Symmetry and Group Theory
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Lecture No. 22
Transformation Operators Form a Unitary Representation for Orthonormal Basis

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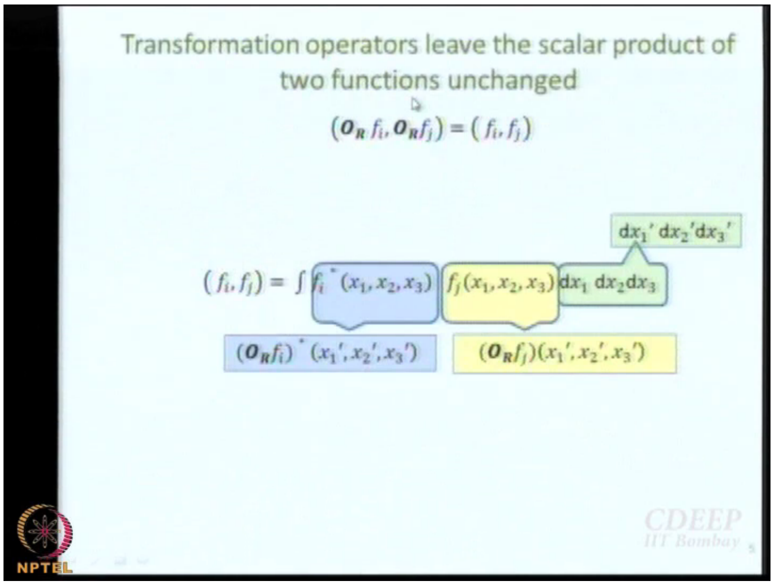

Now with that background let us study 3 or 4 properties of the transformation operators. First once again you are going to use this in the later discussion. The first property is that transformation operators leaves the scalar product of the two functions unchanged. Remember what is scalar product, dot product how are they defined? What is the fi fj? In case if you do not remember I have written it here, this is as you write it fi, fj in brackets and it is defined as integral over all space fi star fj right.

Fi star is the function of x1 x2 x3 fj is the function of x1 x2 x3, what are we dealing with here, we are dealing with functions right which can be represented as linear sum of the Cartesian coordinates x1 x2 x3. I could have written x y z, but x1 x2 x3 is more symmetric then xyz. Good thing is that I can change the subscript and go from 1 2 other that is why I have returned x1 x2 x3 ok. Do you remember this is the scalar product of fi and fj.

What I am now saying is that the scalar product of ORfi and ORfj is the same as the scalar product of fi and fj understand. Now let us prove that do you agree with this fi star in terms of x1 x2 x3 is ORfi star in terms of x1 dash x2 dash x3 dash transform function, in transform co-ordinate is the same as the original function in original coordinates right. So I could see the understanding is being switched on little bit on your face now but you are saying earlier now that is, this is the relevance ok.

So I have worked out the easy one, can you work out the difficult one what is fj, x1 x2 x3, yes ORfj in terms of x1dash x2 dash x3 dash. Now see if you now look at this does not get almost look like the scalar product of Orfi and Orfj. What is left to make this scalar product dx1 dx2 dx3 is there. Instead of this I can transform to dx1 dash dx2 dash dx3 dash right and that is saying little earlier is it not. When you work with a volume element it does not matter if I right Dx1 Dx2 Dx3 or if I write Dx1 dash Dx2 dash Dx3 dash volume element very small volume element are the same.

Without any prick of conscience I can write Dx1 dash Dx2 dash Dx3 dash instead of Dx1 Dx2 Dx3 right. We are substituted fi star by ORfi star in the transform coordinates. And substituted fj in the original coordinates by ORfj in transform coordinates and I have written the volume element in transform co-ordinate as well. So if you agree with that that you see that on the left hand side I have the scalar product of fi and fj. What do I have on the right hand side? The scalar product of ORfi and ORfj right;

So, what we have done is essentially is that we have proved this scalar product of the transformed function is equal to the scalar product of the original function or in other words transformation operators leaves scalar product of the two function unchanged ok. At the moment we might it might seem that something completely arbitrary and far away from Chemistry. Very far away from symmetry is it not. We are going to be little patient to two more classes and we will be back start from whether it will be a better understanding.

Next transformation operators are linear, what is the meaning of transformation operators are linear? We can consider two cases here.

