Symmetry and Group Theory
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Lecture No. 21
Transformation Operators Form the Same Group as Transformation Matrices

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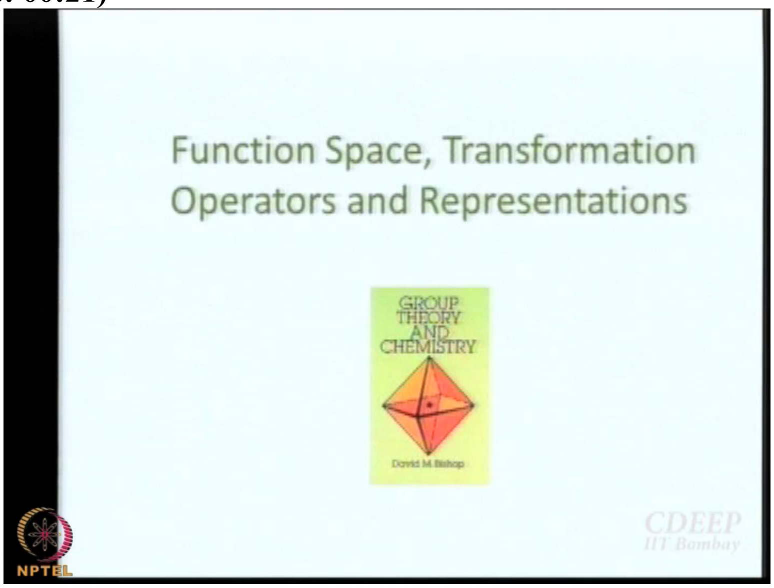

We have started talking about function spaces transformation operator we touched up on the representation little bit that is what we are going to do today. Do not lose the sight of what we are doing all this. We are doing all this because we want to develop a systematic and a generic description of symmetry operations and point group's right. So that we do not have to work out matrices all the time and we do not have to worry about how many reducible representation; how many irreducible representation there are all the time. We want a machine the Black Box which will do it for us once you prepare it right.

Right now what we are doing is we are populating the Black Box, building the Black Box. Once we are done we can put the lead on it and seal it and you should not forget about what you have done right. But then you will see that can be used even without understanding how it works ok. But you should not work like that you should know what is there inside the Black Box. For all these discussion we are following this book group theory and symmetry by David Bishop. This is something that we have talked about when we met last time right.

Long, long ago we talked about the function space. What is the function space? It is no need to be scared because I am using term space here. Your function space is just is a collection of function for now just we call them f1 f2 f3 f4 so on and so forth.

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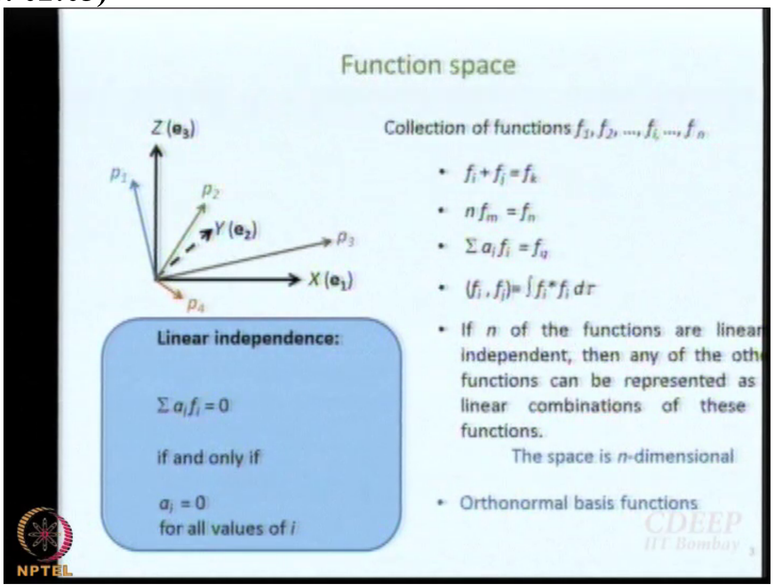

Collection that satisfies some properties, the properties of as follows if you add two functions the sum should also be; the sum should also belong to the same collection or in other words sum should also be a function in same function space, fi + fj = fk, where fk is also belong to the same function space. And the very convenient example that we are using is that of position vectors right. So if you add any two position vectors I think we understand you are going to get another position vector. What is the position vector?

