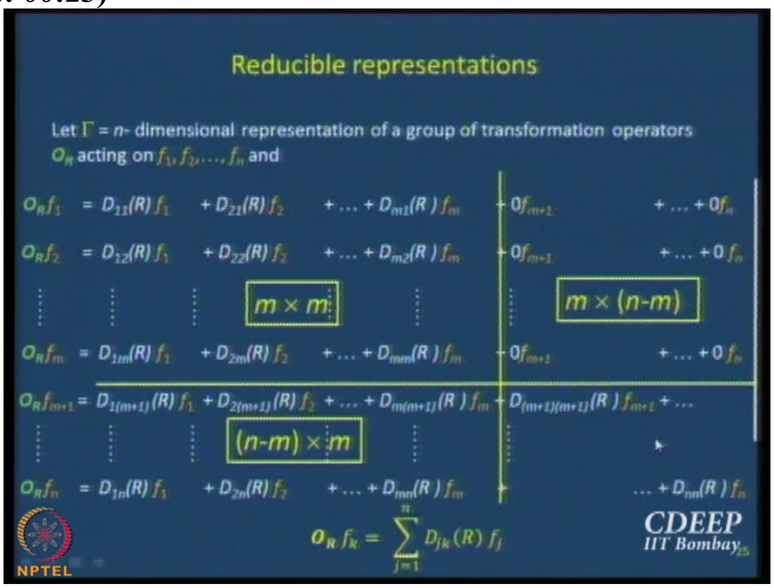
Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology-Bombay

Lecture No. 27
Reducible and Irreducible Representations

(Refer Slide Time: 00:23)



Fine ok, not much is left maybe one and half hours of class maybe I would have gone slower. So, we close today with the deep discussion of what are reducible representations and what are irreducible representations you know this already. But you need to know the; you need to know how to denote this. It will come and handy later on when we go into further discussion. This is how we generally denote the representation.

Which letter is this? Gamma right capital Gamma, so you generate representation by Gamma, let us say Gamma is n dimensional representation of a group of transformation operators OR acting on a basis f1 f2 f3 so on and so forth up to fn right. And let us say this is not a general case, let us say this is what the situation is what is ORf1? ORf1 = D11R f1 + D21R f2 by now you are familiar with this and notation it is not D12 R but it is D21R because we are working with the basis D21R f2 + so on and so forth Dn1 R fn. So what I am saying is that D's Dxy's they can be zero and they can be non zero generally.

But then 0 into f n + 1 0 into f n + e et cetera et cetera up to +0 into fn and the similar pattern holds ORf1 +ORf2 + ORf3 up to so on and so forth ORfn. Have we encountered a situation like this? When you work with xyz and said that principle or when you say that axis of rotation along the z Axis then what happens? Will you not get the similar situation x and y mixed z did not right. X dash first what was this for rotation by theta? Ok you can work it out right sin theta cos theta multiplied by x x dash = cos theta - cos theta? Cos theta then + sin theta -sin theta y you can work that out.

Then plus what into z? 0 into z similarly for y something into x and something into y + 0 into z, so this is just general depiction of the similar situation, the coefficients of all the functions beyond fn are 0 for the transformed function f1 to fn ORf1 to ORfn ok. Let us say like this it is just the extension of what we had for x y and z. So basically some functions by the operation R. Some functions are missing and some functions are not. So, we say that they do not contribute to the first one.

