

Theory of Group for Physics Applications
Prof. Urjit A. Yajnik
Department of Physics
Indian Institute of Technology, Bombay

Lecture - 16
Representation Theory - II

(Refer Slide Time: 00:15)

From representation point of view

$$\begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \rightarrow \text{reducible representation}$$

We can make do with upper corner
 2×2 matrices.

The 3×3 corner entries "1" can be understood
as the trivial representation of all the elements
 \rightarrow Unfaithful representation, but irreducible

With some $\begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$ is a reducible matrix or a reducible representation; in the sense that it seems to be two separate representations being there not getting mixed with each other doing their own business and we could have with upper corner 2×2 matrices. The 3×3 corner entries 1 can be understood as and it is the same entry in all the matrices.

So, as the trivial representation; all the elements this representation is unfaithful, but also irreducible; right you cannot reduce one any further so the representation is irreducible, but it is unfaithful. The upper corners the 6 distinct matrices provide a faithful and irreducible representation.

(Refer Slide Time: 03:11)

The 6 upper corner 2×2 submatrices provide faithful irrep.

Generically, reducible rep has the form

$$\left(\begin{array}{c|c|c} 3 \times 3 & 0 & 0 \\ \hline 0 & 2 \times 2 & 0 \\ \hline 0 & 0 & 1 \times 1 \end{array} \right)$$

in terms of carrier $\rightarrow \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{matrix} 3 \\ 2 \\ 1 \end{matrix}$

The 3 dim, 2 dim & 1 dim subspaces do not mix

PH 520 L / Slide 6

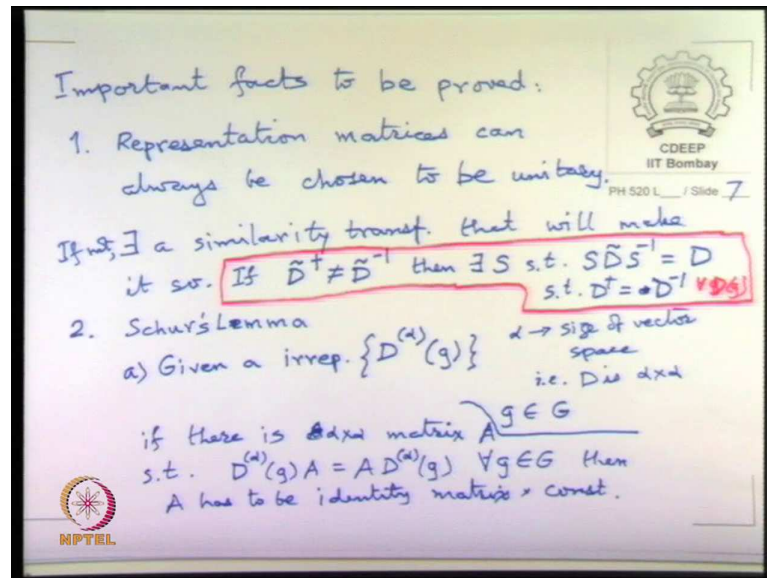
CDEEP IIT Bombay

NPTEL

This short form irrep is very common for saving one the trouble of writing irreducible representation. So, those provide faithful irreducible representation. So generically reducible representation as the form of a block matrix; so it can be 3×3 , it can be 2×2 , it can be 1×1 and then these entries all have to be zero matrices of corresponding sizes ok. So, this is called a reducible representation in terms of the carrier space those components or those planes do not mix with the other planes.

The vectors in this part of the list do not mix with vectors in that part of the list and vectors here do not mix. So, in terms of this is a 3 entries, 2 entries and 1 entry one component and those do not mix; when it is a reducible representation all right. So now, let us write down a few things little bit in advance what we are going to do next? We will see the important theorems.

(Refer Slide Time: 06:18)



One nice fact is that you can always represent such matrices by unitary matrices and in other words there exists a similarity transformation, if you are stuck with some arbitrary representation which is not looking like unitary matrices you can always do a similarity transformation and make it unitary. If not then there are 2 interesting theorems. These are called Schur's Lemmas and there is some variation in various books in how what they call them, but one of them is certainly the more important Schur's lemma the other one is relatively simple. So given an irreducible representation $\{D^{(d)}(g)\}$; where g are group elements and when I put curly brackets to mean the whole group represented by this set of matrices and d usually denotes the size of the carrier space. So, D is $d \times d$ and g is of course, the group element. So, we usually write it like this and often explicitly display the d in decision D ok.

