Quantum Mechanics
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Lecture - 19
Function Spaces - I

Today what we will talk about is vector space, which is the space of functions, okay. Before I get on to that let me.

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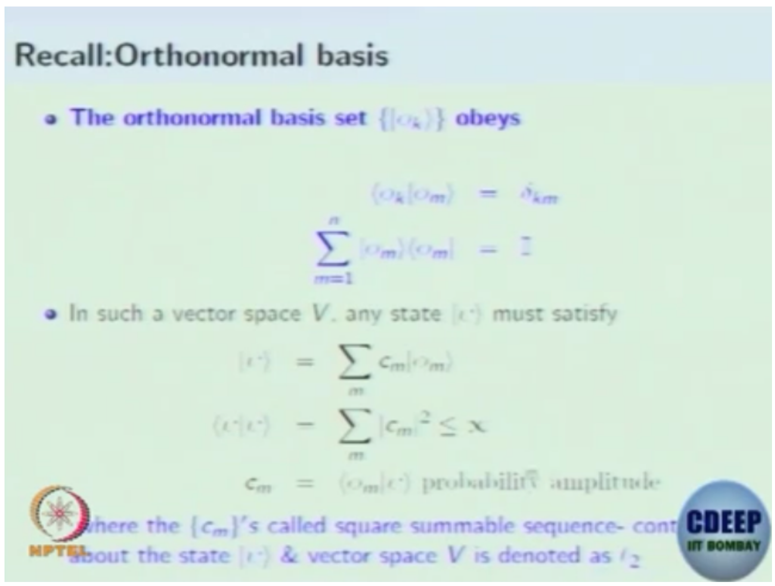

So what all did we do? We said that there is an orthonormal basis set, which we denoted by this angular bracket which is called ket and it obeys the inner product should be delta, Kronecker delta and also we had this outer product. Each of these outer product term is a projection operator, sum over all the projection operators that should add up to be a identity matrix or identity operator. Is that right, and everybody is with me? This is what we did in the last lecture.

So that is the orthonormal basis set, which has to obey these 2 criteria. The first 1 is the orthogonality condition or orthonormality condition. The second 1 is called as the completeness condition. So in such a vector space, any state psi should be, you should be able to rewrite it in terms of the basis set, states in the basis set and there is a complex coefficient Cm. In general, it could be complex if the vector space is complex vector space and Cm is the coefficient.

And you can determine what Cm is by taking inner product on both sides and applying the orthogonality condition, right. So suppose I take an inner product which psi i and phi i, Cm is a constant.

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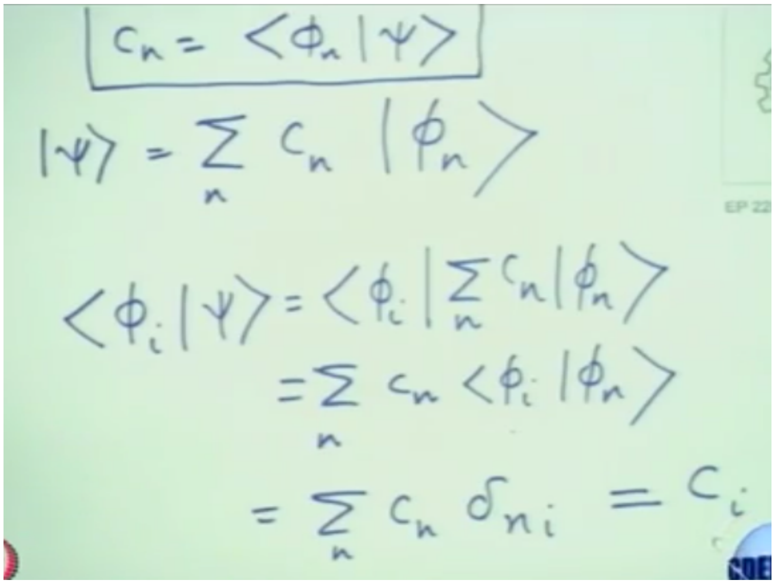

So if I write psi to be summation over n Cn phi n. If I take the inner product phi i with psi, it is phi i with summation over n Cn phi n and I can pull out the summation over n outside and take Cm is also that the property of this, inner vector spaces. I can take out the Cn and you will have a phi i with phi n. What is this? This is orthonormality condition, I will give you a delta ni, so you will have summation over n Cn delta n. So only when n=i, it is going to contribute.