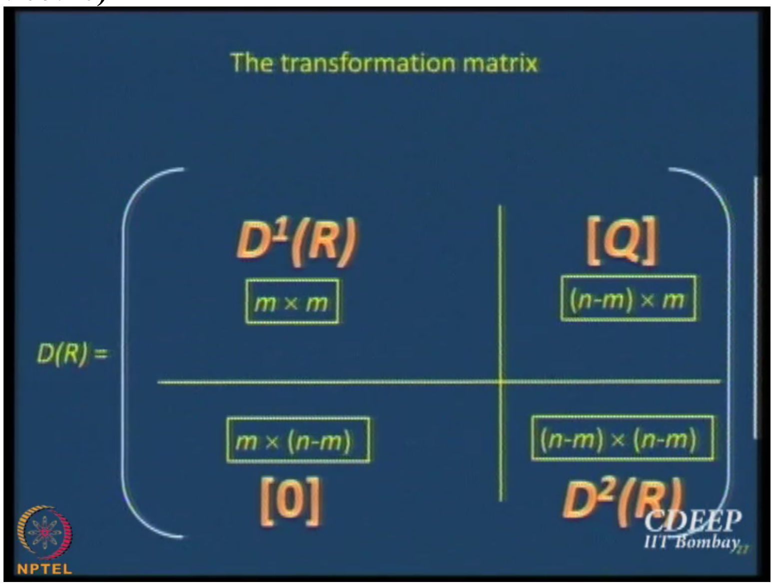
Alright let us say this is a situation. What we are trying to do now is you are trying to see what is the reducible representation means ok. Then let us a situation is like this ORfn+1 we do not know what the coefficient is. Let us say everything is non zero, zero or non zero whatever it is. Let us write D1 n+1Rf1 D2 n+1R f2 so on and so forth plus what will be the last one Dn n+1R fn. And the last one is this Orfn is D1nR f1 + D2nR f2 so on and so forth DnnR fn so on and so forth plus Dnn Rfn ok.

Let us see whether it is 0 or not ok. So now I want to isolate the 0's by drawing these two lines. By then this is a 0 block this is a non 0 block, what are these? We will see ok now this is an equation that we are familiar with now ORfk = sum over Djk R fj right. And you know that the way the coefficients are arranged that is really a transpose of the way they are arranged in the matrices right. This is working on the function on the basis D11 D12 D1n. Should they be down the column or should they be along the row.

It should be along the row right that is what I am saying. Now what is the dimensionality of the block? m by m. What is the dimensionality of this block m+1 n-m into m. Is it n-m into n or is it m into, whatever the matrix or you are talking with a matrix are you are talking about what you get from it n-m into m. How many elements will be there from here to here this is n this is m this is right n-m right.

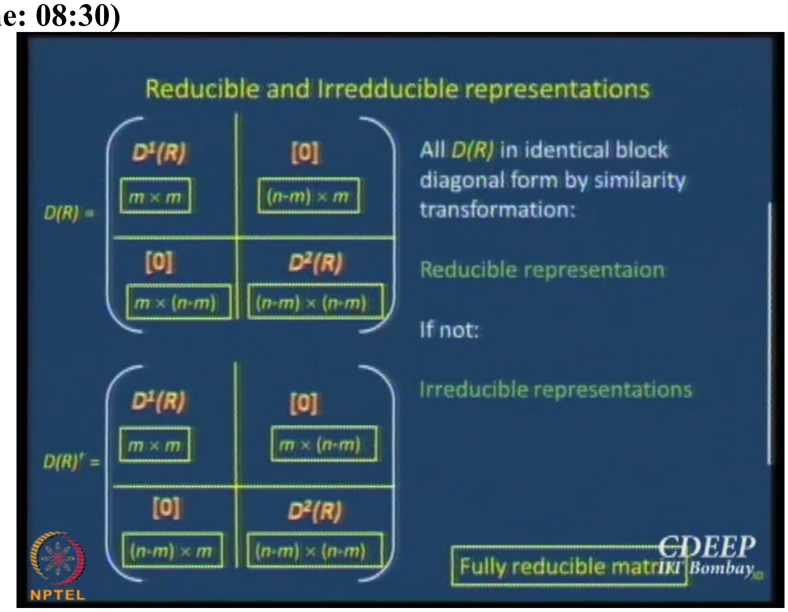
Here we are going down but in actual matrix will be going from left to right. So with respect to the transformation Matrix it is n - m into m. So, as far as transformation matrix is concerned it is n-m into m block ok. What is this? What is the dimensionality is here m into n-m and it is definitely a 0 block is it not. In the matrix all elements will be 0. What is the dimensionality of this? N-m into n-m good thing is there is no confusion whether it is matrix or whether it is operator n-m into n-m is same as n-m into n-m ok.

