Symmetry and Group Theory
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Lecture No. 20
Function Space, Transformation Operators

To do that what we do if first of all we are not very far away from end of this class today right now I do not want to introduce to many concepts in the same day especially we have another class tomorrow. Tomorrow we have class at 5:45 P.M. same place right. First of all let us introduce concept of function space and let us go back to the prefund do not get scared. Function space is not a rocket science it is not very difficult to understand or it is our level it is fine.

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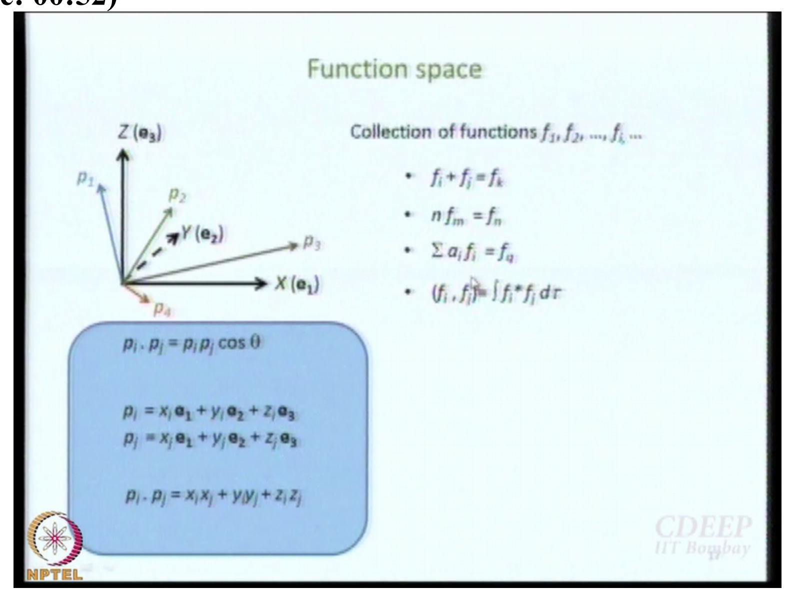

So what you mean by function space is that a collection of functions just put it that way. Do not think of a space where we can sit down and have your basic and all. Collection of functions ok f1 f2 f3 f4 etcetera so on and so forth. In an example of a function space it is a collection of say the position vectors P1 P2 where is P3 P4 are the colours showing on. I do not see them very well. And what you are done as we have drawn this position vectors. In three dimensional space, X Y and Z and the unit vectors based on the vectors e1 e2 e3 as usual, right handed Cartesian system is that right.

It is right handed system or not have you drawn it X Y Z, right handed or left handed the days of left-handedness days are over better be right handed ok. Even position vector it is an example position vectors are examples of functions. Position vectors are something that it is very easy to understand right because it is in tangible space so I use them as an example right. These are examples, this are not general picture, so it is a collection of functions. They have to satisfy certain properties then only you can call that function, function space.

What are the properties first of all fi+ fj = fk, you add up any two functions you get another function. Another function in the sense functions in the same collection. Now think of any two position vectors P2 and P352 add them up what do you get vector addition you get another vector. Where will be the origin of vector be, at the origin, I am calling it origin. Where it will begin, origin of vector will be still 000 right that vector is also function that vector is also be a position vector right.

So this is satisfied by position vectors fi+ fj = fk, got it, fine. What are you trying to do here? We are going to define something completely abstract a function space can be anything right. Then we are going to define an operator. By now everybody is familiar with use of operators and vectors right eigenvalue equation so on and so forth. That is the approach we are going to take we are going to make an operator operate on this functions and then see what comes out.

What will come out is going to be perfectly a general picture which we can use for any system that we want right. So thing is we started with symmetry we talked about matrices today we came back to symmetry and he established some kind of connection between what you discussed in first 3 classes and next 3 classes. Now we are seemingly making a little bit departure once again. It is not really a departure it is just that we are defining same problem of symmetry which is tangible little more abstract term.

The reason why we need abstract definition here is we need generality. So in case I lose you anywhere please do not hesitate to stop me. And we will go back a little and come back but it is important that we understand fine. Second point Nfn = fn, does it work, does it work for position vector? It works if you multiply by scalar still you get position vector to make things more convenient, the direction of the position vector is same as a the position vector as you started with alright, just multiplication by a number scalar ok.