The summation will be gone and you will get Ci. So what we have shown here is the Cn are nothing but inner product of phi n with psi, okay. Is it all right? Each of these coefficients in the superposition of states where phi n are the basis states. The coefficient Cn can be determined by taking the inner product of that state with the basis states. Also you want your vectors, such that the norm is finite which means every set, every vector which we write involves the set of sequence of numbers here or sequence of scalars here.

And that scalars set of scalars should satisfy this criterion, which is called as a square summable sequence and the states which are written in such a vector space, where we have this square summable sequence, that will denoted by Cm of course I have said already. That we denoted by a little l2. So little l2 will, is the vector space which constitutes of all possible states psi, such that the Cm satisfies this criteria or the norm is finite, then you call this vector space to be l2.

So this is discrete set of basis states and we will come to slowly to a continuum set, countable, uncountable, and so on. In the literature, the Cm which is finding, the probability of finding the state in phi n, so that same as what we call it is a probability amplitude and mods Cm square is what we call it is a probability of finding the state. We have done this in the wave function formalism.

I am just trying to rewrite it for you in the Dirac notation that taking the inner product of psi with phi m will tell you what is the probability amplitude for an arbitrary state psi to have a component along phi m. You can treat this to be a set of you know many components in a vector space, that is basis set. So you are finding the inner product of the state, arbitrary state psi to have a component along phi m basis that gives you Cm. Is that clear?

So CM is what we call it as a probability amplitude and the probability should be given by the mod Cm square. It is what we call it as probability, but if you want to define it as probability, then you have to make sure. If this is probability, then the sum of the probability should add up to 1. So you have to normalize it. If it is finite, you can normalize the state and write each of those normalized state coefficients, the mod squared coefficients, which are here.

The coefficients are here mod squared of it. If psi is normalized, then you can call them to be the probability. So such a vector space is what we call, we denote it by l2 and they involve a set of square summable sequence. For each vector, you will have a sequence of complex scalars. So you can either write the state psi just like that or you can give the set of sequences of numbers okay and then we also went on to operators. Is this clear?

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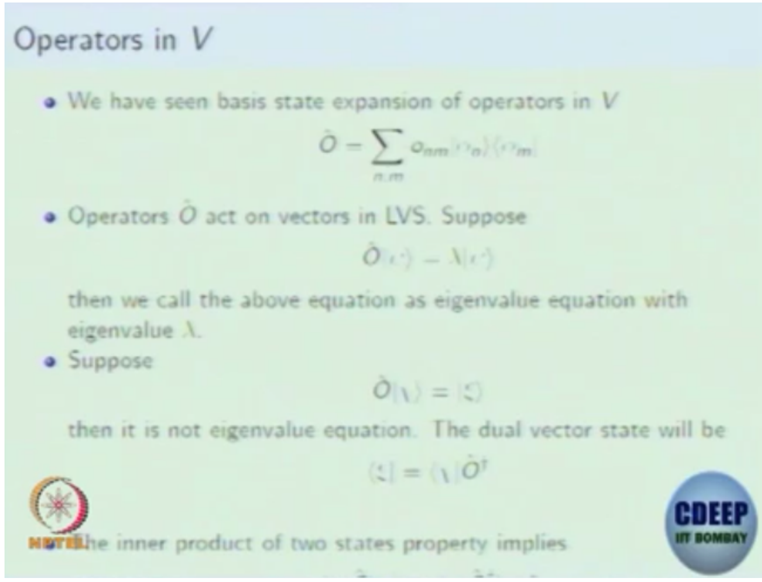

Is the slides and all clear to all of you? Then we went on to the operators just like the basis, any state can be expanded in terms of the basis state. We also went through this operator, which can be rewritten in terms of the outer product of basis states with some maintenance coefficients. We also saw how to write Onm as a matrix element of this operator between the states phi n and phi m. this is what we saw in the last lecture. Is that right?

