Introduction to Quantum Mechanics

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Lecture – 01

Equivalence of the Heisenberg and the Schroedinger formulations – Mathematical preliminaries

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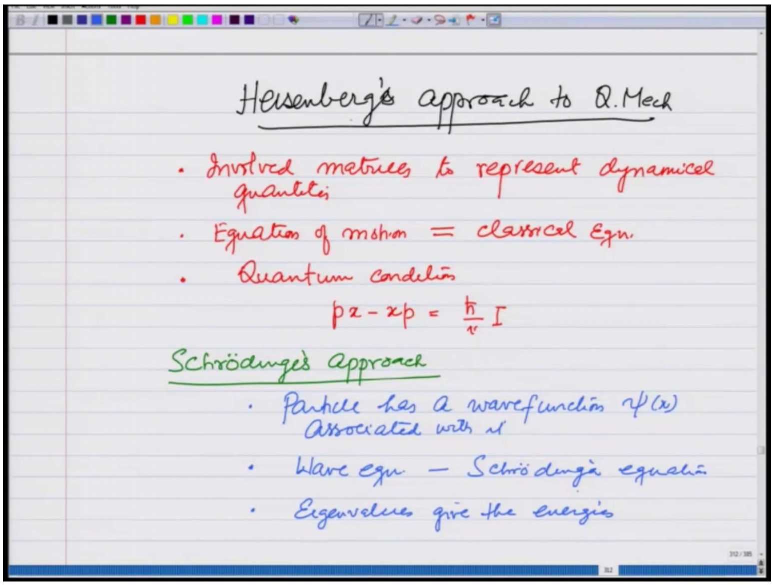

What you have learnt so far in quantum mechanics is Heisenberg's approach to quantum mechanics, which essentially involved matrices to represent dynamical quantities. And the equation of motion was same as classical equation. And quantum condition was represented as p x minus x p equals h cross over I the identity matrice. I we have also learnt another approach which is Schroedinger's approach which is very, very different on the surface from Heisenberg's approach, and what happens in this approach is the particle has a wave function psi x associated with it. Number 2 there is a wave equation known as the Schroedinger's equation, and 3 the Eigen values determined by the boundary condition give the energies.

So, these 2 are very different approaches, but what you learnt is that for simple harmonic oscillators both give the same answers. Is it mere coincidence that both give the same answer or is there a deeper meaning is there any connection? Or are these 2 approaches the same they are just represented in a different way? What we are going to do in the next 2 lectures is learned that actually Heisenberg's approach to quantum mechanics and

Schroedinger's approach to quantum mechanics are one and the same thing. And this will also teaches about how quantities are represented in Schroedinger's approach. For example, we will write the operators for the momentum and so on, and all that requires a little bit of mathematical preparation which I am going to do in this lecture.

So, this lecture is essentially devoted to some mathematical aspects related to the solutions of the Schroedinger equation.

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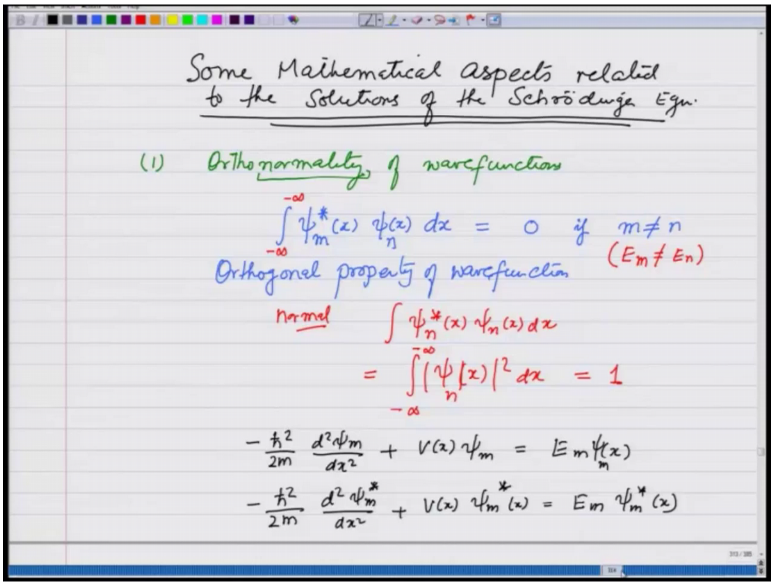