Third is the combination of first and second linear combination of the position vectors sorry linear combination of the functions is also a function there I think you can understand easily.

Take a linear combination of any position vectors what you get is position vector ok. Multiply this vector by whatever number you want does not matter. What is the definition of position vector must begins at origin can point in any direction right can be of any length so, no problem right. So, position vector so for falling in line with definition of function space that we have defined.

Next this is what we perhaps no what is f1, f i, j in bracket yes, what is that called? Another word; scalar product right, scalar products are defined at integral fi star fi d Tou integrated by all space ok that sounds scary. I am scared whenever I see an integral right. Are you extremely scared when I say integral printing mistake. I hope the printing mistake as not continued letter on also, never by delete something; yeah perhaps this is the definition. Let us see what it means? Whenever I get scared by the integral sign I remind myself integral is just summation. Then I am little less scared even my 7 year old son can had ok. When you say addition it is not all that scary.

When you say integration at least I get scared why let us see, let us take an example once again of two position vectors and let us see what the scalar product means. And let us and as you see turn out to be addition of the same form ok. PiPj so printing mistake has not been continued PiPj = Pj cos theta right, j is just the subscript Pj means jth P, not the usual meaning. This is the Pj, PiPj = Pi Pj cos theta right. Let us work it out work this out for the position vectors. To help you all write this Pi = xi e1 + yi e2 + zi e3 and Pj = xj e1 + yj e2 + zj e3, e1 e2 e3 are the base vectors.

Unit vector along the x y and z axis with respectively. Now if you take the product what do you get xi xj e1 e1. What is the dot product of e1 and e1 is 1.What is the next term xi e1 yj e2, xi y1 e1 e2 what is the dot product? 0 right cos theta is 90 right. So this, what you get very simple xi xj + yi yj+ zi zj ok that is somewhat like a sum. That is the sum; this is the sum of products right fine.

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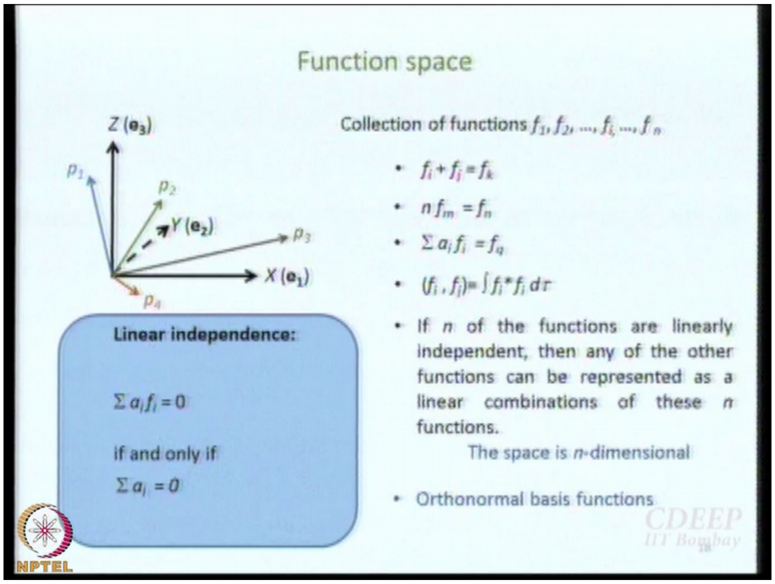

Next one is little unusual in this course that generally we do not have paragraph only the bullet points this is a paragraph. What we are saying here is something that you know very well it is just that I have many words you know if n of the functions are linearly independent, what is the meaning of linearly independent? What is the meaning of linear independence? Yes go ahead exactly you cannot write any vector, any of the linearly independent vectors the combination of the other ones.

So the formal definition is this linear independence means sum over i ai f phi has to no sorry, sum over i ai f phi =0 if and only if sum over i ai=0, no, all this are 0 a1 a2 a3 a4 everything is zero. Second sum is not right, if ai are 0's than is a trivial solution. Otherwise you cannot write sum over i ai f phi =0. Let us take the easiest example that we can understand. x y and z can you write something into x + something into y + something into z = 0.

Can you write how? Something into x + something into y + something into z do not forget what it means something into x + something into y + something into z is a position vector right. When will the position vector will be 0. When the coefficient of x is 0 when coefficient of y is 0 coefficient of z is 0 right, trivial solution otherwise the point is this x y and z take x and y ok if there are non zero resultant it will be in the xy plane right.