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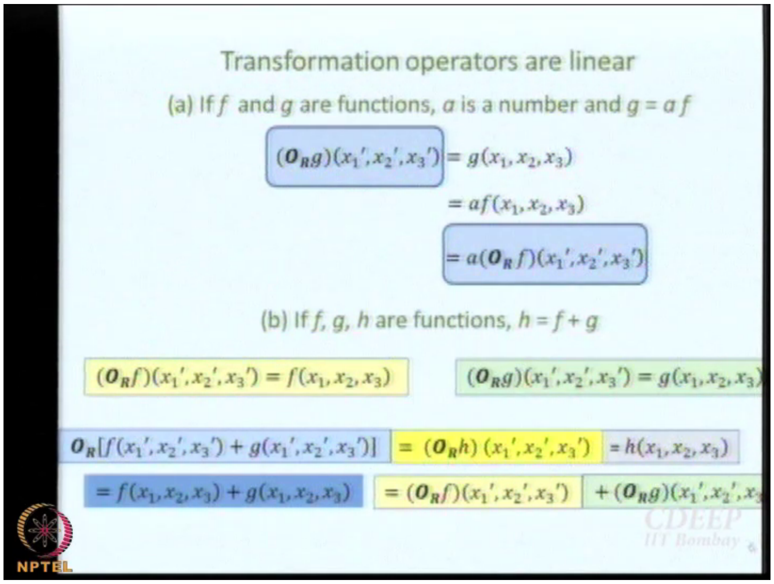

Let us see f and g are two functions a is the number scalar and g = af This case if the transformation operators are linear what should I write? That ORg should be equal to a into ORf is it not then it will be linear. And in the other cases f g and h are three functions. So that h = f+g, ORh should be ORf + ORg right. Example of a linear function sin sin theta + Phi = sin theta + sin Phi, no definitely not. There is not everything in the world is linear ok. Then what is the example of linear function linear operator sorry yeah linear operator. So, let us prove let us see transformation operators are linear.

All operators are linear? No, just you saw right. Not everything is linear, are this is linear let us see. Let us start with this by now if you agree with me if I write ORg in terms of the transformed coordinates is equal g in terms of the original coordinates will you allow me to write that. Now what is g? G is just a multiplied by f, g = a multiplied by f. What will be the next step, what is that? F x1 x2 x3 what is that? ORf x1 dash x2 dash x3 dash and hence proved. What do we have on the left hand side ORg right.

In x1 dash x2 dash x3 dash on the right hand side we have a multiplied by ORf in the same base right. So essentially is ORg = a multiplied by ORf they are both in the same base. This one was x1 dash x2 dash x3 dash and that was in x1 x2 x3 then they would have been a problem they would convert to the same base that is all. Once you convert into the same base we have to write it right. You convince yourself that in the advance School of chemistry linear is boring because nonlinear is here to stay in what I can do with you they are linear ok.

Let us take more interesting example f g and h I forget that to highlight here anyway sorry. I think you allow me to write this pair of equations ORf in the transform co-ordinate system = f in the original co-ordinate system and then ORg in the transformed co-ordinate system =g in the original co-ordinate system right so far so good. So now what do I want to see, I want to see whether ORf+g = ORf + ORg right. So let me write like this, is this ok. Is that ok ORh in transformed co-ordinate = h in the original co-ordinate.

What is h? F+g in original coordinates, I write like this f in x1 x2 x3 + g in x1 x2 x3 now what should I do? What is f x1 x2 x3 is ORf in x1 dash x2 dash x3 dash right and what is g in x1 x2 x3 ORg in x1 dash x2 dash x3 dash hence proved, the background music was very timely it came almost at the time of climax not very most timely. You say or not ORf + g = ORf +ORg everything in the same base that is what we have proved alright, Aachal question, no question good.

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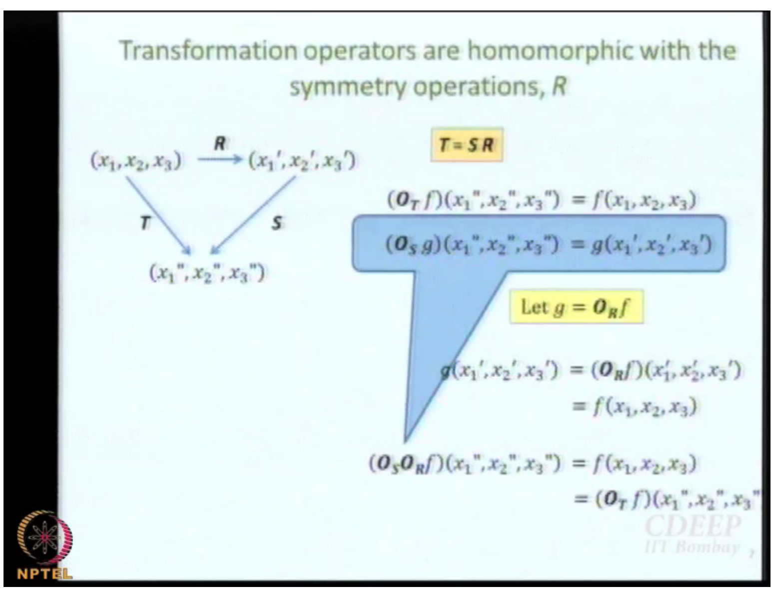

Next I think I have one more one after this we almost done it will take some time. Transformation operators are homomorphic which symmetry operations. What is the meaning of homomorphic? Similar structure that means if you workout multiplication table we have similar structure. Let start with this, let us do the derivation and let us see what we get. Let us see S R T are 3 operations and T= SR that means you start from here start with the co-ordinate system x1 x2 x3 ok.