So, first in that I want to talk about is the ortho normality of wave functions. And let me explain normality is the property that we in first ortho means perpendicular. So, this first I am going to talk about of the ortho behavior or the perpendicular behavior of the 2 way function. So, what we mean by that is, if there is a wave function psi m x and I am going to restrict myself to one dimension. Idea is to give you the concepts one dimension makes it easy. Psi m star psi x product where m and n are 2 indices for the energy level integrated over is equal to 0 if m is not equal to n. So, this is what I am going to call the orthogonal property of wave function.

I am going to explain in a bit what we mean when we say m is not equal to n, what it would amount 2 is that if the energy relate energy related to mth level is not equal to energy related to nth level. So, this is the orthogonal property of wave function which is going to be satisfied. Normal means and that I will explain the second points, normal means that for the same n psi n star x psi n x d x which is equal to integral of mode of psi x square d x is going to be one. We choose the coefficient the constant, we choose the constant in front of psi and such that it has integrated to 1. And the integration is carried to all over the space minus infinity to infinity.

Similarly, in orthogonal behavior is also minus infinity to infinity. So, normal part I will come to normality we in force. Orthogonality that these wave functions are orthogonal in the sense of the way I have explained above it follows. So, let us prove that. So, to prove this let us take the Schroedinger's equations d 2 psi m by d x square plus v x psi m is equal to E m psi m x. If I take it is complex conjugate all the real quantities remain the same psi square over 2 m d 2 psi m star over d x square plus v is real psi m x star same as e is real psi m star x. So, we have just written a Schroedinger equation for psi m for it is complex conjugate as well as the wave function itself.

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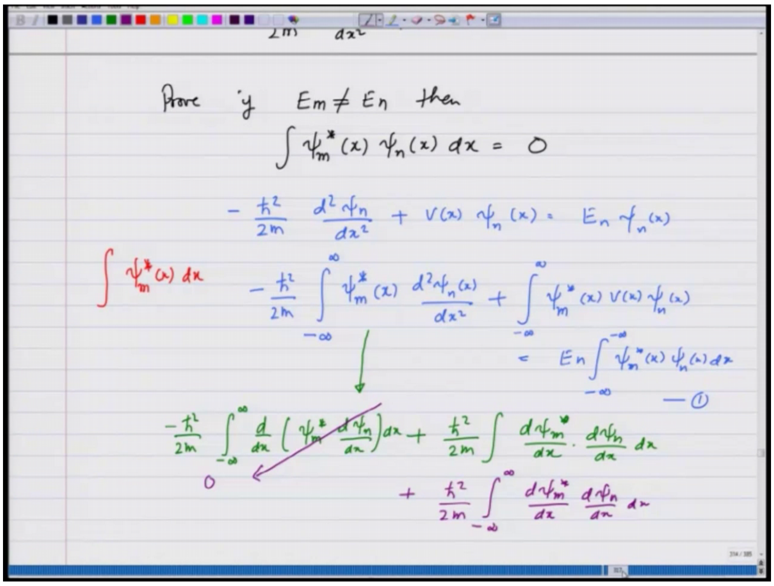

So now I am going to prove that if what we have to prove, now prove if E m is not equal to E n then integration psi m star x psi m x d x is equal to 0. So, let us write the equation for nth level which is minus h cross square over 2 m, d 2 psi n over d x square plus v x psi n x is equal to en psi n x, multiply by psi m star x from the left integrate over d x this is what operation I am carrying out. So, that this equation can be written as minus h cross square over 2 m, integration minus infinity to infinity psi m star x d 2 psi n x over d x square plus integration psi m star x v x psi n x equals en integration psi m star x psi n x d x all integration are from minus infinity to infinity. So, that is equation number 1. Let me simplify the first term this term, which I can write as minus h cross square over 2 m integration minus infinity to infinity, d by d x of psi m star d psi n by d x, plus h cross square is integrated over x over 2 m integration d psi m star over d x d psi n over d x d x.

