

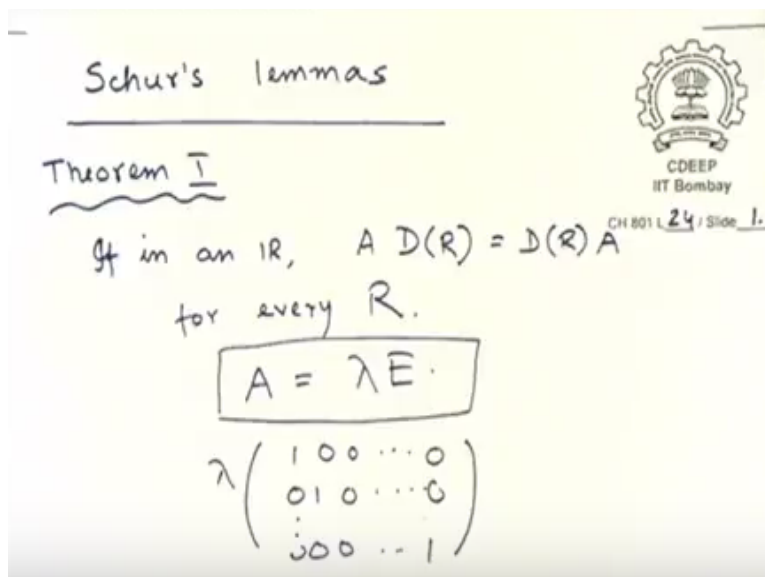
Symmetry and Group Theory
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Lecture - 66

Derivation: Great Orthogonality Theorem - I (Schur's Lemma 1)

What we do is we learn how to derive the great orthogonality theorem. And there also I will leave something for you to figure out.

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See we have used great orthogonality theorem for at least 50% of our course, right? But the reason why we need so much of matrix algebra at the beginning was to do what we do today. We just do not want to use great orthogonality theorem like a black box. We also want to know where it came from. As we will see today, it actually came from a very basic matrix algebra and a lot of manipulation is there but then you people are masters of manipulation anyway.

You know very well when, will have to be multiplied by something and take inverse, let it become C and all that. I think you would be much more comfortable with this than I am at this stage. So before getting on to great orthogonality theorem, the actual part of it, we need to go through what are called the Schur's Lemmas. Schur is the name of a mathematician. What is a Lemma? What was that? Does it have a proof now?

That is an axiom yes. Lemma can be proved as you will. We are going to prove them. So did you follow this Mangalyaan thing, the Mars mission. So in Mars mission or any such space mission they have a big rocket right and along with that they also have some subsidiary rockets, booster rocket and all that, right? So Lemmas are to theorem what booster those subsidiary rockets are to the main rocket.

So lemmas are small theorems that we need to prove, not because they themselves give us some very great intuition but because they help you solve a bigger theorem, okay. So they are something that come in the way. Actually, it must have been the other way. Somebody tried to work out great orthogonality theorem, got stuck. So then you know took a break, worked this out and then went back.

In our case, since we have the benefit of hindsight we are going to work out the Lemmas and then get on to great orthogonality theorem, okay. And they, if you just look at them, they seem kind of innocuous to start with. So there are 2 such theorems. Theorem no. 1 is this and once again please do not memorize anything. Just try to follow. I will, going to ask questions where if you have followed what we have done here you will be able to work out.

There is no need to memorize each and every step. When I was an M.Sc. student the guy sitting next to me in exam started poking me during the exam. He says I know everything just tell me where to begin. He has memorized the entire notes of the year. He just does not know where to start. So once he starts he can go on and on and on. So do not do that, it does not make sense, okay. So this is what theorem 1 is.

So suppose we are working with an irreducible representation. So in irreducible representation what do we have, we have matrices like this. By the way, I have gone back to Bishop's book okay, Bishop's book. What is $D(R)$? Yes. Yeah, but what kind of matrix, what is R ? It is a transformation matrix. $D(R)$ is a transformation matrix corresponding to the symmetry operation R . So what we are saying here is if in some IR we have a matrix which commutes with $D(R)$.

What is the meaning of commutation? Yes. So suppose we have $AD(R) = D(R)A$, now where did the B come from? $AD(R) = D(R)A$ for each and every symmetry operation R. A is a matrix. Let us say A is a matrix which commutes with the transformation matrices of a particular irreducible representation, all the transformation matrices then we are going to prove that this A is lamda into E. What is E? Eigen value? Identity matrix.

And lamda multiplied by E, what kind of matrix is that? Diagonal. What it has another, again among diagonal matrices this is a special kind of matrix. Lamda multiplied by E. What is this matrix called? What will be the value? All the diagonal elements are lamda is it not? It is called a constant, constant matrix, okay? So Dola while you are not there we have changed the date of the exam. It is going to be on a Sunday, 16th okay? Alright. It is a constant matrix, right?

So what we are saying is that in a irreducible representation if there is a matrix that commutes with each and every transformation matrix of that representation then it has to be a constant matrix. That is what we are going to prove. Why are we going to prove this because it turns out to be handy later on when we try to prove great orthogonality theorem. But is the theorem clear to all of us. This is what we need to understand.

If $AD(R) = D(R)A$ in an IR then $A = \text{Lamda } E$. That is what we want to prove, alright? I have created some degeneracy. Okay, let us see. How do we go ahead? We go ahead by doing a similarity transformation. We want to simplify the problem, okay.