(Refer Slide Time: 07:40)



What will the matrix look like Let us get rid of everything else and write the matrix this is what the matrix will looks like? Here we have a block here m by m this is m into n-m, n-m into m, n-m into n-m alright. I called this block D1R block just name it; it is very easy where is this 0, here or here? Here right transpose do not forget this is zero block definitely. I call this a cube we see what cube is in a moment. I call this D2R block. So Matrix can be divided into 4 blocks right.

(Refer Slide Time: 08:30)



This is the same matrix written in a more same size right 4 blocks and do not forget we are talking about an n-dimensional representation and we are talking about the f functions alright. Now let us say that the A function are orthonormal. If the functions are orthonormal what will happen to the matrices they are unitary right. The DR's are unitary if DR's are unitary then you know what that means D of R inverse, what is D of R inverse? The transformation matrix of the inverse of R inverse operation of R;

So, we are talking about the C3 rotation then it is C3 minus rotation or C3 square rotation fine. So DR inverse = DR inverse = DR transpose. I think this is something we have discussed earlier also right. So now this is DR transpose ok all that happen 0 and Q get interchanged is it not. Now the thing is this what is DR transpose? DR transpose as you told me right now is the transformation matrix corresponding to the R inverse operation. Now see do you think R and R inverse are going to mix functions differently.

What R has done is that as a function of R you are seen that there is no contribution of f m+1 f m+2 etcetera up to fn in f1 f2 f3 up to fm. So, do you think that in another separation we are going to have contribution from this f m+1 f m+2 etcetera up to fm elements in the transformed f1 f2 f3 up to fm elements? It is just inverse right it is not possible that the function does one kind of mixing that the not function; it is not possible that the operation mixes a given subset of function on the inverse operation mixes a different subset of functions that is not possible right. What will the difference between plus and minus operations? No coefficients right. Coefficients will be different but for f1 f2 f3 up to a fn the subset of the basis that is used that cannot be different right. So what does that mean? Q is 0 that is what it means. So, Q = 0, ok put in 0, so now see this matrices are block factorized in a certain manner. So, this D1R and D2R or two non 0 blocks, these two are definitely the 0 blocks right.

Can this also be 0 block D2R so if it is a 0 block then what will be the ORfn+1 or let us see what will be ORfn? We have already said that for ORfn the front block is 0 right, 1 to n do not contribute to ORfn, fn what am I saying, right or wrong we have proved that Q block is 0. Where did the Q block came from contribution of f1 to fn f2 to fn so on and so forth up to fn to fm those are all 0's. Now the contributions of f m +1 f m +2 dot dot dot fn these are also 0.

Then what kind of operation is OR? That is why I am saying we have just proved that Q = 0 what is Q? Contribution of which function with which function right, what was the 0 block that we started with, I will go back. What was the 0 block? It is the contribution of fk or fi where i = m+1 to n in fj, in ORfj j where j is 1 = n, j = 1 to m right. Now this is the RO block right Q block, what does the Q block stands for? Contribution of f1 to fn f2 to fn so on and so forth that has been proven 0.

Now if this block is also to be 0 that means none of this original basis functions makes any contribution in the transformed function right. Other words everything is 0 here ORfn = what? 0, what kind of operation is OR? It is an angulations operation that is right. Angulations operation is definitely not a symmetry operation ok it cannot be a 0 block. Sum of the elements can be zero fine but at least one should be a non 0 in a2 block, is this a2 block is it not. Why do you say that? I am saying that the block cannot be 0, if it is 0 then that determinant is 0.

