Quantum Mechanics

Prof. P. Ramadevi
Department of Physics
Indian Institute of Technology – Bombay

Lecture - 20
Function Spaces - II

Okay.

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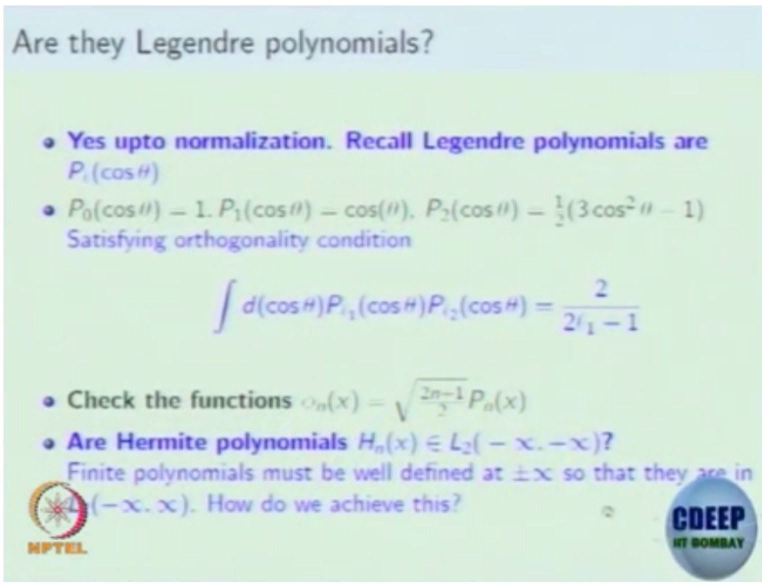

So just to recall your Legendre polynomials, it was not square root of 1/2. The phi 0 was square root of 1/2, P1 was square root of 3/2*X, right. Slightly different, there is some normalization difference, but it is definitely X, P2 is 1/2(3 cos 3X squared-1), if you call cos theta to be X, okay. So there is a root phi/2 in between also, in the front. So there is some mismatch of the overall normalization, but you should also know the condition the Legendre polynomial satisfies is not just 1, okay.

I should have put a delta L1, L2, I am sorry. This psi is delta L1, L2, but there is some factor, which is 2/2L+2L1+1, okay. It is this factor if you try to put a square root here and square root here, then you will see the matching. You wanted to be normalized means, you want this side to be 1. If you want this side to be 1, you can take the square root in the denominator for each of these wave function. So you will find your phi L to be related to your PLs by the normalization.

Okay, so I leave it to you to check that phi n(X) will be actually root of 2n+1/2(Pn(X)). So the next question is Hermite polynomials, the range in which these functions are written, functions of X, that range is we have already discussed, is minus infinity to plus infinity. Then there is trouble. If I write these polynomials at +/- infinity, these polynomials will blow up, right. X to the power of 15 at X=plus infinity or minus infinity square to be very large.

To call them to be square integrable functions, you needed to be less than infinity. How do you achieve this? This is where you try to.

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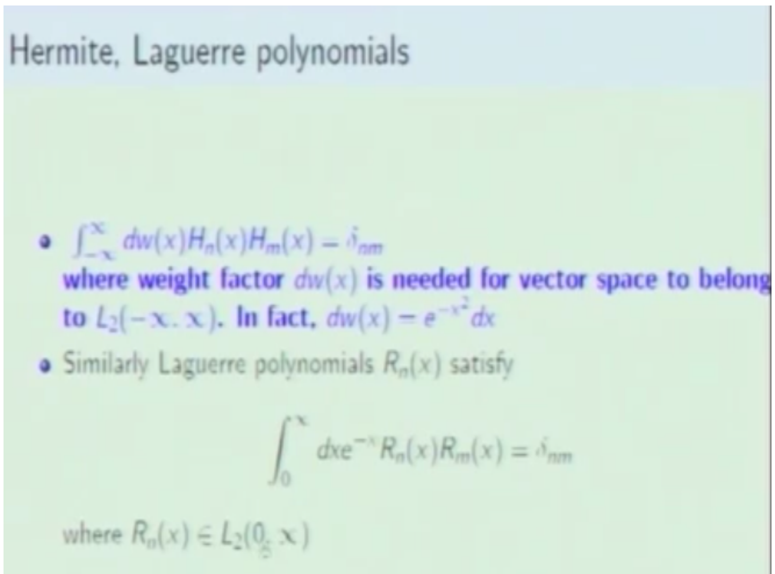

