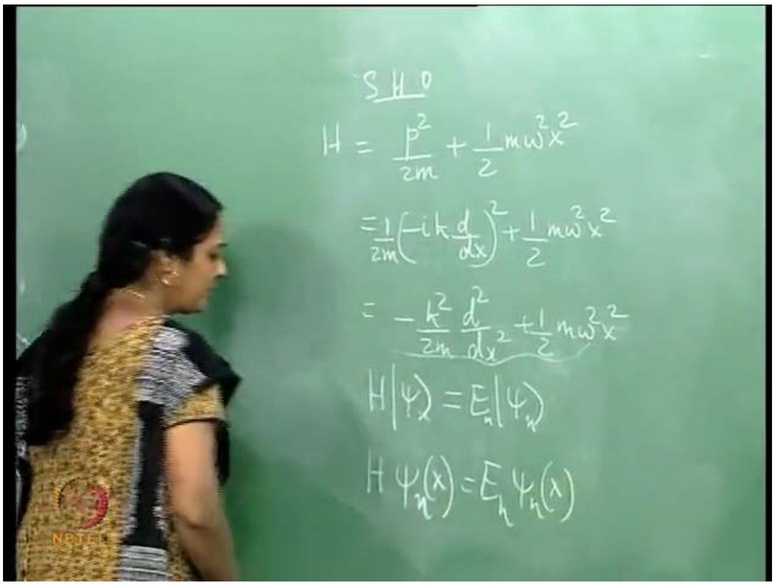

This Hamiltonian acts, I should really be writing in the position representation. H acts on psi n of x, to give me E n psi n of x, where n takes value 0 1 2 3 and so on.

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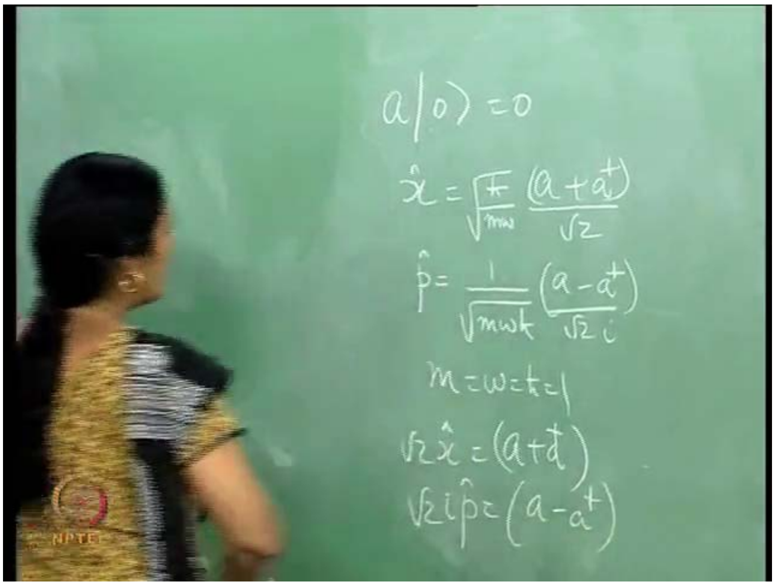

So let us look at that, look at the ground state. You will recall that the ground state, was represented by ket 0 and the annihilation operator destroyed the ground state. But, we also know, that x was a plus a dagger by root 2, which was dimensionless, with a root of h cross by m omega, which are dimensions that were appropriate and p is 1 by root of m omega h cross, these are operators a minus a dagger by root 2 i. Now, suppose for convenience just to illustrate the point, I set m equals omega equals h cross equals to 1. Then I can see, that x is a plus a dagger root 2 x is a plus a dagger, root 2 i p is a minus a dagger.

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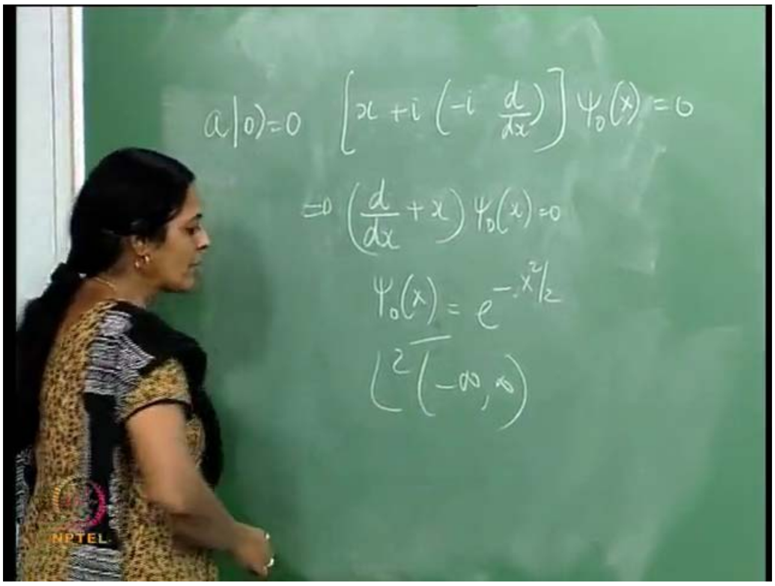

And the equation for the ground state, a on ket 0 is 0, simply translates to the following: a itself is root two x plus i times minus i h cross d by d x. It is just x plus, minus i h cross d by d x. (Refer Slide Time: 43:39) Because 2 a was root 2 times this. So give or take a half and a on ket 0 equals 0, just becomes, turns out to be, psi 0 of x, acted upon by this operator is 0. That implies and I have set h cross equals to 1 so, I can get rid of that there and that tells me that the d by d x, plus x psi 0 of x, equals 0. The ground state of the oscillator in the position representation is clear that the solution is essentially, e to the minus x squared by 2 which is a Gaussian.

So the Gaussian, is a minimum uncertainty state. We have already shown that the ground state of the oscillator is a minimum uncertainty state. We have just now seen that the ground state of the oscillator can be represented by a Gaussian function of x. So, this is an example, of a wave function or a state represented as a function of x. The relevant linear vector space is L 2 of minus infinity infinity in this problem and the ground state happens to be a Gaussian. Now you have seen that the Gaussian is a minimum uncertainty state. It is a different matter that we can check that out explicitly once more, for ourselves and indeed the Gaussian turns out to be minimum in delta x and minimum in delta p.

There are certain very interesting and important differences between finite dimensional vector spaces and infinite dimensional vector spaces, particularly in the context of bounded and unbounded operators. So, I would look at L 2 of minus infinity infinity more closely, in a subsequent lecture and talk about bounded and unbounded operators in this context. Some very important operators turn out to be unbounded operators, in this framework. The function space itself becomes very important, in discussing the Schrodinger formulism of quantum mechanics that is wave mechanics which is what we will take up shortly.