Okay so to proceed further I passingly mentioned about eigenvalues and so on. So let me put it in here. Operator O acts on vectors in the linear vector space. Suppose the operator on an arbitrary state psi, is lambda*psi. What is this equation called? It is an eigenvalue equation. If you have, if you see it as a finite dimensional vector space with matrix representation, you would have taken a matrix operating on a column vector to give you some number times the column vector.

Then it is an eigenvalue equation, the same column vector. So this equation which I have written compactly here is an eigenvalue equation. What is an eigenvalue? Lambda is the eigenvalue. So the state psi is also called an eigenstate of the operator O. So if you take arbitrary state, which are not against eigenstates of this operator, then in general if you have the operator acting on a vector in this vector space, it can give you a new vector, which belongs to the same vector space.

This is possible, right. If you take a matrix, operate it on a column vector, you can get a new column vector. It need not be the same column vector multiplied by a number. If that happens, then it is an eigenvalue equation. If that does not happen, then this equation is in general possible. Just like we wrote a dual vector state, right in the dual vector space, we would like to write the bra notation for these ket. What happens to this equation?

What will happen to this equation? So the equation can be written as, you can write complex conjugate and transpose, which you can call it as a dagger in matrices and that will operate on the row vector and that will give you a new row vector which is the dual state to the psi. So the operator row, when you go to the dual space will become the dagger operator. So the inner product of these two states property. What is the property of the inner product?

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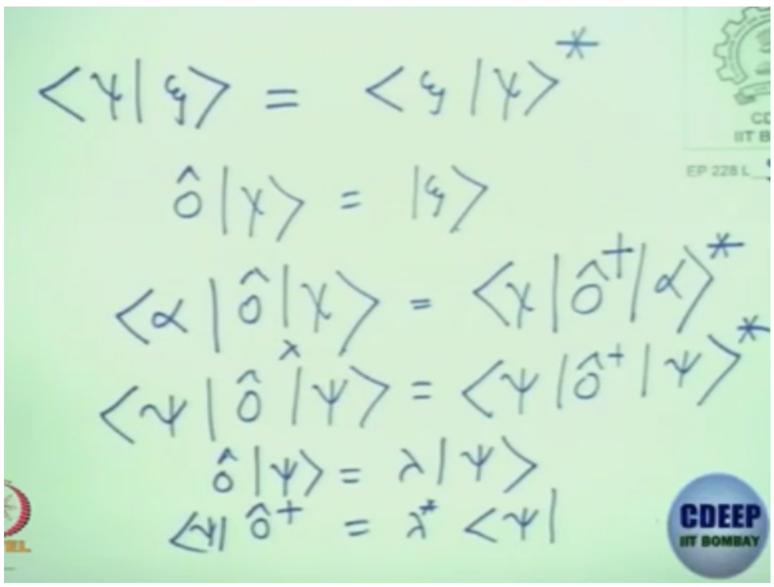

If you had a chi and xi, it has to be, is not it? Okay. If you have an O operator on chi giving me xi okay, so then I can try to write an alpha with O operator on chi that xi. What will this be? Somebody chi with operator dagger, you all agree? And then alpha, so once I write this intermediate equation and use this inner product state property, you can show that this is what is this called. This is called as matrix elements, right.

Matrix element between alpha and xi state and this matrix element if you interchange the row and the column, you have to also take the complex conjugate and transpose. What is that operation called? Adjoint operation, right it is an adjoint operator. It could be a complex vector space. So you have to take the complex conjugate of this result. Is it fine? So this is something which the inner product property forces on you that every operator, which you consider, which acts on vectors in the linear vector space, it has to be obeying this property.