Let us see this is a point right you join a line draw an arrow from the origin to that point, since it is a arrow and a vector that is called the position vector for that point. What is the position vector for this point this is the position vector and this is the position vector and this is the position vector and that is the position vector so on and so forth. So if I act this and that pictorially I get another vector which is also a position vector starts at origin and go somewhere infinite space.

So, position vectors for example satisfy this condition when you add two functions you get that the sum is also a third; the sum is also a function in the same function space ok right. Second thing is if you multiply function by a scalar quantity number then you what you get is function in your same function space. That also is very easily understood by using the example of the position vector 3x, making it very simple is a position vector or not. Let us say 3e1, 3e1 is the position vector along x, 23e1 is also a position vector, 23e1 is 23/3 by e1into 3e1 ok. Now third is if you combine the two then what you write is, if you take a linear sum of the functions.

In the linear sum of their functions is also a function in the function space sum over i ai fi = fq say, fq belongs to the function space. This also I think you can understand very easily with the analogy of the not the analogy example of position vector. Then this is how the scalar product is define dot product, scalar product is a dot product or cross product? Dot product right, scalar product means you take two vectors and on multiply them what you get is this also a vector right.

What you get is a scalar only magnitude right what you are done is that you work it out once again proposition vectors what is Pi Pj you work it out and sum over i sum over xi xj + yi yj + zi zj which is basically is same as integral fi star fj d Tau it is like that in this example we have taken only 3 basis vector ok. This is the definition of scalar product you are going to use this extensively today. So please do not forget what is scalar product?

Scalar product is fi and fj is written as fi, fj in first bracket and it is defined as integral fi star fj d Tau, what is d Tau? Volume element, what is the volume element? Yes kishan, what is a volume element give me a easy answer as usual you are thinking of more difficult answers I will not even seek you. I say it is a small volume right small volume somewhere in the functional space, small volume somewhere in the functional space. I want to define it in a general manner because then things become very easy letter on.

And when it is very small right then little bit of fluctuation does not matter is it not. Then you remember Cartesian co-ordinate to spherical polar coordinates what is the volume element in Cartesian co-ordinate Dx Dy Dz. what is the volume element in spherical polar coordinates everybody knows that is sin theta D theta D Phi it is exactly equal to Dx Dy Dz, is it not, not really. Because after all it is a cardinal, but within the approximation these are both very small we can say that they are more or less equal ok that is what is important to understand.
When you talk about volume element we are really talk about time defined volume so if you change the co-ordinate system it does not matter the volume element in the original co-ordinate is the same can be taken to be the same volume element in the transformed co-ordinate do you agree with this. Example is this r square sin theta D theta D Phi, yeah I forgot here right, r square Dr sin theta D theta D Phi very good right.

And then finally what we said is that if out of all this function we have taken if n of them are linearly independent. What is the meaning of linearly independent this is the meaning of linearly independence sum over ai fi =0, if and only if ai =0 for every value of ai, trivial solution right which means that we cannot express one of these vectors as the linear sum of the other vector. And the easiest example once again e1 e2 e3 or xyz whatever you want to call.

You just take ok x and y something into e1 and something into e2 take the vector sum where will the vector sum be? Somewhere in the xy plane, z axis in the xy plane, no. It is impossible to exactly offset whatever is the value of z, it is not in long z, is it not there along z there is no component along z to be honest right, that is the meaning of linear independence. That sum over i ai fi never be equal to 0, you only case that it can be equal to 0 is when ay when ai =0 for all values of i. And if the all the coefficient of 0 anyway and what is that we are talking about, it is a trivial solution right fine.

So, formally what you say is if n of the functions are linearly independent then any of the other functions can be represented as linear combination of these n functions, once again just understood in terms of position vectors and unit vectors base vectors along the Cartesian coordinates. Take any position vector how do you write it always they are the coordinates write xyz, x1 x2 x3 whatever you want to write. No matter which position vector you take you can represent it completely as a linear sum of the base vector right that is what we are saying here.

