

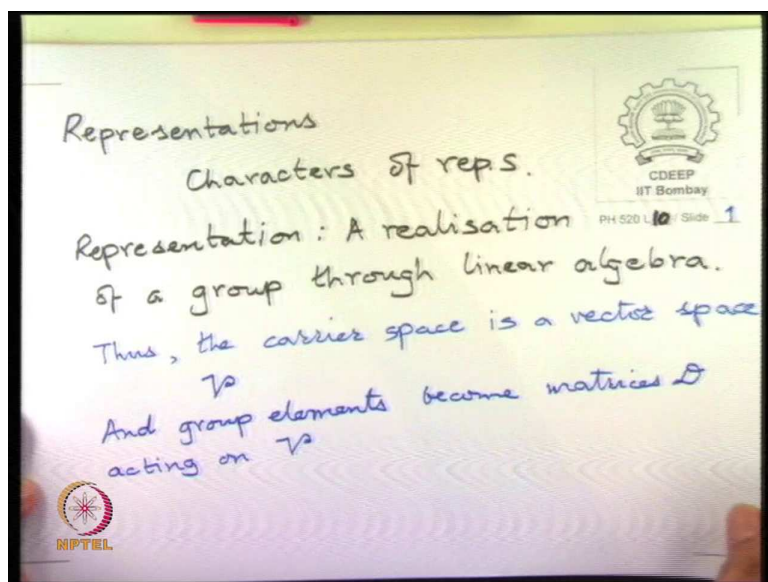
Theory of Group for Physics Applications
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Lecture – 17
Representation Theory – III

So, welcome and we are now moving into the more interesting part of group theory. Where, we learn about representations and we learn a little bit about how it is applied to real systems like molecules. Their the applications are actually extensive molecular physics as well as lattice dynamics, but to lattice dynamics and to condensed matter physics application requires knowing condensed matter physics and lattice structures reasonable well. So, that would really take us out of the main focus of this course.

So, we will stay with the basic methods and the basic concepts and their proves and then apply primary lead to the molecular case, which is a little bit simpler. So, to continue from last time what we are discussing are two things representation and within that characters of representations.

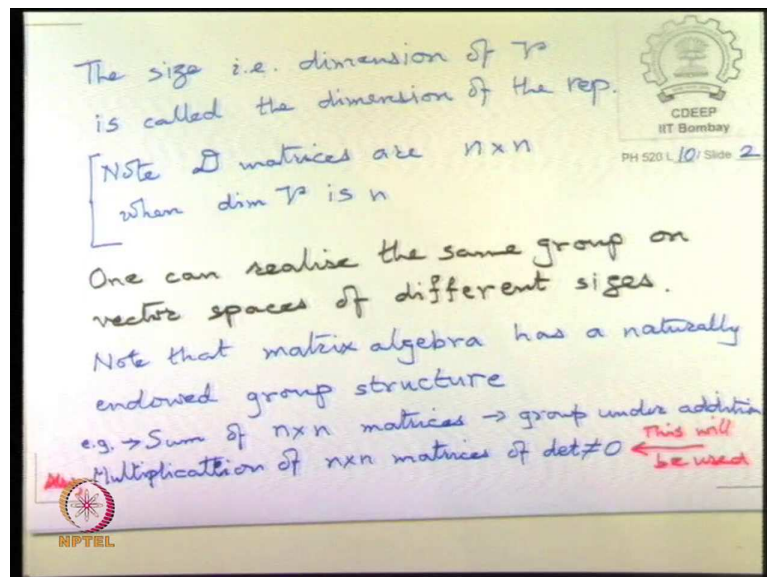
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So, these are the two broad concepts we are progressing on, now last time we had some overview of this, but today we can be a little more formal.

So, we say that; Firstly, a representation essentially is a realization of group operations in linear algebra. This is what it really is what this means is thus the carrier space is a vector space, \mathcal{V} and the group elements become matrices \mathcal{D} acting on \mathcal{V} . The size of \mathcal{V} is called the dimension of the representation.