You try to put a weight factor, okay. Instead of just blindly saying orthogonality condition between the functions, you need to be integrating over the weighted dx, okay. So dw in fact will be needed, so that it will belong to the square integrable functions and you take this weight as e to the –x squared dx, okay. So this orthogonality condition, which we study is with weightage factor of e to the –x squared dx and this is very important if you want to go.

If it is from A to B, you do not need this weight factor, but if A and B are infinity, you need to be careful. You need to put a damping factor, so that the square integrable condition is satisfied, okay. Similarly, Laguerre polynomials, which you will start seeing in hydrogen atom, you know that it is a radial coordinate and the radial coordinate is going only from 0 to infinity in the coulomb potentials, right. So you have an equivalent.

So there is another polynomial, which is called the Laguerre polynomials, but there is a new weightage factor here because this will take care, because you are only on the positive x axis. You can put this weight factor as dx e to the –x. So what will you say Rn belongs to? L2 of 0 to infinity. I am just giving you some flavor of the familiar polynomials, which you see and they all belong to the square integrable functions.

Of course, whenever you hit an infinity, you have to worry about the weightage factor in your orthogonality condition and since it is hitting infinity on both sides, the weightage factor should be symmetric, both x+/- infinity it should damp down. Here only when x tends to + infinity, it should damp down and start thinking about, if you want to look at L2 from minus infinity to zero, what will you do, just for a heck of it, then the weightage factor could become e to the +x.

So that is the orthogonality condition with the weight factor integration to be imposed whenever your limits of your square integrable function hits infinity. Any questions? Clear?

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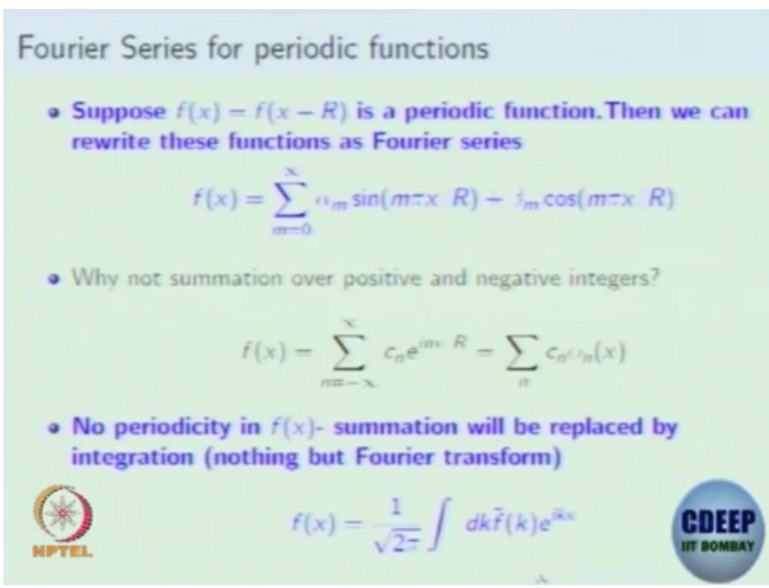

Okay, the next thing I want to get on is functions, which could be periodic, okay. Periodic in a sense that similar rhythm will be there. You go from 0 to L, L to 2L, there is the same rhythm, so on. How do you define that? That you call it as a function f(x)=f(x+R), where R is the, after R steps, again when you come back it is going to be the same. Take the room tiles, each tile if it is identical, you can just work within the tile, the next one will be the same as this.

So how do you put this condition in? How do put this condition in? You try to put this condition f(x)=f(x+R) will force you that you should have a sin m pix/pi R, because when you take x to x+R, then you should get back to the same place and similarly here. Is there a 2 factor? Anyway, so, I am just giving you a flavor that you have to write a series expansion, it satisfies this periodic boundary condition and you can have sin and cos function.