If n of the functions are linearly independent in this case 3 of the functions are linearly independent then any of the functions can be represented as linear combination of these n functions and this space is called n-dimensional. So physical space is therefore 3-dimensional, no matter which point we take in physical space the position vector of that point can be represented as the linear sum of xy and z fine. And finally what you said is that when do we get orthonormal basis function?

When do we get orthonormal basis function? We already have linear independence right so these vector are also orthogonal each other like is the case for xyz, I will normalise them then these are called orthonormal basis function. And once again today we are going to deal with some orthonormal basis function
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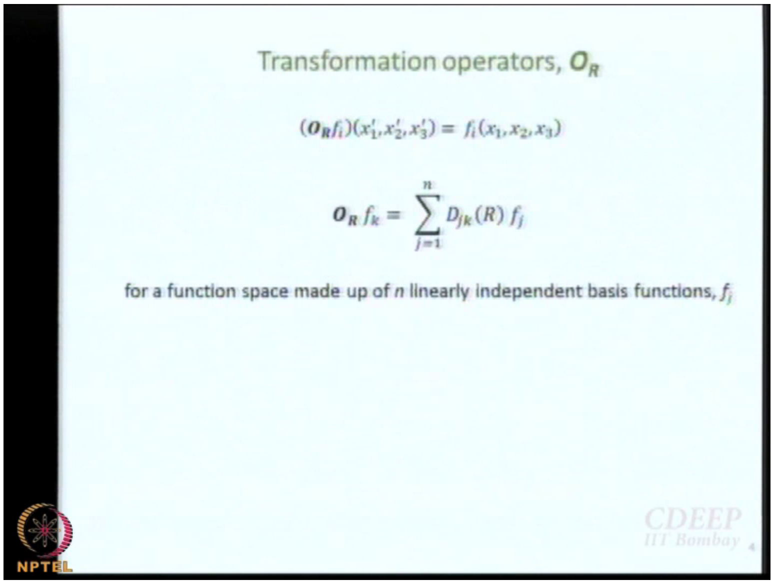

And I think this was where we stopped in the last class, we have defined something called transformation operations ok nothing to be scared of, please do not get scared by the term operator and all is not that scary to be honest. What we said is that the transformation operator is something that is going to take a function and then change it. And what you are going to do is we are going to define a transformation operator corresponding to every symmetry operation. For every symmetry operation capital R we define a transformation operator OR right.

It is just writing the same thing in a different way. What has we defined earlier with respect to each not with respect to for every symmetry operation R have we not worked out the transformation matrix have we not call it DR, right remember capital D and capital R they are in bracket, right or wrong, DR remember transformation matrix now always saying is that we can write the same thing in an operator form.

After all what is an operator the operator is something we do on a function the function changes so we can write as a matrix and make it as a operator also ok. We want to write it in the operator formalism because it make our task little easier when we try to did a great orthogonality theorem and in subsequent discussions that is all, are we clear so far. For every symmetry operation we say that we are going to write a transformation operator. And today for the rest of the day you are going to talk about the properties of the transformation operator.

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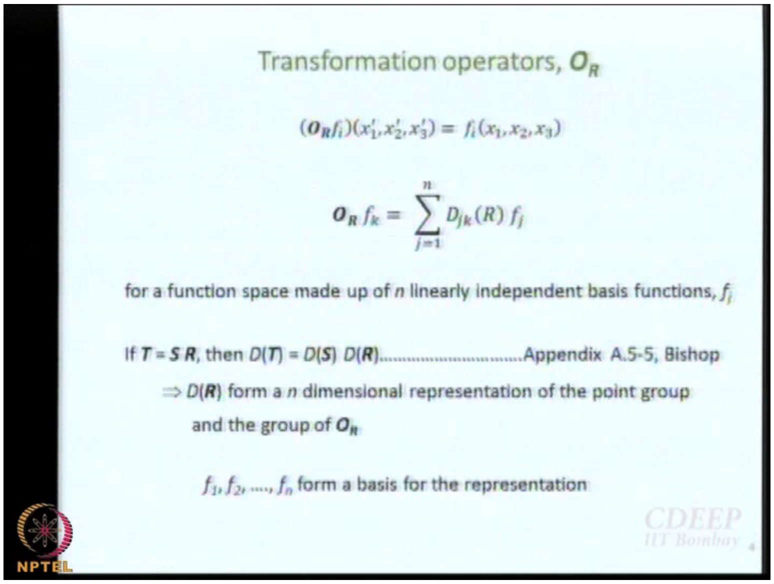