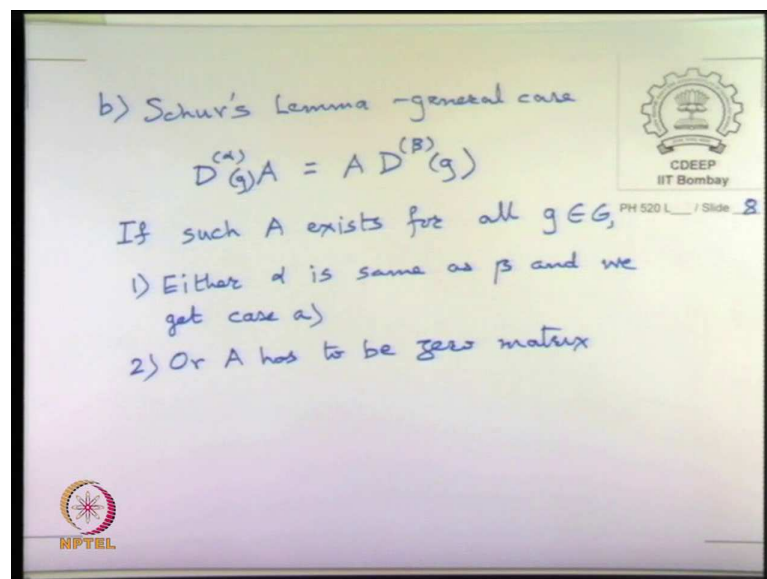
So, we will come to that later what this lemma says is given a particular irreducible representation and if there is a matrix A such that $D^{(d)}(g)A = AD^{(d)}(g)$ for all $g \in G$; then this A has to be proportional to identity times a constant ok. So, this might remind you a little bit about quantum mechanics, but we will come to see it specifically how it applies. The more non trivial lemma that sure proved, so, this lemma looks a little simple simplistic you know you say if a matrix commutes with a every possible matrix in your representation and the representation is irreducible. We know in group theory there is only one element that will commute if for an arbitrary group which is not Abelian. If there is a matrix which commutes with every single matrix I.e. I mean any element that

commutes with every single element; now it has to be a identity because no other element will do it. So, it is now great surprise that A has to be a identity if this is fact for a general group, but a more non trivial lemma which also again looks a bit innocuous, it is really powerful as we will see it later.

Is representation matrices can always be chosen to be unitary and if not if you are ended some representation which does not look like unitary matrices; there will always exist a similarity transformation that will make it unitary. So, there will always exist if this D I am already choosing to be, but it does not matter. So, if $\tilde{D} = \tilde{D}^{-1}$ then there exist S such that $S\tilde{D}S^{-1} = D$; where D is unitary.

But you know my $D = D^{-1}$ and this is for all the g in the group ok. So for all $D(g)$ so the tilde representation which is something arbitrary can always be made unitary by a similarity transformation; so hopefully that I prove before we end today but I am telling you in advance some of the things as preview.

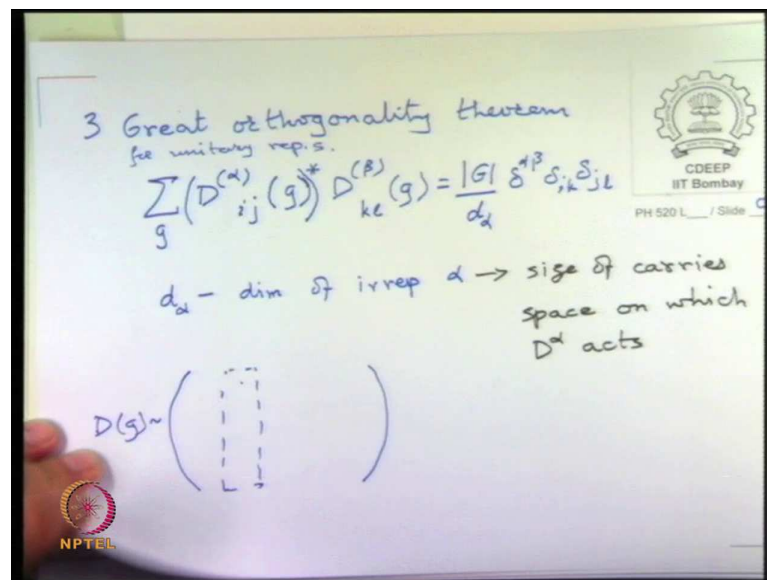
(Refer Slide Time: 14:14)



So, Schur's lemma for the more general case is when is when I have $D^{(\alpha)}(g)A = A D^{(\beta)}(g)$; where α is not necessarily the same rep. So, here I remember I said you have a given representation D , $D^{(\alpha)}$ and I find that given a particular group element D ; its representation matrix D is such that A commutes with it and then this A commutes with all the representation matrices in that particular representation. Now this more general things is suppose I have two different representations $D^{(\alpha)}$ and $D^{(\beta)}$ and there is a matrix