It means it is perpendicular to the z axis right. So, vector sum of something xy plane and something along z is never be equal to 0 is that right. Something in the xy plane and a vector and the vector in the xy plane and vector along z, no matter what the angle is right, this is the angle never be equal to 0, that vector sum never be equal to zero. Otherwise if it is equal to transport that is what I think Shantanu was saying.

You cannot write something like z = ax + by unless everything is equal to 0 ok this sum is not right there is just again. So you understand what it mean by linear independent let us go back to the definition now if n of the functions are linearly independent then any of the functions can be represented as linear combinations of this n functions. Very easy to understand in terms of position vectors and base vectors.

Any position vector take any position vector you always write it as xi e1 + yi e2 +zi e3 ok components, any position vectors right that is basically what we are saying here. If n of the functions are linearly independent, in real space 3 functions that are linearly independent right then any of the other functions are represented as a linear combination of this n functions ok. In other words what we say is that this space is n dimensional.

The space here is 3 dimensional ok just because you have many vectors many functions. Suppose you have 480 functions it does not mean that we are working with we are working with 480 dimension working space. What we have to see is that how many of these vectors are n dimensional. Are linearly independent ok that number will give the dimensionality. How many position vectors are there? 3 position vectors only.

Infinite number of position vectors are there, are we in n dimensional space? No, we are only in 3 dimensional spaces because 3 vectors are sufficient right. Linear sum of these 3 vectors is sufficient to describe any position vector we can think of. So this is the meaning of dimensionality. Not how many vectors there are but how many of these vectors are linearly independent alright fine.

And then when these are orthonormal then it forms what is called orthonormal basis function right. There are many examples for orthonormal basis function xyz is little boring I said so many told so many times, can you think of some other being chemist. Think of another let us just keep it simple think of another 3 dimensional basis function. You are chemist do not forget. And it is a physical chemistry class Px Py Pz right.

Now let me ask one of my favourite questions what is the magnetic quantum of Px orbital. People who are taking 821 courses now do not answer. I think it would have been discussed.

Industry people who did 8226 last semester they also do not answer. Others, Jeeva definitely do not answer, yeah what is the magnetic quantum number of Px, +1 or-1, what do you mean either + 1 or-1 depends on Pz is 0 I agree. What about Px and Py? What is the magnetic quantum number? Both, you are just starting 821 so quite, let us see whether other figure out 103 Ch 103 Ch 107 whatever you studied Ch 425.

What is the 5 Part of n =+1 orbital wave function, what is the 5 Part? Theta to the power of 5, theta is theta, 5 is 5, never that is sequential meet e to the power n = +1 what is the 5 dependent part of the wave function? This is 2, i5, and for -1 e to the power of -i5, e to the power of i5 long x or y, it is out of this world. It is in the imaginary axis right. Px or Py do not have well defined magnetic quantum number ok this is discussed in Atkinson physical chemistry book among other places.

The point is these, these are imaginary wave functions ok if you define the magnetic quantum number only when n = 0, what happens is something in cos theta. Cos theta is along z right, what is theta? I hope you are not forgotten this is theta. Starting from z this angle is theta it can go from 0 to 180 degrees. What is Phi? This is Phi along xy it can go from 0 to 360. R of course everybody knows about R.

Now so if this is theta, this angle then cos theta would be along z, right. So, when n = 0, e to the power i0, what is that? e to the power i0 is 1, so that imaginary part vanishes. So, you get real orbital. And the real orbital is something in cos theta it is align with z axis that is why it is called Pz. So, Pz n= 0 but for n = +1, n =-1 cannot draw them along Px Py. So what you can do is take linear combinations right you add once subtract once and in one case divided by i. Then you get functions the along x and along y.

Just read it from Atkinson's book this evening right. So m is not even defined the reason why I invoke all this is that m = + 1, m = 0, m=-1 right they form an orthonormal basic set and Px Py Pz they form another orthonormal basis understand and of these two basis completely diverse from each other, no, they never common member in this case. But you can generate these real wave functions by taking linear combinations appropriate linear combinations of the imaginary wave function.

So basis can be inter-converted transformation of basis not is impossible it is doable it is done right. This is one meaning of orthonormal basis function right.