The first term can be integrated fully and since psi and their derivatives all go to 0 as x tends to infinity this term is going to be 0. And therefore, the first term can be written only as plus h cross square over 2 m integration from minus infinity to infinity, d psi m star d x d psi n d x d x. And therefore, I can write the Schroedinger equation after this integration as h crosses square over 2 m Integration minus infinity to infinity d psi m star over d x d psi n over d x integrated over plus minus infinity to infinity.

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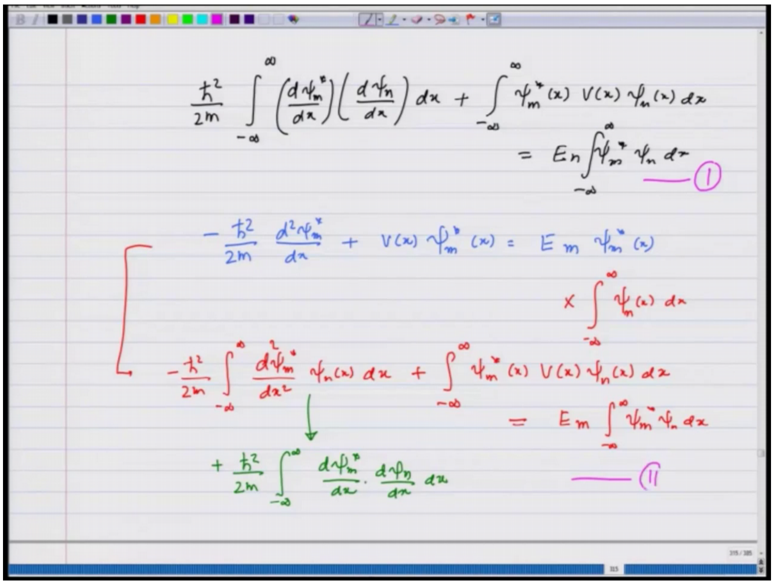

Psi m star x v x psi n x d x equals E n psi m star square minus infinity to infinity psi n d x.

Let me now write the equation for psi m star d 2 psi m star d x plus v x psi m star x equals E m psi m star x this I had did in earlier. Now what I am going to do is multiply it from the right side by psi n x and integrate minus infinity to infinity d x, So that this equation now becomes minus h crosses square over 2 m integration minus infinity to infinity, d psi m star over d x square psi n x d x plus integration minus infinity to infinity, psi m star x v x psi n x d x equals E m integration minus infinity to infinity psi m star psi n d x. I can again show by the same trick as I did earlier, that this term is equal to plus h crosses square over 2 m integration minus infinity to infinity d psi m star over d x d psi n over d x d x. You do exactly the same thing you take one d y d x out and then expand this.