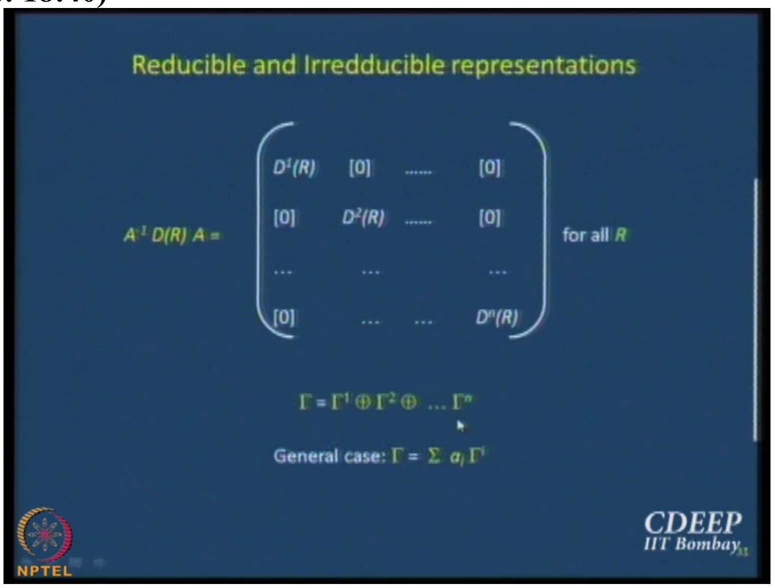
At least one non-zero element in each block is required so in that single non-zero elements prevent you from being a 0 block. Even if there is a non-zero element it cannot be one row completely 0 yeah, so every row must have a non-zero element right. So, a2 cannot be a 0 block. D1R is a block, D2R is another block and this half diagonal are the 0 blocks. What do you call the matrix like this? It is blocked factorized matrix right. It is called fully reducible matrix ok.

So, what is reducible representation? Irreducible representation is a representation in which all the transformation matrices can be block factorized in an identical manner. To start with some DR at least you have some able to perform some similarity transformation in such a way that all of the matrices becomes block factorisable in a particular way. This is something that we have done already before going through all this right. Block factorise done in the matrix in the way remember.

For example xyz for C3v or C2v which one you take to do, C2v perhaps positively what happened to xyz we block factorised in such a way that; we had 3 1 by 1 blocks right but when we took the atoms then we got 1,1 by 1 block 1, 2 by 2 block right. You blocked factorised in the same way. It is not that you are going to put the lines you cut off the last two and last column in one and cut off the first row of the first column no, you have to block factories in the same way right then it is reducible representation right.

If you cannot draw the lines like that even after performing the similarity transformation to a large content then it is an irreducible representation then it is an irreducible representation this is the formal definition. The reducible representation is one in which all the matrix will be blocked factorized in a particular way and the matrices are such a may not be block factorisable. But that should be some similarity transformation that you can do that will make them all block factorisable in the same way, if that is possible then the representation is reducible if it is not possible then it is irreducible right.

(Refer Slide Time: 18:40)



Ok this is how we write it; let us say this is irreducible matrix ok. Here we have all these diagonal non-zero blocks half diagonal blocks are all zeros ok this is how we write it Gamma = Gamma 1 what is Gamma 1? Gamma 1 is the collection of the D1R blocks. What I am saying is that for all R's for all symmetry operations the matrices should have the same form ok collection of all the D1R’s is called Gamma 1. Should I write Gamma 1R, I am writing D1 and then R in bracket why will I not write Gamma 1 and R in bracket?

That is a silly question, why will I not writing R to Gamma, because I have taken all, the R’s why should I write R. See the matrices for one matrix for every symmetry operation. That is why you have to write R in bracket that is a function of R. But then you are talking about the representation when you are taken all the R's. You have to look at the R at the same time. There is no point in writing R inside the bracket anymore. So this is how we write it, so this is what the matrix is look like. Then the representation Gamma is Gamma 1 I will just call it plus.

But just show that it is not really addition it is plus inside the circle I do not know what it is called. Anybody know what the sign is called multiplication inside a circle what it is called yeah it is convolution, it is also called convolution. It is so it is just to de note that all these plus inside

the circle means you are adding blocks. Do not just add them D1R D2R. I have D1R put in 0 and put D2R in its place ok this is blocked addition. Gamma 1 = Gamma 1 + Gamma 2 + etcetera etcetera up to + Gamma n.
It is possible that Gamma n is same as the Gamma 3, are there 3 Gamma 3 or 3 Gamma 4. So the general case is Gamma = sum over ai Gamma i. That is how we write the representation. Reducible representation it is a linear sum of smaller representation and generally we take these, Gamma i's to be irreducible representation. What you say is that reducible representation can be constructed it should not be well yeah.

Reducible representation can be written as the linear sum of irreducible representation, still remember that when I say linear sum here mean that I am doing block addition. I am not just adding up matrices just like that ok. So, this is the definition of reducible and irreducible representation.