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So, you can represent on vector space is a different sizes the size or dimension of \mathcal{V} , in the usual vector space sends that is one way of saying it is the number of basis elements require to represent the vector space to represent all the vectors.

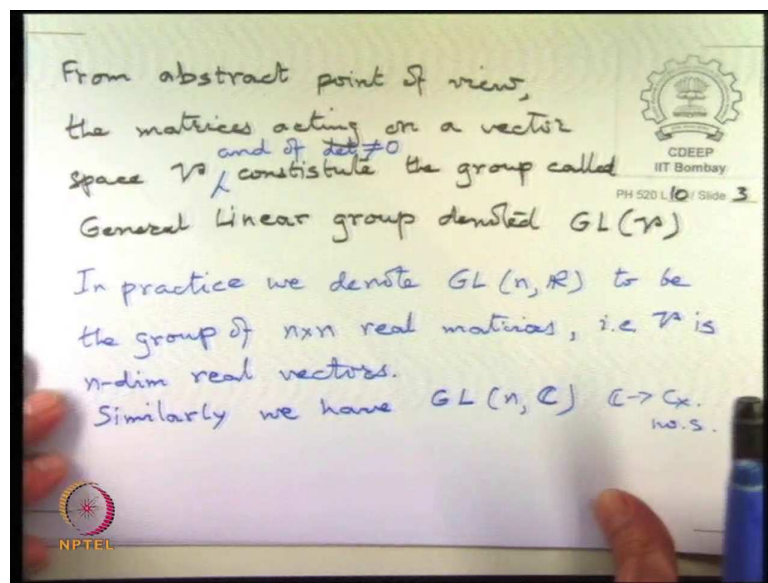
So, the dimension of \mathcal{V} is called the dimension of the representation, this is a little important note matrices $\mathcal{D}^{(r)}$ size $n \times n$, when dimension of \mathcal{V} is n ok. So, at n dimensional representation of a group means that you have $n \times n$ so, actually n^2 is the size of that linear space, but this is the size of the vector space. Now, in general one can represent same group or realize the same group on vector spaces of different size.

So, we will get into a bit of terminology let us also define some symbols. So, symbols to be used are that we already introduce this \mathcal{D} and the \mathcal{V} is the vector space. And the set of matrices, which acts on vector space is called the general linear group ok. So, let us write this down. Note that matrix algebra has a naturally endowed group structure, because I mean even natural numbers have a group structure because you can add things and subtract things. And so, there is some group operation you can identify within your

already existing knowledge of this algebra and here the group structure is that the sum of vectors is a vector and so on sum of matrices a matrices.

So, sum of $n \times n$ matrices is a group under multiple editions, but what we will be using is multiplication of $n \times n$ matrices, which are invertible of determinant $\neq 0$ ok. So, these are the two different types. So, for example, one is this, but the one we will be using is the second one also we have multiplication and that is what we will be using.

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So, we call this set of in the more abstract sense in the linear algebra sense the matrices form a general linear group or the general linear group, acting on a vector space V and well acting on vector space V constitute the group called general linear group denoted $GL(V)$.