Now if you take x to x+R, suppose you take x to x+R, I want f(x) to be same as f(x+R). So you need to make sure that probably you have to put a 2 factor, maybe I missed the 2 factor. If I have the 2 factor, the sin function and cos function is there, okay. Is that clear? This is, you do this Fourier series in many instances and if you have a periodic function, this expansion something rings the bell somewhere. This is what we have been doing.

Whenever we take an arbitrary function in the Legendre function, it is a linear combination of the basis states. Any arbitrary function will be a linear combination of the basis states, just what mechanically I have put in here. Are you seeing the spirit? That is, it is always if you have a set of basis functions, you can write any arbitrary function as a linear combination where with some coefficient, some scalar coefficient alpha m and beta m.

Here I have taken the basis functions as sin functions and cos functions with the same. Actually there should a 2 here and m is going positive values. Why positive? Why cannot we have negative values? It does not really matter for the sin functions and the cos functions, but you could equivalently write this in a different way. What is the equivalent way? Excellent. So you can write this as a e to the power of 2inx/R. Yeah, yeah 2pi x also, thank you. That is it.

So it is 2 pi*inx/R, okay. I will correct these things in the file, but please note down yourself also. So what is the basis functions here. These are the coefficients and this should be the basis functions, correct. Here these 2 are the basis functions, many of them, same here. Each basis function, you can give a subscript n depending on that n. Formally, I am writing this as summation over n, Cn phi n(x).

This phi n, I choose it to be orthonormal and I can write my f(x) in terms of that. So in this particular example, this phi n is nothing but there should be a 2 pi factor here in the exponent and that factor is your phi. If suppose I do not have this periodicity, suppose I do not put this periodicity, this periodicity allowed us to write this expansion, which satisfies that periodicity, but if I do not have this periodicity, I have to replace this summation, by an integration.

What is that integration called? nothing but Fourier transform. So if you take a free particle, which is not bound anywhere, there is no periodicity, suppose you put a free particle on a circle, make the particle and to move on a circle of radius R, what happens. When it comes back after 2 pi rotation, it is at the same point. So you have to put this periodicity condition f of theta=f of theta+2n pi and then that forces you to have a Fourier series.

The same happens even when you do spherical coordinates in the hydrogen atom. Phi angle has that property. You need to make sure that your phi angle, when you make phi to be phi+integral multiples of 2 pi, nothing should change. The wave function because it is a same point, but if you have a real line going from minus infinity to plus infinity, it is not like this angular coordinate. There is no periodicity. Unless I give some condition that there is a repetition, it take a real line.

Then I do not have any periodicity, so it can, you have to replace your summation by an integration and that is your familiar Fourier transform with basis functions as e to the ikx, here basis functions are to ikx and your Cn analog is your Fourier transform components f tilda of k. There is no periodicity, know, if you try to put in the f(x) and f(x+R) are not related. See if you try to put it as a finite series of summation, that periodicity will happen with this basis functions.

Even with this basis functions. If you do not want any periodicity, this has no periodicity, that is all I am trying to say. Think about it, so that is the way to view a finite series summation, which is Fourier series for periodic functions and for no periodic conditions put in, you will replace it by a Fourier transform, okay. So if I ask what is f tilda of k, just like here if I ask here what Cn, what will you do, you will integrate f with the star of this, right.

The same thing here, f tilda of k is the inverse Fourier transform, which is nothing but the star of this is e to the –ikx multiplied by f(x) integrated over dx. It is as straight forward as it can be. Do you understand? If I want to find what is f tilda of k, that is the coefficient for in the super position, you need to take the star of this basis function with f(x) and integrate, okay. So someone can question why is there a 1/root 2 pi here?

The only thing is that if you do it again, you need to make sure that your Dirac delta function definition is satisfied, there are many conventions, some people put in the Fourier transform or 1/2 pi and in the inverse Fourier transform, they do not put it. You could do the other way. There are many conventions. In this course, let us follow this convention that we put 1/root 2 pi for both Fourier transform and the inverse Fourier transform.

There are many conventions, but we will confine to this. So everything is correct as long as you do not follow half the way 1 convention and another half way another convention. If you follow 1 convention throughout, you will get the correct answers, okay.