First property we have discussed already and this is something of central importance that keeps coming back to haunt us. That is ORfi in transformed coordinates = fi in the original coordinates, make sense because what you do is if you take the function and performer C3 rotation whatever it is. Then its coordinates in the original coordinates system would change and the function value would also change. However if you simultaneously turn the coordinates what will happen? There is no relative displacement right.

So the function value will not change so show the value of the transform function in the transform co-ordinate system is the same as original function in the original co-ordinate system, make sense fine. OR defines transformed function you get this very clear that something that we will use very quickly and very frequently after this. So please get the physical meaning of transform function in the coordinates being the same as the original function on the original coordinates.

Some of them are trivial observation right it is not because seemingly trivial observation is going to be used later on to prove all the properties of the transformation operators right, does not make sense or not, does not make sense is it just that sound silly right. If you think sound silly then you got it right, that means that you have understood what it actually means ok. It should sound silly if you have understood it at this point of time ok. Transform function in transform co-ordinate system is the same as original function in the original co-ordinate system ok then I am I go ahead.

Now next the another thing that is important very important to understand write it OR fk sum over j = 1 to n Djk R fk, how am I writing the functions f1 f2 f3 f4 f5 dot dot dot fk dot dot dot last is fn. I write it as a column vector right and what is this DjkR that is the matrix element of the transformation matrix corresponding to operation R, what is DR? How did we define DR? DR is a transformation work matrix that you work on earlier for the symmetry operations ok.

Now see this makes sense here what am I doing here? If I say sum over j = 1 to n then I write DjkR what am I doing? D1 k the first one D1k, then D2k did you get to here or here, down D3k down D4K below that dot dot dot Dn, so what I have written here really a column of the transformation matrix what about fj? fj j = 1, so DjkR first row sorry D1kr is first row and which column kth column right kth column.

Then D2k which row which column second row the same kth column ok that is all we are going that kth column. And what about fj and j = 1 is f1, then j = 2 is f2, j = 3 is f3 so on and so forth. Now is that how you multiply matrices, we multiply column with column? You multiply row with column. Why are you multiplying column with column now? You are doing transforming so, do not forget what you have discussed in last class. What are we done? First we transform the coordinates and second we try to work with the base vectors.

So the effect on the base vectors is opposite right, you remember what we are shown there. This is your position vector and this is your co-ordinate system now if I rotate like this rotate the position vector like this. Which side is the elevation clockwise or anticlockwise? Clockwise, whether you rotate the position vector clockwise or whether you rotate the co-ordinate system anticlockwise effect is the same right.

So, the ttransformation that takes the coordinates clockwise or going to rotate the base vector in anticlockwise manner, so it is going to be the transpose right. Since you are working with the coordinates with the functions here, we have to work with the transpose off the transformation matrix do not forget that. This is something that you have worked out in your previous class or class before that? Previous class right please do not forget that.

OR fk is sun over j = 1 to n DjRfj we are multiplying by the multiplying column by column, that is because Matrix that we really working with is the transpose of the matrix that we get from this transformation matrix right. Please read this from Bishop’s, understand if you are not confused at the first time you are not read it right. Please read this part from Bishop's very, very carefully then only you will understand and come back and ask if there is a question ok. Do not forget that what we are working with what is f?

F is one of the; fi's and fj's of the n linearly independent basis function they are like your xy and z that is why we have to go down the column Djk not Dkj right. So you are working with linearly independent basis function here please understand that simple. Otherwise at your age it is very easy to memorize everything and write it down in the exam but that does not does not make any sense please understand what is going on ok. You are working with n linearly independent basis function do not forget that ok.