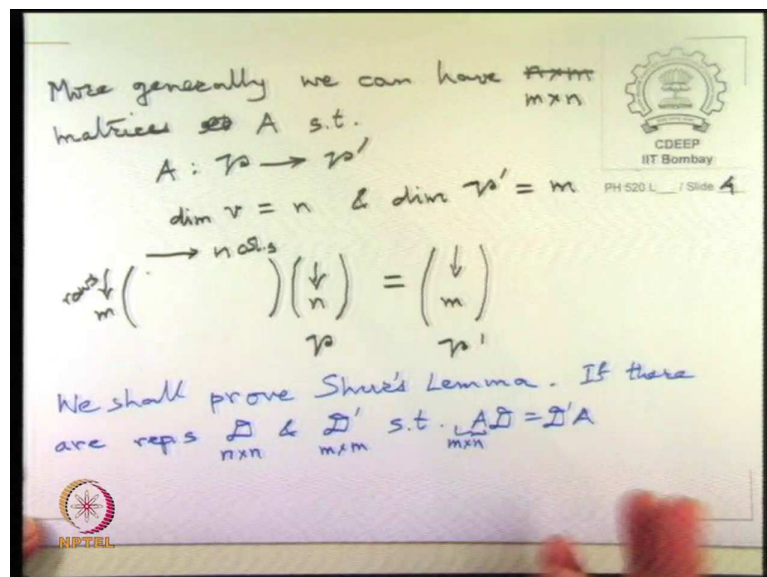
So, there are special cases of this which we use this notation $GL(V)$ we will be using for a short time for 1 or 2 lectures, but in practice we denote $GL(n, \mathbb{R})$ to be the group of $n \times n$ matrices real matrices, i. e the vector space is identified to be n dimensional real vectors. And, similarly we have $GL(n, \mathbb{C})$ here all the entries can be complex all the $n \times n$ metrics entries can be complex and the vector space is likewise complex it has complex components.

So, this will be one of our notations that will be required, when we are dealing with representations, but $GL(n, \mathbb{R})$ has no restriction, you can have things that will have zero

determinants. Then the then the no sorry I am very sorry very sorry take that back, because the inverse will not be defined unless. So, I think we should at that here. So, matrices the of the type I myself get carried a being doing this all the writing. So, we already emphasize that we will be using the second type. So, of determinant $\neq 0$ from abstract point of view matrices and acting on a vector space and with determinant $\neq 0$.

Thank you, otherwise it will not constitute a group. So, here it was. So, we already said that we want only those that have determinant $\neq 0$. So, this is called the general linear group.

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Now, we want to move towards the other notation we use is that the in general you can also have, we can have $n \times m$ matrices, such that A matrices and we denote them a such that $A : \mathcal{V} \rightarrow \mathcal{V}'$. And clearly the by the matrix so, we are switching between the concrete notation of a matrix and a linear operator.

But, the point is that since it acts on \mathcal{V} it must have as many rows as the size of \mathcal{V} . So, if $\dim \mathcal{V}$ equal to so, if it is n it is number of row is n write and $\dim \mathcal{V}' = m$. So, just to not get lost let us draw this. So, I have n entries here this is \mathcal{V} . So, I must have as many columns. So, number of columns must be also n . So, that I can multiply this then the number of row and suppose it produces and m dimensional vector \mathcal{V}' .

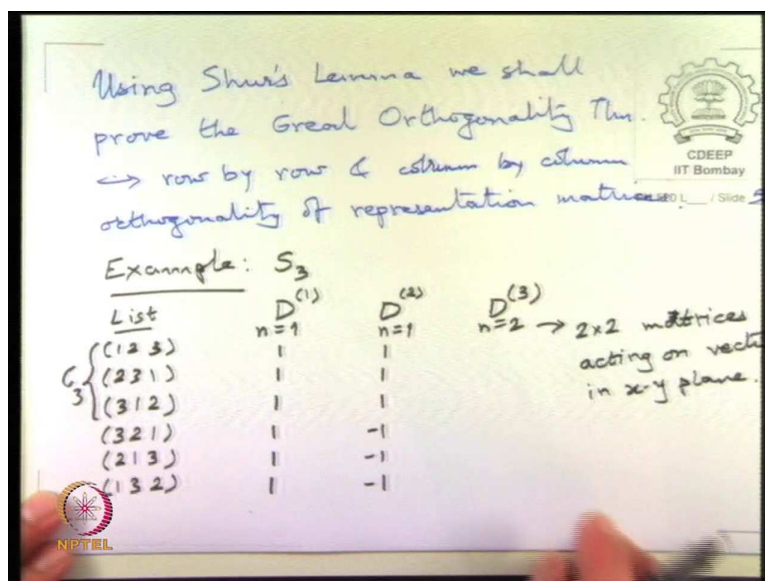
So, the number of rows here n columns such a matrix we call $m \times n$ matrix. So, that is right. So, if we have n dimensional \mathcal{V} and it gets mapped into an m dimensional \mathcal{V}' then the matrix must have m rows and n columns. This we will need for a little while it is not going to be part of major group theory, but in order to prove some important things about representations, that have different sizes we will need this for next 2 lectures. So, we also have operators of this type which map $\mathcal{V} \rightarrow \mathcal{V}'$.