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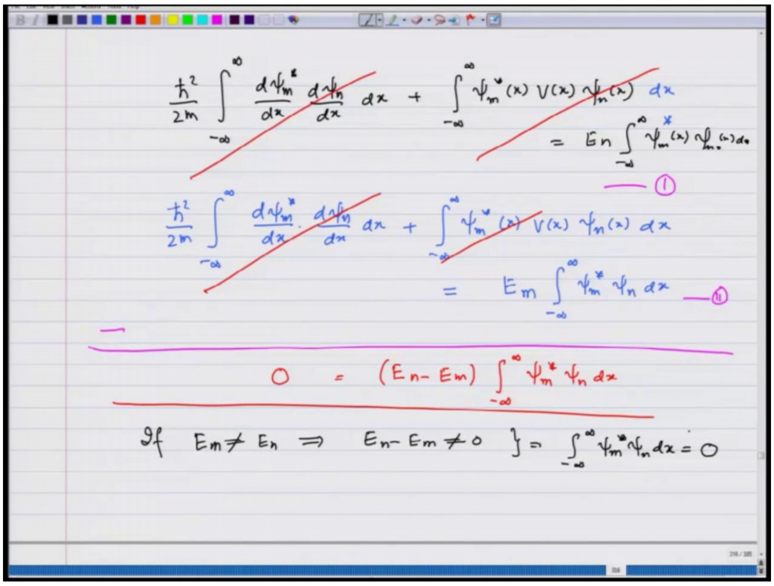

So, I have got these 2 equations let me remember them number 1 is this one, that I wrote on top and number 2 is this equation. So, I have h cross square over 2 m integration minus infinity to infinity d psi m star d x d psi over d x integrated plus integration minus infinity to infinity psi m star x v x psi n x equals E n integration minus infinity to infinity psi m x psi n x d x this is my equation number 1. And equation number 2 is h crosses square over 2 m integration minus infinity to infinity d psi m star over d x d psi n over d x integrated over x, plus minus infinity to infinity psi m star x v x psi n x d x is equal to E m integration minus infinity to infinity psi m star there should be star on top also there is d x psi n d x. This is my equation number 2. Subtract 2 from 1 and when you subtract you notice that the first one cancels. So, does the second term. So, what you are left with is 0 on the left hand side is equal to E n minus E m integration minus infinity to infinity psi m star psi n d x.

And now, you can write if E m is not equal to E n which implies E n minus E m is not equal to 0 it immediately means that integration minus infinity to infinity psi m star psi n d x is equal to 0. Therefore, you prove the first property of orthogonality of the wave functions, that is one thing we will require later and this is always going to be true in the case of Schroedinger’s equation because we require nothing just the solutions of the

Schroedinger equation. The Eigenigen functions whose Eigen values are different, they are orthogonal.

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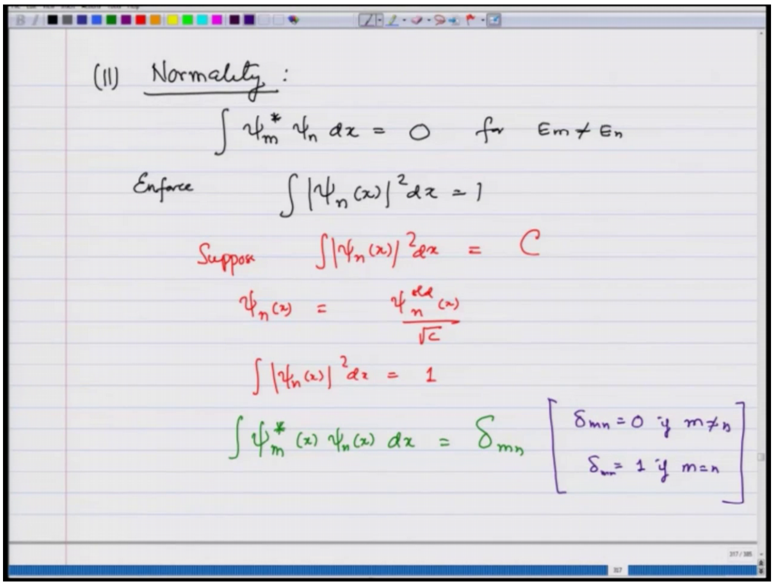

Number 2 this is the property we are going to enforce is normality. And this will have significance later when I will discuss on interpretation normality is going to be. So, we already seen that psi m star psi n d x is 0 for E m not equal to E n. And we are going to enforce that integration for the same index mode square d x be equal to 1.