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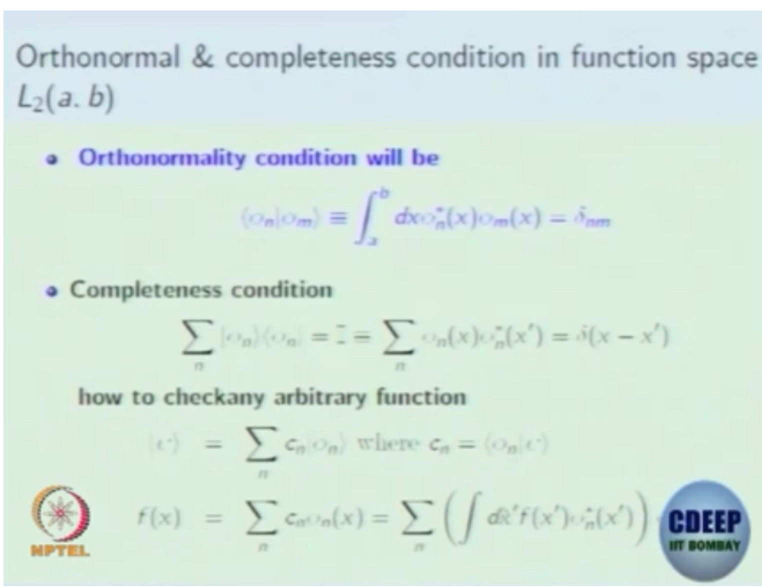

So just for putting in the completeness here, so for an L2 space between A and B, the inner product, which we define for a finite dimensional vector space, in the function space, you will put in this integration of dx between A and B, phi n/star phi m to satisfy this orthonormality condition. You know what is the Dirac delta function? No or yes?

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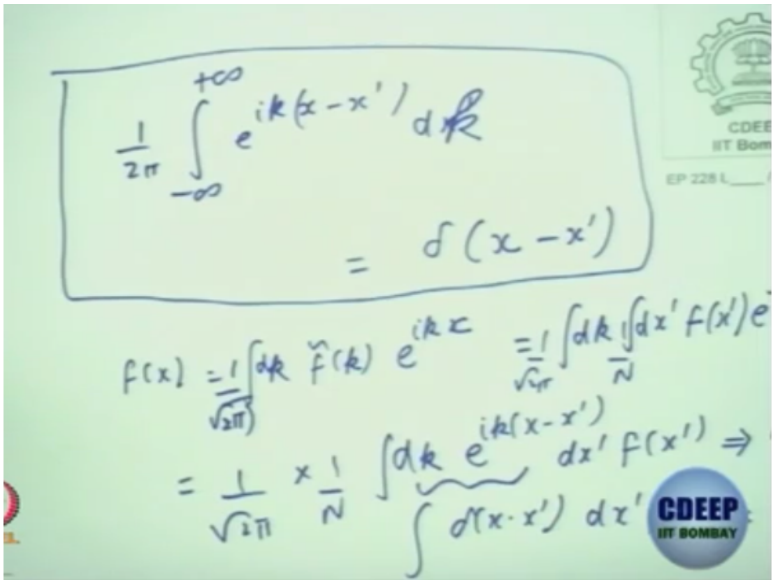

So 1/2 pi integral of e to the power ikx-x prime/dx prime is what delta function, something wrong, dk. Is that correct? I need to satisfy this property. When I take a function of x, which is integral of k, f tilda of k, e to the power of ikx, suppose I introduce this 1/2 pi and I replace this f tilda of k as this, then you will also have this e to the ikx, is that right? And 1/root 2 pi was here already, I do not know what I should put here. Let me keep it as 1/n.

So this will be 1/root 2 pi 1/n integral of dk e to the power of ik(x-x prime) f(x prime). I want left hand side to be same as right hand side and that forces me to choose this. Is this clear? At some places, they would have used here 2 pi and then the inverse Fourier transform normalization will be 1. That is all this. So this will imply n has to be, this is known definition. That we do not want to violate. That is the Dirac delta function definition.