So, before we go on let me just try to do as an interlude because now we are going to do something a little more technical where what we want to next prove is Schur's Lemma, but we will see an example of where we are going after I state Schur's Lemma.

So, next we shall prove Schur's Lemma actually it is such an interesting thing that it is a theorem by itself, but you will see later why it is called lemma because Schur proved it on the way of proving something much bigger. So, we shall prove Schur's Lemma, which basically says that if there are representations \mathcal{D} and \mathcal{D}' such that $A\mathcal{D} = \mathcal{D}'A$ ok. Such that that size of A matches the required $m \times n$ thing. So, \mathcal{D} is let us say $m \times m$ this is $m \times n$. So, just picking from here this means that this is $n \times n$ and this is $m \times m$, then it can take a $n \times n$ matrix if you multiply it by an $m \times n$ matrix.

Then, it will convert it into a $n \times n$ matrix and then that can be multiplied on the right by an $m \times n$ matrix right. So, if there is an A such that it kind of commutes with two representations that converts one representation into the other, then this A has to be trivial or it has to be identity or $\mathcal{D} = \mathcal{D}'$ and A is proportional to identity matrix, where n will be the dimension of that \mathcal{D} .

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So, using this theorem, which we will prove is called the great orthogonality theorem.

The great orthogonality theorem roughly speaking is row by row and column by column orthogonality among representation matrices. Now, a little example and the example is the very exciting one that we have been considering for a while this is the S_3 . Which is just to remind you again two ways of thinking it is either all the permutations of 3 objects, but geometrically it is also the symmetry operations of an equilateral triangle.

Because, you get C_3 if you just rotated, but then if you flip it along the 3 altitudes then you get improper rotations. So, if you include those as well then you get 6 elements and that is what is S_3 and we have been writing out ok. So, we will so, one way to write these elements is to denote them, the list of elements is we write out in the usual permutation way, but I think the space will not be enough well let us just write it once $(2\ 3\ 1)$.

So, this is cyclic permutations and you can see that the cyclic permutations are the usual C_3 elements $(1\ 2\ 3) \rightarrow (2\ 3\ 1) \rightarrow (3\ 1\ 2)$ so, it just rotating the triangle. Now, we do an anti-cyclic permutation. So, we say $(3\ 2\ 1)$. So, that becomes anti cyclic and then cyclic permutations of the anti-cyclic form also work, I hope that already has $(1\ 3\ 2)$ ok. So, the first 3 form a proper subgroup which is just C_3 I can write it on the left hand side there is space here forms just the subgroup C_3 and then these involve flips. Now, what the next thing we do is write out the representations for this.

So, one thing that I should have talked about in the generalities is faithful versus unfaithful representation which emerges now. So, consider a representation D of size 1 ok. So, actually this is 1 is label and it is I think at the or here we write it is size $n = 1$ ok, that is where I represent all elements by 1.

So, this is the trivial representation, which is available for every single group – discrete, continuous whatever you have. Now, this does not look like a very exciting representation because it is mapping every operation into one of course, under multiplication any group multiplication table will be satisfied.

So, that is a very silly way, but it turns out that like we have 0 in addition this representation anchors all the irreps ok. So, the representation is irreducible, completely unfaithful, it is not homomorphic, it does not preserve the formalities homomorphic, but it is it kills the information detailed information about the group. So, such a representation is called unfaithful. So, there is another representation also of size 1.