Suppose it is not one suppose. So, let us write suppose integration psi n square d x is equal to some number c. That I can always defined a new psi n x which is equal to the old let me write this old psi n x divided by square root of c, So that this condition of normality is going to be enforced because I can always multiply solution of differential equation by constant. So, I can redefine its. So, normality is enforce therefore, in general I am going to write that psi m star x psi n x d x is equal to delta m n where delta m n is the prone gal delta. So, on the side I will just write that delta m n is equal to 0, if m is not equal to n and is equal to 1 if m equals n.

So, we have one discuss the property orthogonality, number 2 a convention that going to enforce normality on the wave functions, and third which I will require again is completeness of wave functions.

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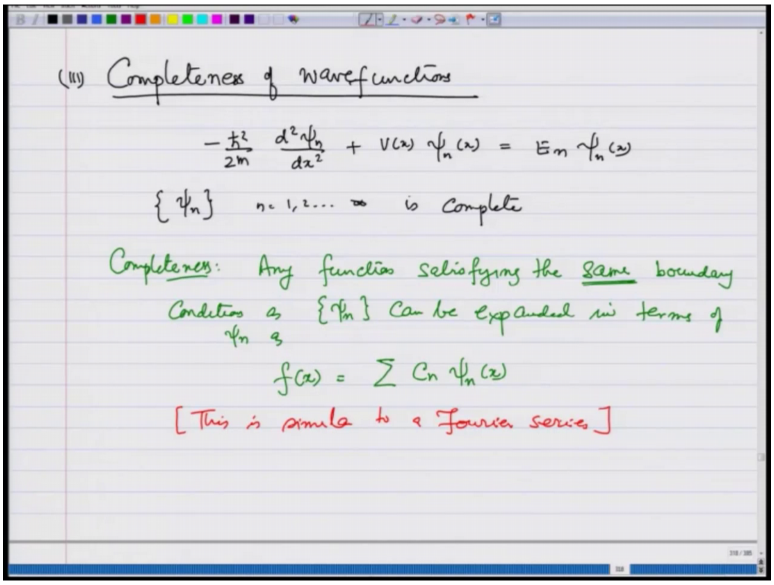

This is the third property, and that is when I write the Schroedinger's equation minus h cross square over 2 m d 2 psi n over d x square plus v x psi n x equals E n, psi n x then the set psi n where n runs from 1 2 all the way up to infinity is complete. I am not proving it. So, you can say assuming it, what it means is that any completeness any function general function satisfying the same and that is emphasize same boundary conditions as the set psi n can be expanded in terms of psi n as f x equals summation C n psi n x. And if you recall from your mathematics this is similar to a Fourier series, where we assume and may be you heard this term earlier that the sin function cosine function and exponential function they form a complete set for those periodic functions.

So here, there are the boundary conditions for the periodicity here the boundary condition satisfied is that satisfied by psi n.

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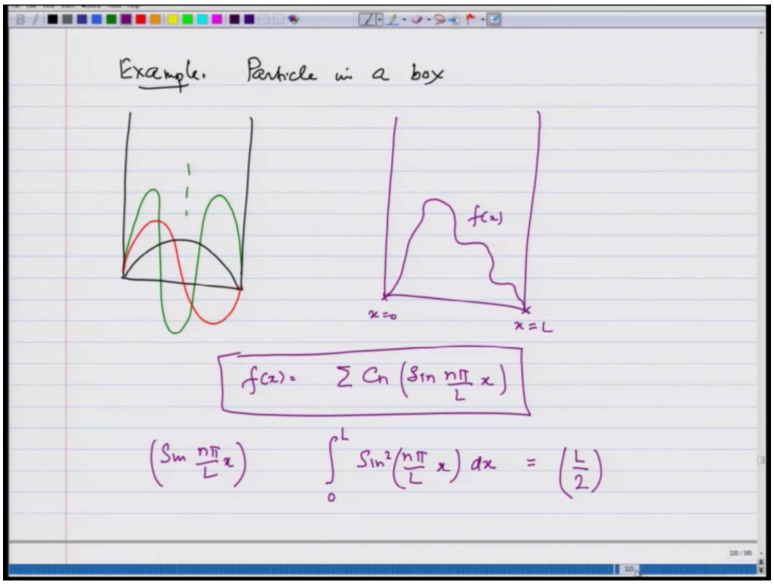