Now this is something that I am not going to prove because you understand this intuitively anyway that is T= SR then the transformation matrix DT is the product of transformation Matrix DS multiplied by transformation Matrix DR, do you believe me when I say this. TSR are the symmetry operations they are the symmetry operations. What I am saying is that if T is SR then the corresponding transformation matrices are also product of each other DT= DS into DR. I think this is something come to you intuitively.

If not please look at it appendix A.55 Bishop ok. So now think is since that is so; we have shown earlier that day symmetry operations from this representation of the point group right. So now we can say that the corresponding matrices also from n dimensional representations of the point group. There is a connection between what we have discussing now and group theory. Remember we have drawn the group multiplication table long, long ago when you are much younger.

So there if I have to take any function if T = SR, what I am saying is that you take the corresponding matrices and multiply the transformation matrices also from the same group multiplication law. You will get the same table if you use the matrix without knowing what is the change? First works out the matrices without looking at the molecule just perform matrix multiplication you will get the same multiplication table right. So, the matrix themselves forms the representation of the group are you ok with that.

If you have a question please ask, do you agree with me that these symmetry operations form a group right. So will you believe me if I say that corresponding transformation matrices that you work out how to get the transformation matrices by using some bases are the other. Illustrate any basis we have taken n linearly independent basis functions fj right. Taking that taking those I worked out the transformation matrices. So do you believe me when I say that the transformation matrices will also multiply in the same manner as the actual symmetry operations multiply?

If T = SR Dft will also be equal to dfs multiplied by DfR bracket means off right. So what I am saying is that that is the case then if I look at the matrices now think of C3v what are the symmetry operations? E C3 C3 square Sigma V Sigma V Sigma V. For these you remember using xyz which are n linearly independent functions where n = 3 we have worked out the transformation matrices right, if I those matrices side by side what was the dimensionality of those matrices.
What by what I use xy and z as basis. So I got 3 by 3 matrices right I will just Sremind you of those difficult matrix all the 3, the matrix for E 100 010 001 ok very difficult, 3 by 3 right, n = 3.So all the 3 matrices that I had using xyz that they are not 3 by 3 matrices ok. What was it for say C3; what is it for C3? I will give you the most difficult line, I give you the third row 001 then minus half root 3 by 2 minus root 3 by 2 right and rest of all is 0's is it not.

Once again you got matrix by 3 by 3 matrixes similarly you got something for Sigma V. So if I write all this matrices side by side what I am saying is they form representation of the point group and the dimensionality is n. The example that I have chosen earlier C3v n = 3 are all by 3 by 3 matrices. So this forms a 3 dimensional representation. I am just stating that you understood 3, 4 classes ago and in a little more complicated language. Since you understood it is so easy easily that time. I am trying to make little more confusing now that is all ok.

Think of an example which you have done already it is easier to understand. What I am saying is that if I take the matrices, what I am saying is that DR DR, R is variable operation symmetry operation. I do not mean this R. All the matrices, all the transformation matrices and n dimensional representation of the point group alright. And they also form a representation of the group formed by the transformation operators. Once again it sounds as if hitting the obvious. But that it is important that believe and understand, understand and then believe what I am talking about now it is going to be important later on. Basically what we are saying is that you just take a symmetry operation, think purely like a chemist.

See what is the effect on the atoms and all and work out a group multiplication table you get something. Now take the matrices perform matrix multiplication right, so instead of E write DE, instead of C3 right DC3, instead of C3 square write D of C3 Square instead of Sigma V write D of Sigma V so on and so forth. And then carry on the matrix multiplication ok. So, you will get the same exactly say multiplication table as what you get using the symmetry operations. Now if you use OR the operators.

Then also you get the same multiplication table that is all we are saying ok. Now if you look at the matrices n by n matrices. They form and n dimensional representation of the point group as well as the group formed by the transformation operators, ok with this. And this is I think something you definitely understand is f1 f2 f3 etcetera fn they form the basis of their representation like x y z from the basis of the C3v or C2v and that OhA and hB form basis for C2v.