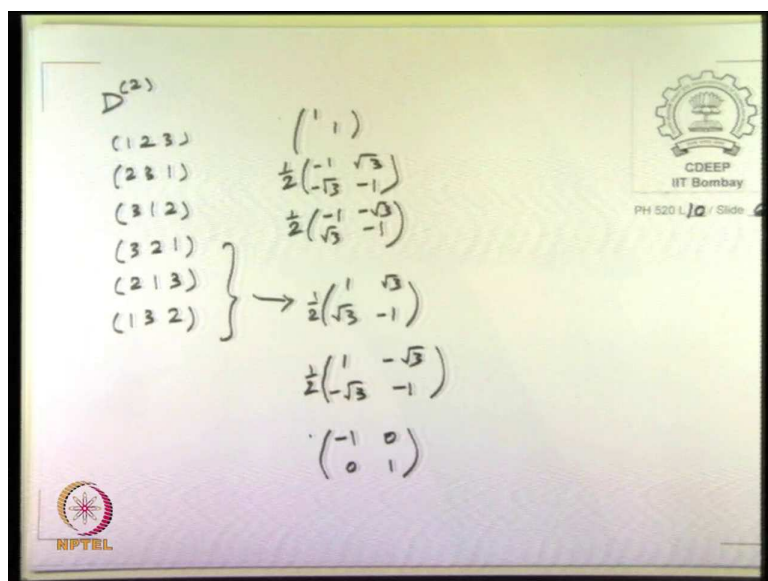
So, the other representation is also 1 dimensional where you put all the proper rotations has +1s and all the improper rotations has -1. So, 1 1 1 1 and -1 -1 and -1, the reason why this works is you remember that if you do an improper rotation, which amounts to say flip, but if you flip twice not necessarily are about the same altitude, but even some other altitude if you flip the triangle twice then it will come back to a form which can be got by simple rotations.

So, product of any two of these will give you this and product of these by themselves from a group. So, this 1 1 and 1 is effectively that trivial representation of C_3 and the other elements of S_3 , which are improper rotations get represented by -1 and then they have the correct property.

And the other representation you can think of is the 2×2 representations, which are the

$3\pi/2$ rotations and the improper ones, $\begin{bmatrix} 1 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -1 \end{bmatrix}$ and those. These are the 2×2 matrices acting on vectors in xy plane.

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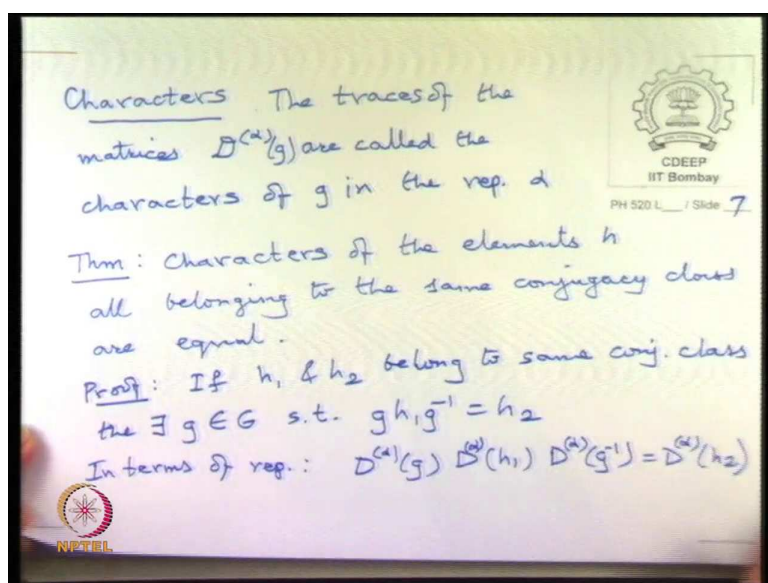


So, let us write those down. So, the D_3 for the same list but the this one is just $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, then

the next one is $\begin{bmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{bmatrix}$. And the next one is $\begin{bmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{bmatrix}$, then for these we start with one

of them gone improper. So, these are $\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{bmatrix}$ and so on. So, there is a 2×2 representation of all these operations like this.