For example so, let us take an example would be let us say particle in a box. So, in the particle in a box if you recall wave function is this function second one is like this, third one is like this and so on. And we assume that this forms a complete set and therefore, any function some arbitrary function which vanishes at the boundaries x equals 0 and x equals L, this is sum f x can be written as f x equals integration C n we call these wave functions these functions are n pi over L x, because this satisfies the boundary condition and the C n can be determined. So, this means that this forms a complete set.

Now, it is as I said convention is to normalize the wave functions. So, the sin n x is not normalized, because let us see what is the integration. If I integrate from 0 to L sin square n pi over L x d x this comes out to be L by 2.

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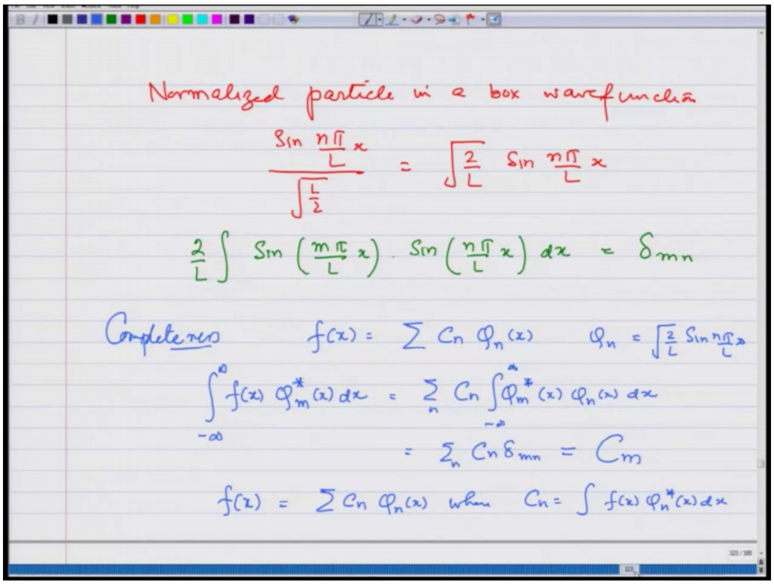

And therefore, to normalize it, I have to write. So, normalized particle in a box wave function would be sin n pi over L x divided by square root of L by 2 which is square root of 2 over L sin n pi over L x. And what an ortho normality is that integration 2 by L sin m pi over L x sin of n pi over L x d x is equal to delta m n. So, that when m equals n it is one. And when m is not equal to n it is 0, which you can check yourself. And the claim is for completeness that affects that satisfies the same boundary condition can be written as C n time is normalized wave function, let me write this as phi n x where phi n equal to square root of 2 by L sin n pi over L x.

How do we determine C n? I will multiply f x by phi m star x d x integrate from minus infinity to infinity, which in this case becomes 0 to L which is equal to summation n C n phi m star x phi n x d x minus infinity to infinity, and by ortho normality this becomes summation over n C n delta m n and this equals c m. So, we have also determined c m; that means, f x is equal to summation C n phi n x where C n is nothing but integration of f x phi n star x d x, that is completeness needs.

Now, I am going to write completeness in a different form and that is useful later, writing completeness in terms of dirac delta function.