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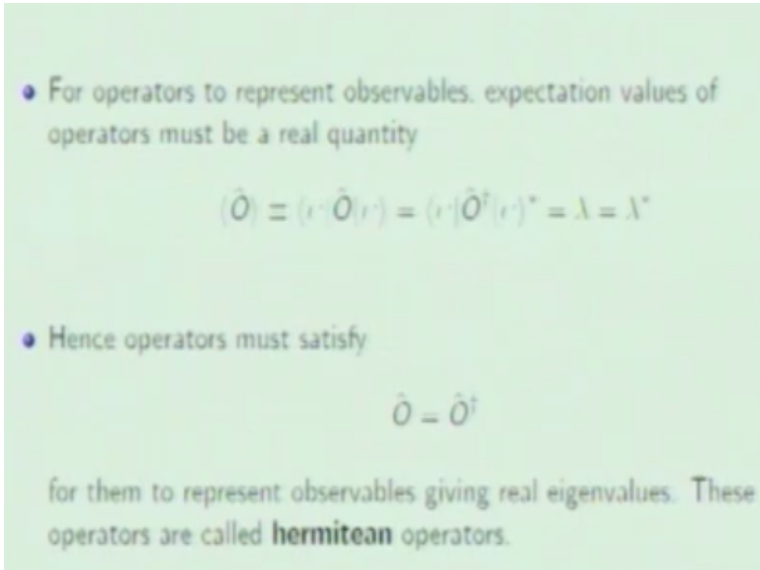

So the next question is we want even though mathematically we call it as operators, we want to make contact with physical observables. Some of the observables are what is the position of the particle? What is the momentum of the particle? You can also have functions of them like you know angular momentum of the particle, energy of the particle, kinetic energy of the particle. You know all kinds of things are all observables.

When I ask you what is the kinetic energy of the particle Ehrenfest theorem, if you remember, the expectation value should behave like your classical results, which means classical results when you study, you always got what? Real, real values, right. You never got complex values. So we expect at least expectation values to be for observables, not for any operator, but operators which can be mapped to observables in physical systems, you want those expectation values to be real okay.

So this is something which you have to keep in mind. So for operators to represent observables, expectation values of operators must be a real quantity. So suppose you take the eigenvalue equation which we had, O/phi was lambda*psi and use the state psi to be normalized, then this expectation value which is equivalent to, suppose the state is prepared in a specific phi. You are given the physical system is in the state psi, and you are asked to find what is the expectation value some operator.

Let that operator correspond to observables. You can take this to be a position operator or momentum operator, just for keeping some kind of a dictionary. So that expectation value is if it is prepared in the state psi, will be formally written as the inner product or the matrix element of the operator in the state psi and just I was telling you about this property that if you interchange the ket and the bra, the initial state, you know the kets state with the bra state, what do you have to do?

You have to make this as both are same. So actually the alpha and xi, which I had, alpha and chi is the same, but O becomes O dagger and you have to do a complex conjugate. So this is what I was showing here right. Suppose I want to write psi O phi, that will be and if you also insist O hat on psi is lambda*psi for any operator lambda could be complex. So if I want to write what is psi on O dagger, it is lambda star on psi.

Lambda in general unless it becomes mapped to an observable, lambda is in general complex. At this conditions, this condition which I have written tells you it is lambda right. O/psi is lambda and this condition tells you it is lambda star. So the expectation values which you find forces that the inner product property forces that lambda has to be equal to lambda star. So this is something which we get provided there is some small thing which I missed here.

These two are looking one and the same provided as an operator equation also you should be able to put this as O operator. So this is what it will turn out to be. So this tells us that it is, so for physical observables, for physical observables in quantum mechanics, in quantum systems the real eigenvalues will force O=O dagger. So this is what we call it as a Hermitian operator okay.