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Now, we defined the character of a representation, the trace of matrices. The traces of matrices $D^{(\alpha)}(g)$ are called the characters of g in the representation α .

Now, the main consequence of this is that the characters of matrices belonging to the same conjugacy class are all the same ok. So, result or theorem are equal this is because if h_1 and h_2 belong to same conjugacy class or conjugate to each other same thing. Then there exists $g \in G$ such that $gh_1g^{-1} = h_2$, but now we in terms of a representation this would mean $D^{(\alpha)}(g) D^{(\alpha)}(h_1) D^{(\alpha)}(g^{-1}) = D^{(\alpha)}(h_2)$.

But, we know that the $D^{(\alpha)}(g^{-1}) = (D^{(\alpha)}(g))^{-1}$, this is because you have to get identity matrix out of this multiplication. So, if it is the inverse this is because $D^{(\alpha)}(e) = I_{n \times n}$ for α n dimensional. So, if the representation α is n dimensional then identity matrix has to be represented by the identity matrix of that size.

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are equal. ... belong to same conj. class

But $D^{(\alpha)}(g^{-1}) = (D^{(\alpha)}(g))^{-1}$

This is because $D^{(\alpha)}(e) = I \leftarrow \begin{matrix} \text{for } \\ (\alpha) \\ n \times n \end{matrix}$

$\therefore D^{(\alpha)}(g) D^{(\alpha)}(h_1) (D^{(\alpha)}(g))^{-1} = D^{(\alpha)}(h_2)$

$\therefore \text{Tr}(D^{(\alpha)}(h_1)) = \text{Tr}(D^{(\alpha)}(h_2))$ Thus proved

Using $\text{Tr}(ABC) = \text{Tr}(CAB)$

$\sum_{i,j,k} A_{ij} B_{jk} C_{ki} = \sum_{i,j,k} C_{ki} A_{ij} B_{jk} = \text{Tr}(CAB)$

Thus $\text{Tr}(ABA^T) = \text{Tr} B$

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And therefore, the inverse of a particular group element has to be represented by the inverse matrix of that group element ok.

Therefore, coming back to this now we take trace of both side of $D^{(\alpha)}(g) D^{(\alpha)}(h_1) (D^{(\alpha)}(g))^{-1} = D^{(\alpha)}(h_2)$. So, if we take trace, then $\text{Tr}(D^{(\alpha)}(h_1)) = \text{Tr}(D^{(\alpha)}(h_2))$ because under trace you can cyclicly rotate the matrices. And so, you can bring the $(D^{(\alpha)}(g))^{-1}$ to this side $(D^{(\alpha)}(g))^{-1} D^{(\alpha)}(g) = I$, so, it will become right.

Using, $\text{Tr}(ABC) = \text{Tr}(CAB)$ everyone knows this yes, if not I will write it here it is a 1 line proof. Because note that this is same as what is the matrix $ABC = \sum A_{ij}B_{jk}C_{ki}$, but once it is tied up like this it is equivalent to $\sum C_{ki}A_{ij}B_{jk}$ correct. So, we have suppress the explicit statement of summation, but we can put it in if you like. So, then it is also explicit that there is no commutativity issue these are just numbers and there is a big summation over i, j and k . And so, this is just visually to help us to bring C here, but once brought here we can think of this as $\text{Tr}(CAB)$ ok.

So, because of this $\text{Tr}(ABA^{-1}) = \text{Tr}(B)$ right, which is what we have used. Therefore, all elements belonging to the same conjugacy class have exactly same character so, thus proved.

But, as an appendix we just say that this is the property we have used; So, now, to go back to our example.