Perform R operation let us say x1 dash x2 dash x3 dash perform S on x1 dash x2 dash x3 dash you get x1 double dash x2 double dash x3 double dash right. And then T = SR I can draw this arrow here and go directly from x1 x2 x3 to x1 double dash x2 double dash x3 double dash by the operation of the S. So will you agree with me on this OTf in x1 double dash x2 double dash x3 double dash is f in x1 x2 x3. I know it is little bit boring same thing over and over again but then the thing is but I have no option but to go through this, if I have to derive the orthogonality theorem.

These are like necessary evils ok with this same same boring out things Transformer function in transformed co-ordinate is same as original function in the original co-ordinate that is all. Similarly Of g in terms of the double dash coordinates is g in terms of the dashed co-ordinate. Now let us say g = ORf. You are transforming the coordinates so far now you are transforming the functions. Now let us say g = ORf, you agree with me on this now. I have written ORf in the place of g in the same co-ordinate system g = ORf I have just started the basis x1 dash x2 dash x3 dash from both the sides.

Now but then ORf in x1 dash x2 dash x3 dash is nothing but f in the un-dashed co-ordinate right it is jugglery. It is very simple jugglery only one concept. So then what is OSg in x1 double dash x2 double dash x3 double dash, first of all instead of g I can write ORf right. And right hand side I get x1 x2 x3 this is equal to OTf in the double dash co-ordinate. So basically get the same thing that we are saying earlier. Do you have the same character table, you get the same group multiplication table no matter where you stay symmetry operation or the transformation the transformation mattresses are the transformation operators right.

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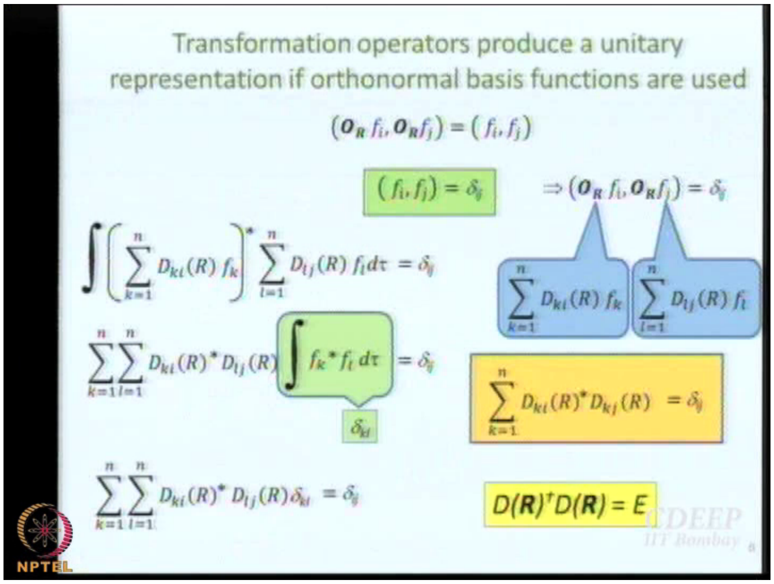

Last for today and the most important transformation operators produce to our favourite terms unitary representation if orthonormal basis functions are used. So, now see we are slowly homing into the take home message. What we are going to show tomorrow is that you take any representation. It is possible to perform a similarity transformation and make it unitary. Eventually we are going to deal with only the unitary representation ok that is the reason why. So we see tomorrow that you convert any representation into unitary representation by a suitable similarity transformation.

So before that you need something that to be understands. The transformation operators produce unitary representation when you use orthonormal basis function. Have we looked at that the example of this already does not ring a bell? Are you too confused with this OR and DR and dash and double dash all that. Remember that those transformation Matrices we talked about using xyz once again. Have we not shown that it is orthogonal? Orthogonal is a special case of unitary right.

Essentially we are proving the same thing we have demonstrated now what we have said already using the transformation matrices we obtained using xyz. Let me check that time he talked about matrices. We got not only unitary matrices but also orthogonal matrix not orthonormal orthogonal matrices. Those are all real if they are not real then they would have unitary that is all ok, something that we have demonstrated already using C3v transformation matrices.