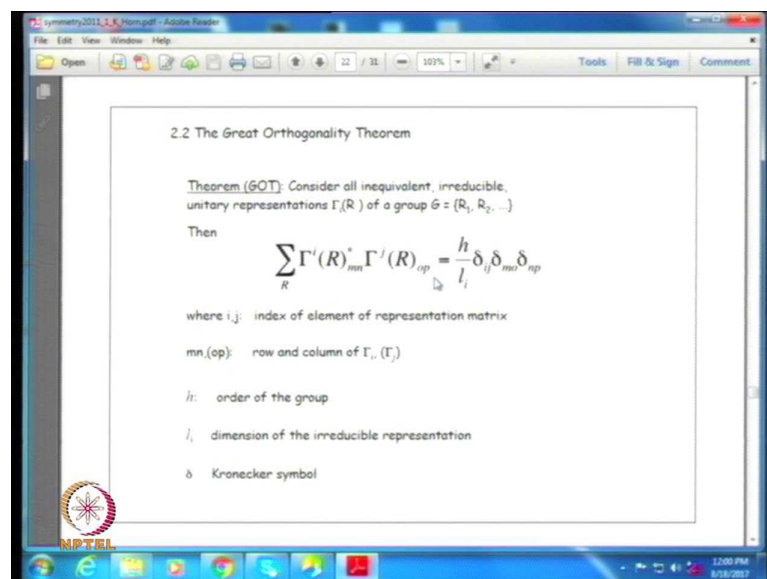
A satisfying this for all g ; then the statement is that either we have to go back to the previous case or A has to be zero. So, we will see this and in more detail later; there is the third fact the third thing which is going to make our knowledge of group theory much more impressive is called great orthogonality theorem.

(Refer Slide Time: 16:53)



Since it is stated here I can in the notation of this these slides uses Γ instead of D .

(Refer Slide Time: 17:16)



So, consider all inequivalent, irreducible unitary representations $\Gamma^{(i)}(R)$ of a group and his all notation is different. So, group g ours we write small g_1, g_2 etcetera. So, sum over

all g of $D^{(\alpha)}(g)$ and $D^{(\beta)}(g)$. So, there is summation over group elements and it could be some two different representations. If you do this then this product this summation over all g will produce a $\delta_{ij} \delta_{mn}$; in the sense that m has to match o , n has to match p and the representation index, the size of the representations also has to match ij and there is a front factor which is order of the group as a whole and divided by the size of the representation over which you are doing this sum in so since anyway l has to be set equal to j it is the common value of l .

So, let me write it in our notation,

$$\sum_g (D_{ij}^{(\alpha)}(g))^* D_{kl}^{(\beta)}(g) = \frac{|G|}{d_\alpha} \delta_{\alpha\beta} \delta_{ik} \delta_{jl}$$

where d_α is the dimension of the representation. I think rest is clear and for this is for the unitary representations.

This is going to be a very powerful theorem, because it says that the matrices in any irrep have to be constrained in this particular way. So, in some sense it is like imposing conditions on all the rows and columns of all the representations, but there is a summation over all g . So, if you have a so, it is some statement of this kind but if I have a $D(g)$ which is looking like this then it is a statement about the column vectors and row vectors in this when I sum over all g and multiply the corresponding elements ok.

So, that is what it is, I have to draw the corresponding $D^{(\alpha)}$ but it is going to be essentially a statement about the representations matching has to be and the row wise and column wise you have to have so and you can think of this summation over g by stacking up all the elements g above it. So, it is a sum of elements of this kind. For finite size representations I am not sure as you know our knowledge will extend to the large number like 6 in and the irreps will be size 3 we what we saw is pretty much what we are actually going to handle, but it illustrates the general things and you can always look up the tables ok. So, now I think I will spend some time proving this theorem that you can always make a representation unitary.

(Refer Slide Time: 22:10)

Theorem: Given any rep \tilde{D} we can make it unitary.