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rove the Great Orthogonality Thm. CDEEP
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→ row by row & column by column
orthogonality of representa

Example: S_3

List	$D^{(1)}$ $n=1$	$D^{(2)}$ $n=1$	$D^{(2)}$	
(1 2 3)	1	1	(1 2 3)	$\begin{pmatrix} 1 & 1 \\ \frac{1}{2}(-1 & \sqrt{3}) \\ \frac{1}{2}(-1 & -\sqrt{3}) \end{pmatrix}$
(2 3 1)	1	1	(2 3 1)	
(3 1 2)	1	1	(3 1 2)	
(3 2 1)	1	-1	(3 2 1)	$\left. \begin{matrix} (2 1 3) \\ (1 3 2) \end{matrix} \right\} \rightarrow \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
(2 1 3)	1	-1	(2 1 3)	$\frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$
(1 3 2)	1	-1	(1 3 2)	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

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So, returning to our example we have these representations. So, we see that we can calculate characters of our representation the characters in this case are trivial traces of 1×1 matrices are the values themselves. So, the trace of everything here is 1. Then the so, that at least ensures that everything in the same conjugacy class is the same. Here the trace of the 1 is connected to identity by usual rotation are all 1.

But, the trace of the improper rotations are all -1, but at least there all similar and remember the idea of conjugacy was that essentially asides from a change of basis; a conjugacy element does the same thing that another member of the same class does. So, these three which are essentially flips the either flip around the vertical what is altitude or the once that are cross like this, but there all flips. So, geometrically they have the same operation and you can rotate one into the other.

But, just doing that rotation does not change it is character in this sense it is its character; it is like it is property. So, the character of these three remains the same and therefore, they have the same character -1. The more interesting thing is the characters of these and we can write so, the letter use for character is χ .

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D_3		$\chi^{(3)}$
(1 2 3)	$\begin{pmatrix} 1 & 1 \end{pmatrix}$	2
(2 3 1)	$\frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$	-1
(3 1 2)	$\frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$	-1
(3 2 1)	$\left. \begin{matrix} \rightarrow \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \\ \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \\ \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \end{matrix} \right\}$	0
(2 1 3)		0
(1 3 2)		0

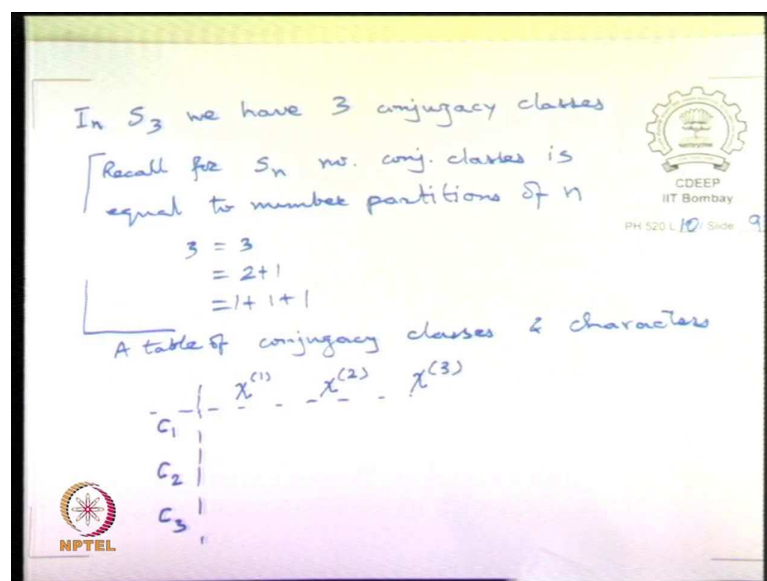
So, $\chi^{(2)}$ values here are 2 then this is equal to $-1/2 - 1/2 = -1$, this is -1 and then these if we see we will add $1/2$ and $-1/2$ so, 0 0 and 0. So, the character the character of these group elements in the representation, which we have called D_3 because 2 is that one with flips signs D_3 .

So, D_3 : the character of identity is 2, the character of these two which are proper rotations is -1 and -1. So, these two remember that the identity is always in it is own conjugacy class, because $gh_1g^{-1} = h_2$, but if h_1 happens to be identity then gg^{-1} will always give identity.