And xyz base and we are going to show that now for general case. But the message is transformation operators produced unitary representation if you use orthonormal basis function. To do this we start from something that we learn from the short while ago that scalar product remains the same ok.

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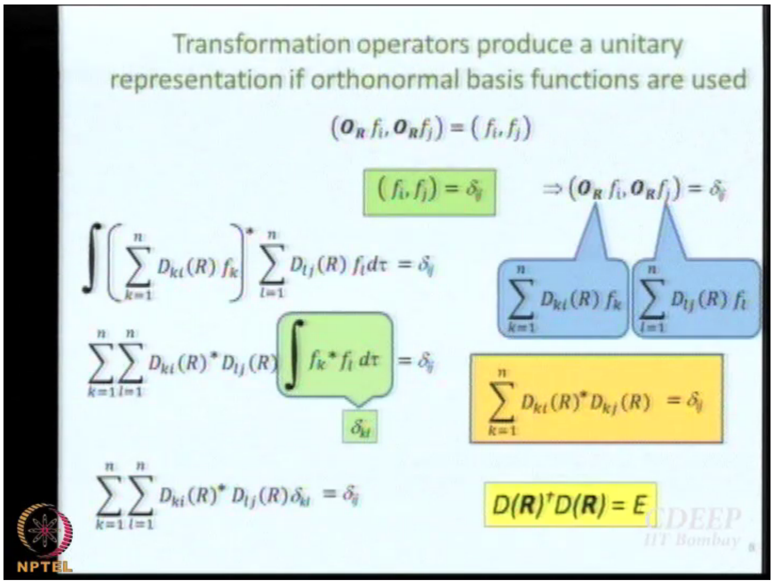

That the scalar product remains same ok, scalar products of the transformed function is same as the scalar product of the original functions ok. Now using orthonormal basis function right, so, I am allowed write this the scalar product of the function is what? Kronecker delta right which implies that the scalar product of the transformed function is also Kronecker delta right, I hope you are not forgotten this what is ORfi?

So in this light we are summarising everything that we have been discussed today. Sum over k D kiRfk that ORfi and ORfj is sum over l = 1 to n DljR fj fl sorry alright remember this. So now what is the definition of the scalar product? Integral f1 star f2 D Tau, so if I write that integral I get little bit scary looking integral, it is not actually scary it is just integral f1 star f2 D Tau. It is f1 a little big ok, it is still scary or it is ok, not scary.

Now let us make it little less scary again. I have integral I have summation it is scary to me. I get scared when I see a integral sign and to make things worse I have two summations as well I have to get rid of this as many as possible ok. How can I get rid of this, one thing I can do if I can collect the integral. I can take the summation out anyway you are integrating over what? You are integrating over all space right. Space not necessarily a Cartesian space.

Space is a function space ok. Now if I am integrating over a function space will you allow me to take this D the matrix elements outside the integral sign and leave only the function inside the integral sign that will scary me less. What will I write in the next line sum over k DkiRfk no fk, sum over k DkiR the sum over l DljR integral fk fl D Tau right? When I write integral fk fl D Tau life becomes little bit simpler why? Because I am using orthonormal basis function write this is what it becomes.

That is the dot product of the orthonormal basis function that is also a Kronecker delta right Kronecker, Kronecker everywhere. So now how does that help me simplify something what are the terms that will survey what is the meaning of a Kronecker delta = 1 when k = l, n = 0, for k not = l. What is the variable k or l, I am summing over k summing over l, I want to get rid of one right. Let me get rid of one, can I get rid of one I have just returned The Delta kl then I think more. How do I get rid of one?

Like this I can get rid of l put l = k those terms will survive I still have one summation but it is ok I leave it one summation I can work. Two summations is too much. So, sum over k Dkl star Dkj = delta ij, what are they, they are matr ix elements ok. Now what we can do is we can put in explicit values k = 1 to n, to start with k = 1, put k = 1what do you have, D1 iR star D1jR right. So that going to be? That is going to be one i = j, i is going to be0 when i is not equal to j. So, if you go on expanding this what are you going to get?

If you go on expanding this will you not get the unit matrix this is what you get right. If this is what is satisfied is not for the matrices to be unitary. Look at this, this is ki and kj this is basically you are working with the matrix element of this hermitian conjugate or adjoint. So the adjoint multiply to give you the unit matrix that is the matrices are unitary ok. This is the most important message we have taken today everything else was really preparing for this the transformation operator produce a unitary representation if orthonormal basis functions are used ok. We stop here today.