Proof: We need $S \tilde{D} S^{-1} = D$

s.t. $D^\dagger = D^{-1}$

Consider $S^2 \tilde{D} (S^{-1})^2 = S D S^{-1}$

$D^\dagger = (S^{-1})^\dagger \tilde{D}^\dagger S^\dagger = D^{-1} = S \tilde{D}^{-1} S^{-1} \quad (2)$

Claim $S^2 = \sum_g \tilde{D}^\dagger(g) \tilde{D}(g)$

Constructive

Finally we shall take $S = \sqrt{\sum_g \tilde{D}^\dagger(g) \tilde{D}(g)}$

So, the proof is constructive proof. So, we will we are looking for such that $D^\dagger = D^{-1}$. So, we write this statement as consider the statement that $S^2 \tilde{D} (S^{-1})^2 = S D S^{-1}$ and then we write it in the form. So let us write this out first, so $D^\dagger = (S^{-1})^\dagger \tilde{D}^\dagger S^\dagger = D^{-1} = S \tilde{D}^{-1} S^{-1}$.

So, we can rewrite this as a condition on requirement for S; so the construct that works, so now, what we do is that we can rewrite this statement by transferring yes.

(Refer Slide Time: 25:34)

Consider $S^2 \tilde{D} (S^{-1})^2 = S D S^{-1}$

$D^\dagger = (S^{-1})^\dagger \tilde{D}^\dagger S^\dagger = D^{-1} = S \tilde{D}^{-1} S^{-1} \quad (2)$

Claim $S^2 = \sum_g \tilde{D}^\dagger(g) \tilde{D}(g)$

Statement (2): Try $S^\dagger = S$

$S^{-1} \tilde{D}^\dagger S = S \tilde{D}^{-1} S^{-1}$

i.e. need S s.t. $(S^{-1})^2 \tilde{D}^\dagger S^2 = \tilde{D}^{-1}$

... for every g

So, we will make one further assumption that $S^\dagger = S$. So we try to look for S which is Hermitian, then the statement 2 is of the form $(S^{-1})\check{D}^\dagger S = S\check{D}^{-1}S^{-1}$ and therefore, need S such that $(S^{-1})^2 \check{D}^\dagger S^2 = \check{D}^{-1}(g)$ for every g .

(Refer Slide Time: 27:16).

sum $S^2 = \sum_g \check{D}^\dagger(g) \check{D}(g) = S \check{D}^{-1} S^{-1} \quad (2)$

i.e. need $>$.

Then with proposed S^2 , check so-

$$\check{D}^\dagger(g) S^2 \check{D}(g) = S^2$$

$$\Rightarrow \check{D}^\dagger(g) \left(\sum_h \check{D}^\dagger(h) \check{D}(h) \right) \check{D}(g) \stackrel{?}{=} S^2$$

$$\Rightarrow \sum_h \check{D}^\dagger(g) \check{D}^\dagger(h) \check{D}(h) \check{D}(g) \stackrel{?}{=} S^2$$

$$\Rightarrow \sum_h \check{D}^\dagger(hg) \check{D}(hg) \stackrel{?}{=} \sum_h \check{D}^\dagger(h) \check{D}(h) = S^2$$

So, now we have proposed that S^2 is of this form, $S^2 = \sum \check{D}^\dagger(g) \check{D}(g)$. So, let us write some h and write this summation. So, S^2 is so what we do is that we try to convert it into a property for S^2 so take this statement and write it multiply on the left by S^2 and on the right by \check{D} ok. So, this \check{D}^{-1} comes here, this S^2 remains here this is here and $((S^2)^{-1})^{-1} = S^2$. So, this is what we are trying to check.

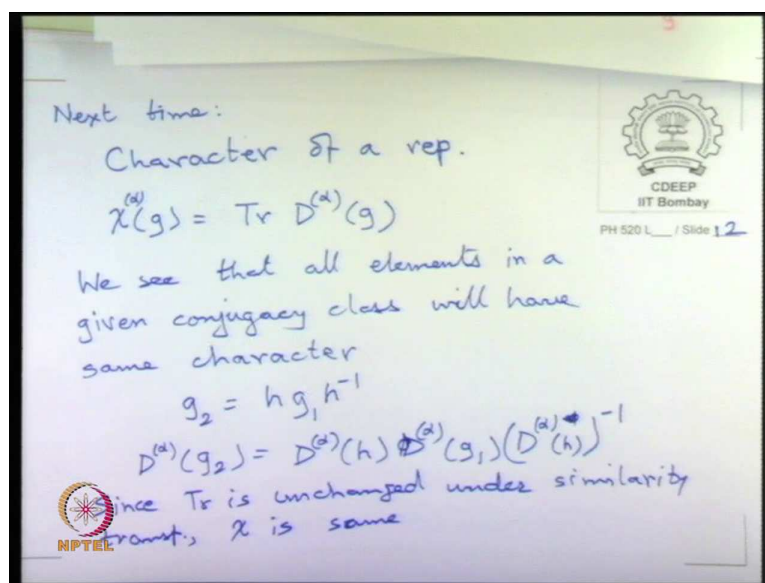
So, question is $\check{D}^\dagger(g)$ and then let us say summation over h and our proposal for this is $\check{D}^\dagger(h) \check{D}(h)$. So, we substituted S^2 and then put $\check{D}(g)$. Now we take the $\check{D}(g)$ inside. So, this is the question, is it equal to S^2 ? And then once we take it inside it become $\sum \check{D}^\dagger(g) \check{D}^\dagger(h) \check{D}(h) \check{D}(g)$. But now remember that as far as the \check{D}^\dagger goes because the representation is as far as this is same as $\check{D}^\dagger(hg) = \check{D}^\dagger(hg)$.