It is in fact from minus infinity to plus infinity. Dx prime is there, so you have to do the integral over dx prime, this will give you a delta function, so this is delta of x-x prime and then integral over dx prime, f(x prime) will turn out to be f(x) provided n is root 2 pi. This delta function I have written is because n is root pi. So we are going to follow convention where we will put 1/root 2 pi for Fourier transform as well as 1/root 2 pi for the inverse Fourier transform.

Some books if you go and see, for Fourier transform, they will have 2 pi, inverse Fourier transform, there would not be a normalization. It is fine. Finally, you know left hand side and right hand side should match and this normalization is just a convenient normalization where I do not need to remember for inverse should I put or should not put, those confusion I would not have if I put the same normalization for both Fourier as well as inverse Fourier transform.

This is the convention I am going to follow. Okay, what is the completeness convention. When the finite dimensional vector space, we have done this, right. The outer product of phi n with phi m is identity. What will it be this side? See I have to have a summation over n, and this is identity, just like a delta n, n kind of thing, right. So what will this be? We will replace the phi n. So whenever you have a ket, I am putting the function and whenever we have the bra state, we put it as a star function.

This is what is the convention I am following. Summed up over all ns, what will this be? The continuum position space, you cannot have Kronecker deltas, what will this be? It would be the, how do verify that this is correct. Take it as a postulate now. Suppose I take an arbitrary function f, then you need to be able to show that if this is an identity operator in the function space, f(x) should not be affected, right. You agree? Let us do that. How to check?

That in function space, this is an identity operator. So arbitrary state psi, just to recall superposition of basis states, Cn is given by the inner product phi n with psi. So f(x) in the function space also you could write it as superposition of phi n(x) and what is Cn here? Cn can be replaced by an inner product state. That inner product is nothing but, I put an x term just to keep track that we doing a dummy integration, okay.

I do not want that to be confused with this X, which is already here and that dummy integration f(x) at x prime will be f(x prime) that is known, then this inner product I told you that I need to take, when I take an inner product, the bra state will become the star of the function, so which is what I have done here fn*x prime f(x prime). So it is exactly the same as what I have written here and you can see that if you take the summation inside.

Take the summation inside, phi m*(x prime) phi n(x), if I put it as a Dirac delta function, is that correct, summation can be moved. Integration and summation can be swept. Then are we consistent. Do we get f(x)=f(x), when you do the dx prime integration, this one will give you the Dirac delta function and you get f(x)=f(x). So this is just a verification, but there will be a systematic way in which we will write this.

In function spaces, the completeness condition will be this definition, which involves Dirac delta function, okay.

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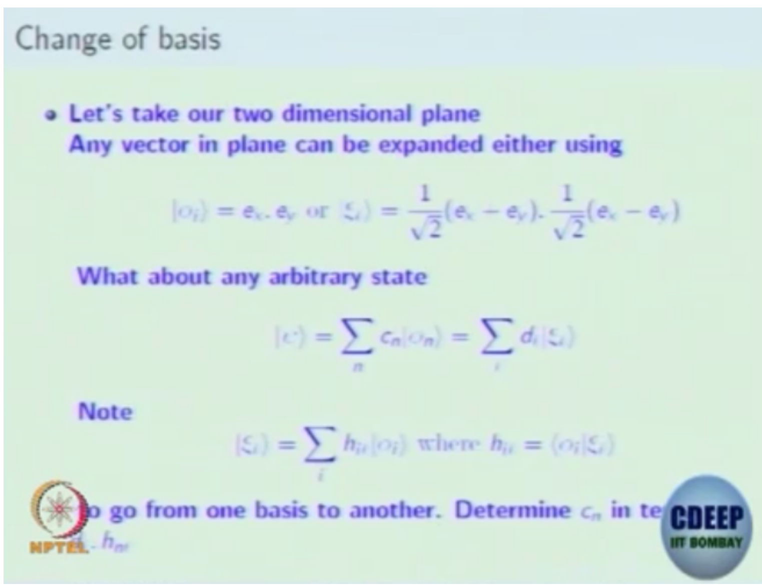

Let us now get on to some more playing around with the basis functions as he already pointed out that the orthonormal basis can be more than 1 possibility, which at least you can be familiar in your 2 dimensional plane, you can have phi i 2 basis functions in 2 dimensional plane as ex, ey and you can also have another basis function, which is a 45 degree rotated basis. This is allowed right. Both are, both can be used as allowed orthonormal basis function in 2 dimensions.