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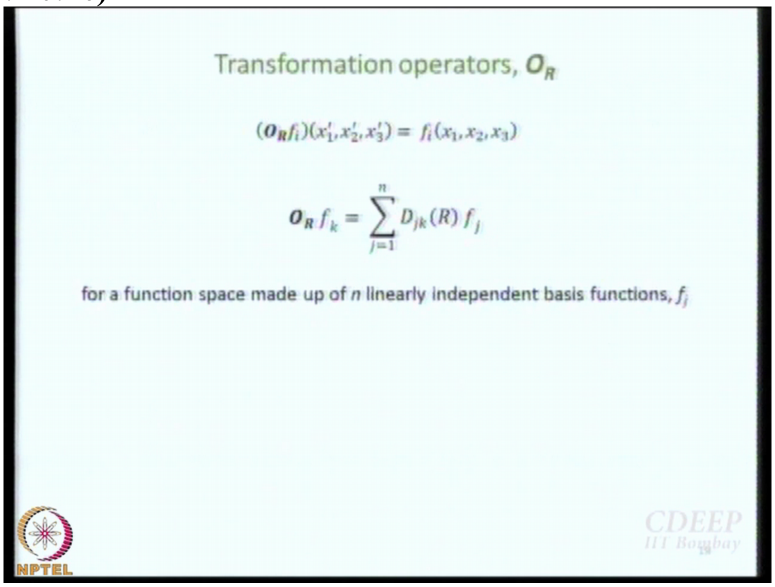

Second last slide now I hope you have at least some idea of what basis functions are right what a function space is? We are going to take the function space and we are going to make some operator operate on the function space. What is our goal? Why are you are you are we doing all these, to get the A at end of the semester. But other than that to get let us without being a spoilt sport let us say we want to develop a generalized method right of knowing how many reducible representation there are? What are the dimensionality and what they are ok? But of course it will come from great orthogonality theorem.

And they are inter-convertible also and you take linear combination and this + or - 1 can become xyz. Similarly you could have taken the 5 D orbital's, the orbital's which work been Bishops book I want to leave that for now because I want to handle D orbital's after midsem when you talk about inorganic complexes. The D orbital's also has affinity do you know why dz orbital's called dz orbital's or dxy is called dxy or dyz is called dyz that is better way of putting it ok we will come to that just.

The question is when I was in school we had this wondrous story everybody has it that some guy wanted to get into jail because it was winter. So, he broke window police did not catching him lot of things finally wanted to get it from, he got caught. There were Cops was used there and we had a question why cops called a cop. do you know why cop is called a cop, any idea, such a good question. Somebody wrote some other question I copy that police man used to have copper helmets, so Cops from copper, that is why cops is called cop.

So similarly well and why Dxy is called Dxy Dz square is called Dx Square. We will also learn D z square is only a nickname, most of us as nickname and good name right. So Dz square is not a good name DZ is a square is only a nickname we learn what the good name is but that is for another day. For now what we are trying to do is we have defined the basis. Now we want to define the transformation operators. Today we will stop at the definition we will not go any further because nothing will transform ok.

What basically you want to do is, if you want to write transformation operators for every symmetry operations and this is what is going to happen when the operators operate. ORfi in the transformed co-ordinate system x1 dash x2 dash x3 dash is in the transform co-ordinate system. So the transformer function in the transformed co-ordinate system is going to be the same as the original function in the original co-ordinate system does that make sense.
Co-ordinate system not the base vectors. See you remove this point, so it has become something else but you move the co-ordinate system along with this same exactly same transformation then in; there can be two kinds of co-ordinate systems right. One is the rotating or let not say rotating molecule fixed or centre of gravity fixed in the reference frame and other is faced fixed co-ordinate system. One can be absolute other can be along with the molecule of course my left hand right hand turn will never meet again.

So, you can transform the co-ordinate with respect to each other right. What we are saying is that you studied NMR spectroscopy right. In NMR spectroscopy you studied the rotating frame of reference or let us take it even easier simpler example. Have you seen the record player in ancient times people use to listen to music from which are like big huge CD's in colour black right. You see record is like a CD, when the player is in action what happens you see that it rotates ok.