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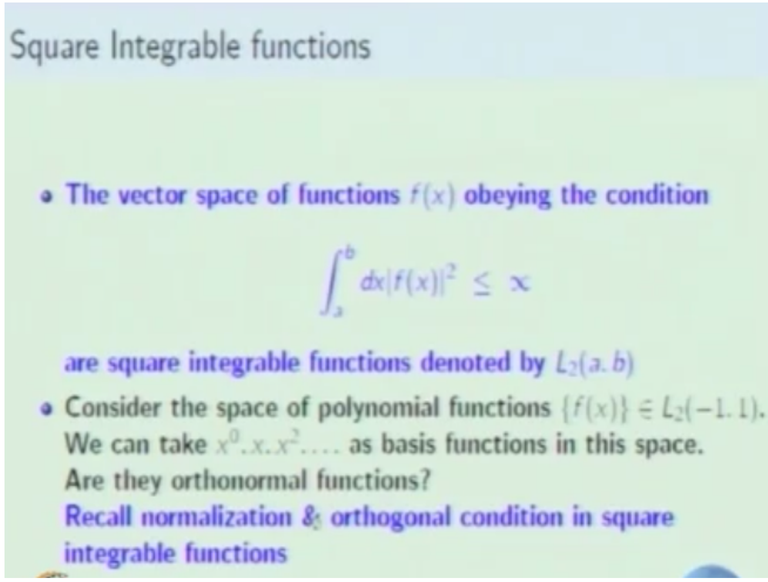

So now I am slowly moving on to the familiar square integrable functions, which I have already dealt within the first week in the context of wave functions. I thought I need to spend some time because you do get a flavor of Hermite polynomials. We did do this Hermite polynomials for harmonic oscillators and then we go to hydrogen atom, we start seeing the Laguerre polynomial and so on. So I thought you should get a feel of these polynomials.

The set of polynomials is also a vector space. Suppose I take these Hermite polynomials, the collection of all these Hermite polynomials forms an infinite basis set countable and you can write any arbitrary function or arbitrary polynomial in terms of these Hermite polynomials. So in that sense, this defines the functions which are polynomial functions, which can define for you a vector space okay. So what are the criteria?

We have seen this in the case of wave functions. Let us take arbitrary function f(x). The mod of f(x) squared integrated over dx between the limits. Let us put a limit A to B, if suppose you have a particle in a box with coordinates of particle, box coordinates to be +L to –L or +A to B, so that should be the integration limits and we have defined that the square integrable functions, where we did wave functions, but we keep to be a general functions here.

They have to satisfy this criteria that it should be not equal to, it should be finite. Sorry, I do not know why I put in equal, should be </=. Please correct it. So these are square integrable

functions. Unlike the earlier case where I talked about square summable sequence, here these are square integrable functions we denote, at least in the literature, it is denoted as L2 and then you also give the boundary points between A and B okay.

So let us take the simplest set of functions which belong to L2 of -1 to +1. You understand what I mean? X takes values from -1 to +1, fine. This is a simplest set of basis function. We can think of polynomial powers. Powers of X, X to the power of 0, X, X squared and so on. Does that form a good basis? Can we write any polynomial using that basis? Yes. Do they form an orthogonal basis or non-orthogonal basis. Non-orthogonal basis, right.

At least we know when we do this. They function formalism, they form an non-orthogonal basis okay and they are not orthonormal. So you know how to do normalization. Normalization is similar to this and orthogonal condition is if you have 2 functions f1 and f2, like 2 stationary states in your particle in a box. If you integrate psi 1 the first excited state with the ground state, you know it will be zero right. That is the orthogonal condition.

So you want to do it on these basis and we cannot do because they are not orthogonal functions. Then what do you do? I want to get orthogonal functions or orthonormal functions. Gram-Schmidt orthogonalization, we need to do Gram-Schmidt orthogonalization in the function space, clear. So now you can yourself start doing it.