Because this reverse multiplication just produces the corresponding representation of the hg element; applied in sequence. But now all you have to do this is summation about the whole group this h , this summation ran over the all the group elements. This is only relabeling the summation because a constant g is multiplying all of them on the right. So, this is same as $\sum \check{D}^\dagger(h') \check{D}(h') = S^2$ ok. So, if we were given any arbitrary \check{D} all we do is, so this is a constructive proof.

Some proofs in mathematics are such that they give you no clue how to actually carry it out; they just prove the existence, but this actually constructs explicitly for you for what you should do. You take your funny representation \check{D} which is not unitary and just construct this matrix S^2 which is summation over all group elements of their corresponding $\check{D}^\dagger \check{D}$. So finally you can say $S = [\sum \check{D}^\dagger(g) \check{D}(g)]^{1/2}$ are all going to be positive.

So, this is going to be non-trivial matrix and you can take its square root in the sense of the square root of matrix is defined that is not a problem ok. So, long as the determinant is non zero. So, you can take the square root and that is what will work as the matrix that will render any representation unitary. So, this is one of the first theorems and the kind of trick we have used is going to be repeated for other things that will prove.

(Refer Slide Time: 33:38)



So, in closing let me just say the next interesting thing is that the word character when used for rep seems a little strange, but we will later see that it actually represents some characteristics of a molecule. So, that is why probably comes ok.

In mathematical term it is very simple, it is a trace of the matrix of the matrix representing the element. So, character $\chi^{(\alpha)}(g) = \text{Tr } D^{(\alpha)}(g)$. In the representation representing a matrix element g , the character is just the trace of the matrix and one thing we can immediately see that all elements in a given conjugacy class will have same

character. This is because conjugacy relation was that $g_2 = hg_1h^{-1}$ then g_1 and g_2 are in same conjugacy class.

But now we have to write out $D^{(\chi)}(g_2) = D^{(\chi)}(h)D^{(\chi)}(g_1)(D^{(\chi)}(h))^{-1}$, but you remember that under similarity transformation trace does not change. So, the character will come out to be the same ok. So, what was in group theory language some abstract concept of conjugacy classes, in matrix language it is simply similarity transformation and so the character will remain the same.

So, this is we will see that this is an important thing. This is why the number of elements in a conjugacy class is important, they can some and we also know geometrically that conjugacy basically means the same kind of operation done after something else; like the mirror flip is essentially a conjugacy class because everything in it is whether you have rotated ones or rotated twice, the flips you do later or essentially the same things. So the χ_v , $\chi_{v'}$ and $\chi_{v''}$ they will be all in the same conjugacy class.

(Refer Slide Time: 36:47)

Blue boxes: Γ_1 Red boxes: Γ_2

We will learn in a moment that there are three irreducible representations for the group C_{3v} . The third one (Γ_2) consists of the following "matrices" (without proof)

+1 \rightarrow E, C_3, C_3^2 -1 \rightarrow $\sigma_v, \sigma_v', \sigma_v''$

In fact, you can see this χ_v , $\chi_{v'}$, $\chi_{v''}$, the trace is 0 for all of them. So, all 3 are essentially same kind of transformations, they are flips is just that one is around this axis, one is around that axis, one is around that axis. So, geometrically conjugacy class contains elements that do essentially the same thing ok; it is just that they got mixed up through some other transformations earlier like a rotation and then that character will come out to be the same.

The character of these two is equal to -1 . So, at the trace of this is equal to -1 . So, if you include this silly; so this is a reducible representation and in the reducible representation the way we define character so far did not say whether it is for reducible or irreducible.

But I can tell you that when we restrict to irreducible representation it gives a more reliable representation of which conjugacy class you are in and you will find well in fact, in this case because these two add up to 0 ; we are the trace of all these threes $+1$, whereas, trace of these two is actually 0 because, upper is 0 . The trace of the identity element is always equal to size of the representation; because it has ones as many ones as the representation space on which on the carrier space on which is it is acting ok. So, we will stop here today.