Two dimensional vector space, you all agree with this, right. Suppose I work in this basis, I want to go to this basis, you can still do that. How do you do that? This state is a linear combinations of xi 1 and xi 2, phi 2 will be a linear combination of xi 1 and xi 2 with a different linear combination coefficient, so we know how to play around. Sometimes, some basis will be useful. Sometimes the other basis will be useful.

So you need to know how to go from one basis to the other basis. So what about arbitrary state. I could work out the arbitrary state either as a linear superposition of this basis, equivalently some other linear superposition of this spaces. You are all with me and then you note that xi l basis also can be written as a linear combination of the phi i basis. To keep track of the indices on the left hand side and right hand side, I put 2 indices here following this convention hi.

How will you relate Cn to dl, you can substitute this xi l as hil*phi i here, right and you can hil is of course the inner product of phi i with xi l. To determine Cn in terms of dl and hnl, I have already told you that xi l, you can substitute this and it is a complete basis.

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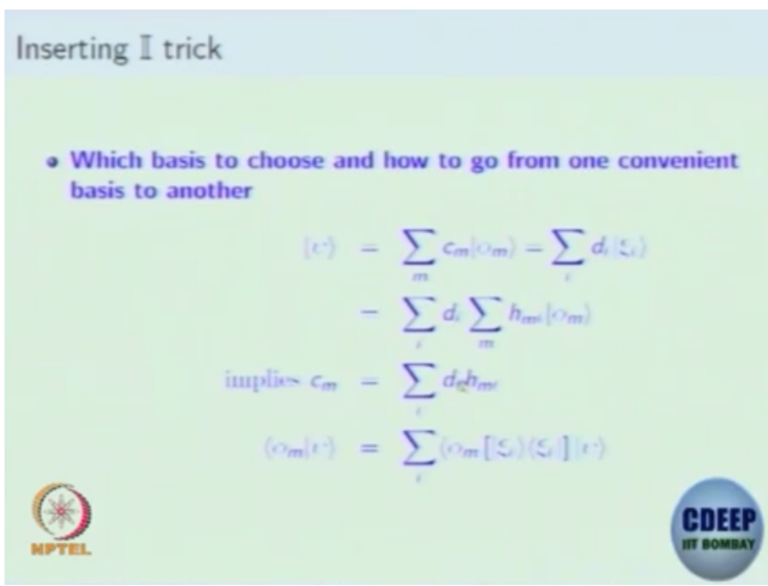

You can compare the coefficients and determine what is Cm in terms of ds and hs. H relates the 2 bases, dl is the coefficient, which I found in the xi basis and Cm is the coefficient, which I find in phi basis. So what is this playing around, just wanted you to appreciate that if you take an inner product of an arbitrary state, so this is the probability amplitude Cm in the basis phi. This can be rewritten; you can keep the outer state phi m here.

So you can write dl as phi m with hml as phi m with xi l, right. Is that right? And what about dl? Dl is xi l with the arbitrary function. So I put this in square bracket, can you see why. What is the square bracket the summation over l, it is an identity, okay? The left hand side is same as right hand side. Whenever you want to get to a new basis, you can insert identity operator anywhere in between.

So here I could insert an identity operator and write the identity operator in the basis, which is a xi basis, okay. So this is a trick which will help us whenever, you see that, suppose, you have a state which is oriented at 45 degrees, you want to look at that state. It is much more convenient to work with xi l basis. If suppose you have things only on the x and y, it is much easier to work with the phi basis, okay.

So depending on the convenience of a situation, you may be able to go from 1 basis to the other basis. So this equation is from 1 basis to the other basis for an arbitrary state. It is nothing but this coefficient if you insert a unit operator in the other basis, that will give you this equation. Conversely I could put an unit operator in between this state and then I can reinterpret this as hml and this 1 as dl, okay.

I am explaining it in 2 dimensional familiar plane and in the Dirac notation, so that you know that this can be done for any dimensional, finite dimensional vector space. So I will stop here.