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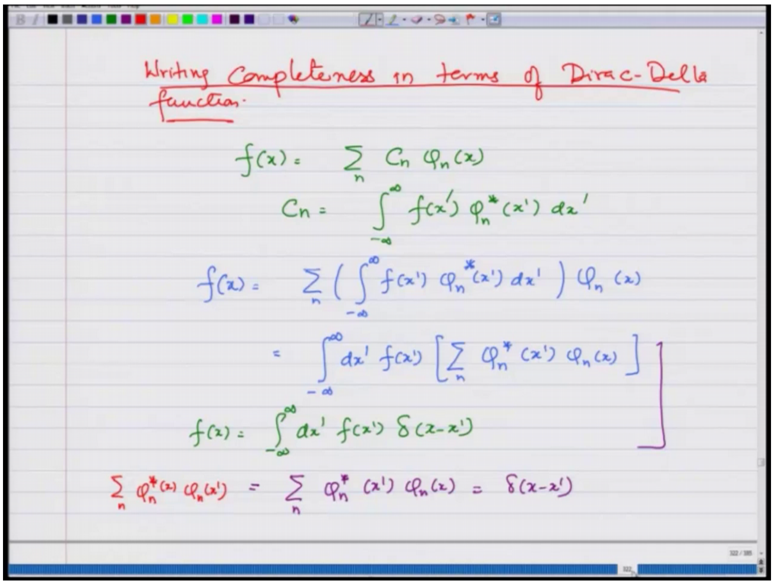

So, what we have just said is that in f x is equal to summation n C n phi n x where C n is equal to integration minus infinity to infinity, f x and let me write this f x prime phi n star x prime d x prime. Because x prime is a dummy variable x I am using earliest. So, I do not want to use that again and then I have f x is equal to summation over n integration minus infinity to infinity f x prime phi n x prime star d x prime time's phi n x. I can rearrange terms and write this as integration minus infinity to infinity d x prime f x prime and then take the sum inside because that acts only on phi n star and phi n x prime phi n x sum over n. This is what completeness is given us.

Now, I also know that f x is equal to minus infinity to infinity, and d x prime f x prime delta of x minus x prime. And this immediately tells me these 2 things together tell me that the summation n phi n star x prime phi n x is equal to delta of x minus x prime. Which I also can write as switch the indices summation n phi n star x phi n x prime s 1 and the same thing because delta function it does not matter if I change x and x prime indices. So, this is another way of expressing completeness.

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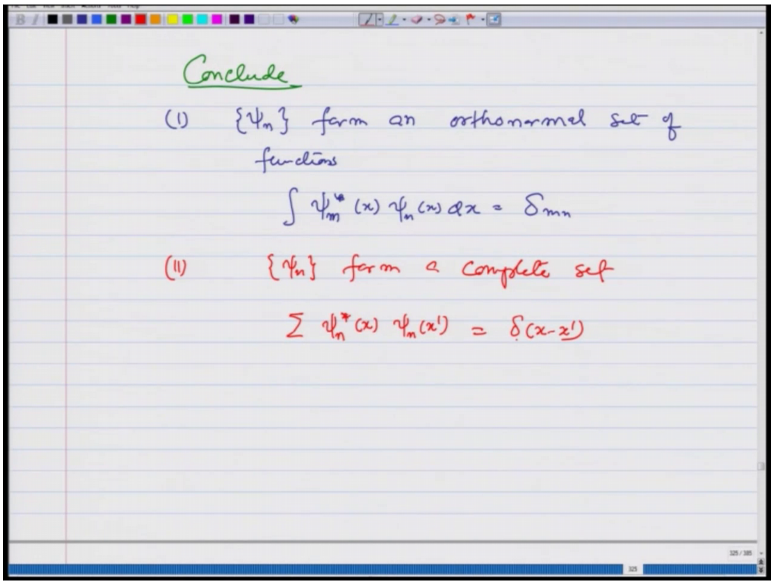

So, let me conclude this lecture with introduction to mathematics by writing number 1, psi n form a an ortho normal set of functions. And what that means, is integration psi m star x psi n x d x is equal to delta m n. And the other property that psi n normalized form a complete set and that means, summation psi n star x psi n x prime is equal to delta x minus x prime.

In the next lecture I will use these properties to show the equivalence of Heisenberg's and Schroedinger's approaches to quantum mechanics.