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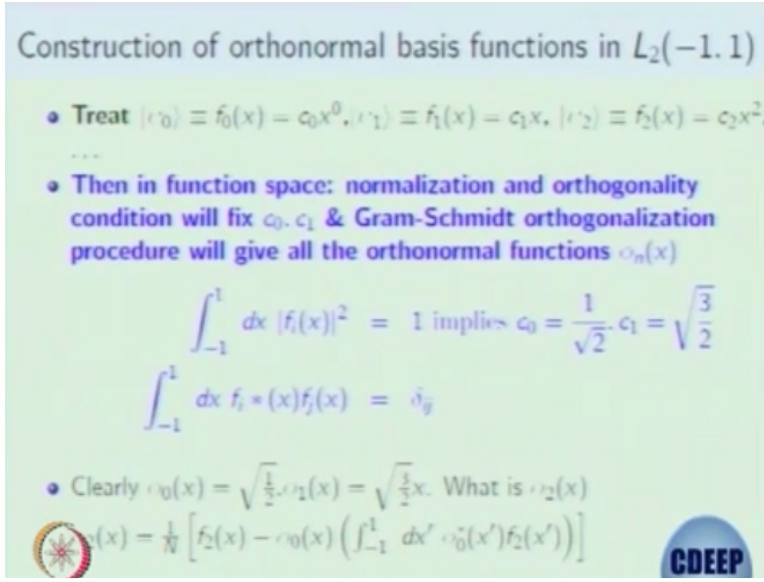

Let us treat the initial state. It is another, it is a function. We will put some normalization, C not times X to the power of 0 okay. So then what do we do? First we need to normalize this function, then we will call that as phi 0. So let us do that. Similarly, we will call psi 1, which is equivalent to the next function, which is just linear in X. Psi 2 is the third function, which is quadratic in X. So these are the basis function, which is the non-orthogonal basis and I am going to do Gram-Schmidt orthogonalization.

So what is the normalization condition? It is an L2 of -1 to 1 correct. So you integrate from -1 to +1. Can we take this polynomial for you know, can you go to X to the power of n also here, where n is very large, the basis functions? You can why because the boundary regions are only -1 to +1, you are not crossing that. So X to the power of infinity is, it can at most have 1 or -1 at the boundaries. 1 to the power of infinity is 1.

So in some sense this basis function is an allowed basis function for the L2 of -1 to +1. You cannot do this if you make it to be - infinity to + infinity, that is the problem right? you do see that, but we need to think of this. Hermite polynomial is the harmonic oscillator situation. What did we do there? We tried to take it from - infinity to + infinity, but there are some subtlety. We need to come back to that subtlety.

You can yourself see here the Hermite polynomials, they do not satisfy this condition. They satisfy with some kind of a damping factor here. You have seen it, right. So we will come back to that, but right now let us confine ourselves to L2 of -1 to +1. So what is C not here 1/root 2. Similarly, you can take from C1(X) subtract out the projection of the state okay. So this will be a normalized function actually.

You try to fix what is C not, and then use that and then you can show that this is 1, but if you try to do this, in the limit -1 to +1, what happens to the orthogonality between f0(X) and f1(X). It is 0? No or yes? That is an even function. This is an odd function and this is going from -1 to +1, you can show that f not with F1 is orthogonal. So when I want to write what is the next state, first state is trivial, you can choose this to be a normalized to be belonging to the orthonormal basis set.

The second state when I have to do from psi 1, I have to subtract the projection of this function on to f0(X) in the function space, which I do not need to do, because this is.

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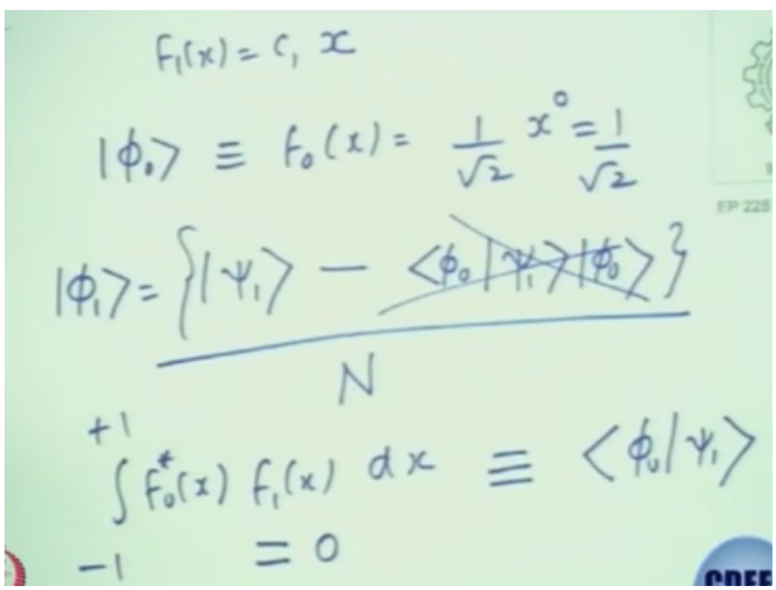