Have you seen movie honey I shrunk the kids everybody has seen that movie suppose somebody has shrunk you and you hopped on to the record player, would you see rotating anymore. Of course more tangible example is there do you see that the Earth is moving, we do not because we are on the earth? Then if we stand outside when we see the earth moving right that is the point. We do not perceive the change in earth because Earth is rotating we are rotating along with it. So the transformed R's in transformer earth coordinates is the same as the original R's in the original earth coordinates.

That is what I am trying saying to say ok does it make sense now. ORfi in the transformed co-ordinate system is the same as original fi in the original co-ordinate system. What is e? Fk, ik these are just arbitrary letters it is does not needed. Right now we are in this line have you understood that line next then we go to the next story. Next story is whatever you are written earlier ok.

Suppose we are you are working with functions space made of n linearly independent basis function, here I should have written fk actually, actually I have written fj, no fj is fine, for this fj is fine. Suppose if you are working in the function space where you have n linearly independent basis functions ok. We have already seen the relationship like this right, we have written it earlier. What is e dash? What is e1 dash? E1 dash is nothing but who ORe1, transformed basis vector.

And here you see we are talking about linearly independent basis function like your e1 e2 e3 we just write earlier equation in different form. On the left hand side we have ORfk, where fk is the particular function chosen from n number of linearly independent basis function quite clear, k is a particular function maybe 186th function. K equal to 186 levels ok. So ORfk that means the transform co-ordinate transformed kth co-ordinate that will be sum over j we got it right sum over j = 1to n, DjkR what is DjkR? R corresponds to the symmetry operations DJk is jkth matrix element of the transformation matrix correspond to the R.

And do not forget I read Djk here because I have constructed B matrix using transformation of coordinates not the basis right that multiplied by fj summed over j = 1 to n. So this is more or less what we did earlier also when we talked about that C3 operator example right is it not.

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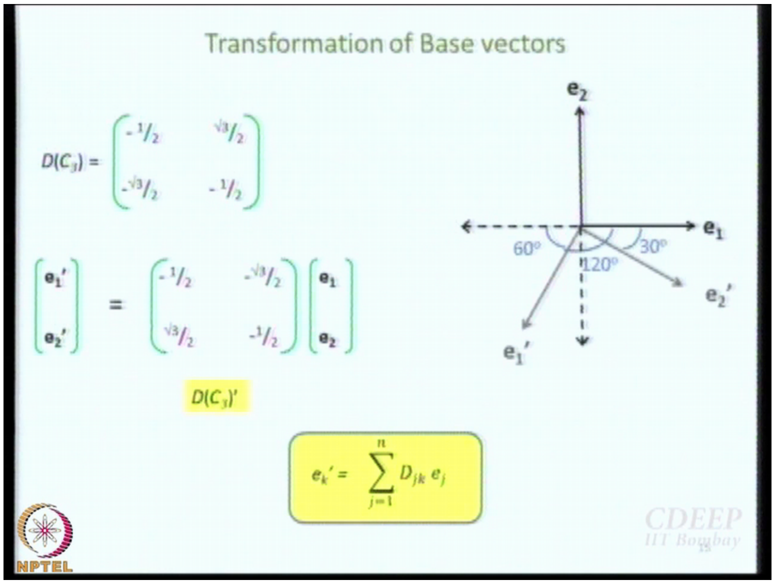

Here is ek dash instead of ek dash we are writing ORfk that is the only difference. When you make OR operate on fk you get this right that equals to sum over j Djk ej all you are done is that we have specified R in little in little more explicit manner make sense. I think we will stop here and when we come back tomorrow and we start from here. What we will see here this turn out to be what are called unitary operators. Back to unitary and then we need to know two more things what are equivalent representation, what are unitary representation.

Once we have done this, then we are ready to derive what are called Schur Lemaa, Schur is some European surname Schur Lemaa and from there you are going to arrive at the great orthogonality theorem. So I think by next Wednesday at least we should be there, if not on Tuesday definitely on Wednesday we will have derived great orthogonality theorem and then in Friday class what we will do it using great orthogonality theorem we start deriving the character tables.

After that let us see I am in two minds weather will talk quickly about vibration I am little reluctant to do that because it is discussed in Ch42 or just we will get into what we did last year in this course talk about what is called symmetry adapted linear combination and discuss valence bond and orbital's theories. Please I am going to send this right away this presentation please go through it once before you come tomorrow it is only tomorrow not for away. Please go through this but that we are ready to take this that tomorrow thank you.