So, identity is in its own conjugacy class. So, this is by itself, it has character 2. These two are in the same conjugacy class because they are essentially proper rotations by hundred and twenty degrees and they have the same character, that character turns out to be -1 in this representation and all these improper guys have the same character which is 0 ok.

So, we can now create a table which is somewhat like a multiplication table, but now only of the characters.

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In S_3 we have 3 conjugacy classes

Recall for S_n no. conj. classes is equal to number partitions of n

$$3 = 3$$

$$= 2 + 1$$

$$= 1 + 1 + 1$$

A table of conjugacy classes & characters

	$\chi^{(1)}$	$\chi^{(2)}$	$\chi^{(3)}$
C_1			
C_2			
C_3			

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We have the class of character we have 3 character classes and how do we know this there is also a theorem recall for S_3 for S_n number of conjugacy classes is equal to the number of partitions of n , this theorem we proved by writing the notation in terms of cycles, through cycle notations we check this.

So, here we have $3=3=2+1=1+1+1$. So, there are three ways of partitioning 3 and therefore, the root should be 3 independent conjugacy classes, which we also see directly in terms of this list because they split up like this. So, clearly there is this conjugacy class this and this.

So, we denote the conjugacy classes by C and then write out their characters. So, in the vertical column we write C_1 , C_2 and C_3 . So, in other words we label the rows by the

character class or the conjugacy class and here we write the character of the corresponding representation so, $\chi^{(1)}$, $\chi^{(2)}$, $\chi^{(3)}$.

So, just to repeat what we are doing is instead of writing the big table I could write this table ok, which generates some generic list, some generic way of writing out the elements. And then for each element in three different representations I write out their matrix representations full-fledged.

In principle I could have returned some D_4 , some D_5 etcetera whatever, but I could create a gigantic table or a gigantic list of what is a group element and which matrix it is represented by, but what we find is that from geometric point of view it is only the character that matters.

So, instead of listing all the group elements we only list the conjugacy classes C_1 , C_2 and C_3 and instead of listing the entire matrix representation we simply write the character of that characteristic class in that representation. So, we can read back and write down what the characters of first two. So, by the way this is the C_3 , you know it is that represented the cyclic group of size 3.

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Example: S_3

List

C_3 { (1 2 3), (2 3 1), (3 1 2), (3 2 1), (2 1 3), (1 3 2) }

$D^{(1)}$ $n=1$

$D^{(2)}$ $n=1$

$D^{(3)}$ $n=2 \rightarrow 2 \times 2$ matrices acting on vectors in x-y plane.

A table of conjugacy classes & characters

	$\chi^{(1)}$	$\chi^{(2)}$	$\chi^{(3)}$
C_1	1	1	2
C_2	1	1	-1
C_3	1	-1	0

Anyway unfortunately in books the mix up all the symbols anyway. So, it does not matter and from contexts you know which is which. So, I have called here the conjugacy

classes C_1 , C_2 and C_3 . The conjugacy class of 1 is the identity and for identity we know the character of this and this is just 1 and 1.

And then in the representation number 3 the character or the trace was equal to 2, then this remains 1 and 1 boringly nothing changes. And here for this we see that these two which form the class C_2 both have character just 1 and this has character -1.

This conjugacy class has character -1 of improper rotations. And finally, we can write out these happen to have 2 and then because the diagonal elements were cosines of hundred and twenty degrees adding them we got -1. So, this is -1 and the character of this is 0. Now, we claim that it is not necessary to build any bigger table, for most at least the molecular physics applications it is actually sufficient to just know the conjugacy class table and not the big multiplication table or the big matrices themselves.

Also, how do you know how many representations you should take well it we will prove that there are no more irreducible representations? So, these are all the reducible irreducible representations there are for S_3 and these are all the conjugacy classes there are for S_3 . This fact followed from our theorem about partitions that there are only 3 of these.

It also turns out that there are only exactly as many irreps as their a conjugacy classes, which is something to be proved later ok. But, so, this example makes it graphic what we are talking about and the fact that this is all that you will in general need to understand or split up the vibrations of a molecule and relative intensities of lines and so on.