So phi 0 which is equivalent to f0(X) is 1/root 2 and X to the power of 0, which is nothing but it is 1/root 2. So I want to find out what is phi 1, I will start with psi 1- right, you take with phi 0 as psi 1 with phi not and then whatever is the numerator, you have to put that in a product and put that as a normalization. This is what you would have done in a finite countable vector space. Now we need to write what is this inner product.

Inner product in the function space will be f0(X) f1(X)*dx between -1 to +1. So this is equivalent to your phi0 psi1 and what is just going to be? What is f1(X)? f1(X) is C1*X, clear? F1 is C1*X. So this is going to be what? It is a constant and X integration from -1 to +1 will be 0. So you do not need to worry about this term. You can just take psi1 and normalize that phi 1, which will give you your C1 and determine what is your next state phi 1 right.

So you can write, what is phi 1, which is what is that? What does the C1 coefficient, can you check it? Okay so do you get root 3/2, square root of root 3/2. Next 1 what is the thing which you should worry about? It will not by the same logic, it did not have an overlap between on odd and even function. This is even and this is odd. Same thing will happen for the projection on to the state, but will this have a projection on to this state.

So you have to do the Gram-Schmidt orthogonalization by taking the projection of the psi 2 states with the phi 0 or psi 0. Can you try it out? So use this properties phi 0 is root of 1/2, phi 1 is root 3/2*X. So those 2 are straight forward, just from normalization condition itself, you can fix it, these 2 functions. What about the third 1? Phi 2(X), can you try it. The same procedure take the f2 function, subtract out phi 0(X). That is the projection along phi 0.

In the functional space, the inner product will be replaced by the integration. X is a dummy variable, so I call it as X prime because I already have an X here. I do not want to confuse, is that okay? -1 to +1 because that is the vector space square integrable functions on L2 of -1 to +1. So you take the inner product of the state f2 along phi 0 in function space or in the wave function notations. This is what you would have done.

So I am doing Gram-Schmidt orthogonalization for the function, is this clear? I have the initial state. I have to also normalize later. The normalization is whatever is in the square bracket, whatever you get, you have to take the mod of that square bracket, integrate over dx between -1 and +1 and fix the normalization. Will you do this step? Finally, from this, what to C2? What this phi 2, both I need to know. Can work it out just straightforward integration to be done.

Are you all trying, at least verify or check whether C2 is root phi/8 and phi 2 will be phi 2(X) yeah. So I put it in a form, you can check that phi 2 (X) is normalized by that I mean phi 2*phi 2 integrated over X between -1 to +1, you can show to be 1. That is one check. Something is clear here. If phi 0 is just a constant phi 1 is a linear power in X, phi 2 involves even power, that is power X to the power of 2 and X to the power of 0.

So this 2 denotes the highest degree, but it can go on to the lower degrees. This is exactly what you see in which polynomial, Legendre polynomial. Sure you would have done multiple expansions of PL of cos theta. So I did not do anything. I just applied the Gram-Schmidt orthogonalization in the function space. I am systematically determining the phi 0, phi 1, phi 2, which turns out to be Legendre polynomials and that set belongs to L2 of -1 to +1.

Legendre polynomials are typically written as what, PL of cos theta, right? Cos theta takes values from -1 to +1. So this belongs to PL of cos theta is an element of L2 of -1, okay. Let me stop here.