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Let $Z = X^{-1}AX$ be diagonal

$$D'(R) = X^{-1}D(R)X$$

$$ZD'(R) - D'(R)Z$$

$$= X^{-1}AX \underbrace{X^{-1}D(R)X} - X^{-1}D(R)X \cdot \underbrace{X^{-1}AX}$$

$$= X^{-1}A \cdot D(R)X - X^{-1}D(R) \cdot AX$$

$$= X^{-1} [A D(R) - D(R) A] X$$

$$= 0$$

$$P = \boxed{ZD'(R) = D'(R)Z}$$

$$\boxed{P_{ij} = ?}$$

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And what we do is we say let z be x inverse AX and let this z be a diagonal matrix. Diagonalization is usually the first step of any problem that has got to do with matrices because the moment you diagonalize life becomes much simpler, right? Of course, here it is apparently if you go look at the theorem we believe that this matrix is diagonal already, right? Constant matrix is λ into V .

So in any case we believe that it is diagonal but there is no harm in doing a similarity transformation on that also. Suppose we take E and do a similarity transformation what do we get? We discussed this long ago when we were talking about group theory. We get back E is it not? So similarly, you take a diagonal matrix, do a similarity transformation there is no issue, okay. But now, suppose I perform the same similarity transformation on the transformation matrices. $D \text{ dash } R = X \text{ inverse } D(R)X$ okay. Should this cause diagonalization?

I am using the same matrix X or even if I do not write the first line, what I am saying is $D \text{ dash } R = X \text{ inverse } D(R)X$ and $D(R)$ are the transformation matrices in an irreducible representation. So my question is should $D \text{ dash } R$ be a diagonal matrix or even a block diagonal matrix. $D \text{ dash } R$, should it be a diagonal matrix or a block diagonal matrix or none of the above if $D(R)$ represents the symmetry operation, the transformation matrix corresponding to symmetry operation of R in an irreducible representation.

It cannot be diagonal or block diagonal. Why because see that is what why you are saying irreducible representation all the time? If $D(R)$ is the matrix corresponding to an irreducible representation then you cannot diagonalize it further is it not? It is as good as it gets. Understand what I am saying. It cannot, so D dash R cannot be diagonal or block diagonal because you have already reached the smallest unit in $D(R)$ itself.

Do not forget $D(R)$ are the matrices in a, an irreducible representation. You should not be able to reduce it any further. Is that point clear? Because that is what we are going to need a little while later, alright? Agreed? Fine. Let us get ahead. Next is very simple, okay? What did I say? I said that A and $D(R)$ commute with each other. Let us see if Z and D dash R will also commute with each other, okay? Let us see. $Z D$ dash $R - D$ dash $R Z$ is equal to what?

What is Z ? X inverse AX is it not? So X inverse AX and what is D dash R ? X inverse $D(R)X - X$ inverse $D(R)X$. X inverse AX . We have reached something that is very convenient. Why? Because here you are multiplying X with X inverse, right? So that becomes E . So this becomes X inverse $A D(R)X - X$ inverse $D(R)AX$. So similarity transformation plus similarity transformation is equal to similarity transformation of the sum.

So I can write it like this. X inverse $A D(R) - D(R) AX$. This step are we all okay, Anchal. Yes, sure. All you have to do is start from here and expand. You see we will reach here, okay? Now what is this? $A D(R) - D(R) A$? That is 0 because A and D are commute. So if you take a similarity transformation of 0 what do you get? Unless it is a creation operation it has to be 0. There is nothing right? And you create. You act like Brahma or God.

God said let there be light and there was light. So unless you can play God you cannot take 0, perform a similarity transformation and get something that is not 0, okay? So $Z D$ dashed $R - D$ dashed $R Z$ that is also equal to 0. Or in other words Z and D dashed R commute with each other, alright? What are we trying to prove? We are trying to prove that A is a constant matrix. We are not there yet.

But what we have done so far is that we have proven that these similarity transformations that we generated they are also commuting with each other, right? So now what we will do is we are going to talk about symmetry, not symmetry sorry matrix elements. So it does not matter if you multiply Z by D dashed R or you multiply D dashed R by Z you get a third matrix, right, the product.

So let us say I call it the product matrix P . By using the rules of matrix multiplication, can you tell me what will be the expression for P_{ij} ? The ij th element of matrix P . What will it be? AB?

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$$P_{ij} = \sum_{k=1}^n z_{ik} D^i_k(R) = \sum_{k=1}^n D^i_k(R) z_{kj}$$

Z is a diagonal matrix.
 $z_{ik} = 0$ unless $k=i$
 $z_{kj} = 0$ " $k=j$

$$z_{ii} D^i_{ii}(R) = D^i_{ii}(R) z_{jj}$$

$$\underline{D^i_{ii}(R)} [z_{ii} - z_{jj}] = 0$$

$z_{ii} = z_{jj}$

So will you let me write it like this P_{ij} is equal to it is $Z D$ dashed R is it not? $Z D$ dashed R and I want I here. So will you let me write iP and then what will be the matrix element of D dash R ? Okay, let me write ik , $P I$ will use later, ik and kj . And then sum over what, k , 1 to n . And that will be equal to, if I write it the other way round, I can write it the other way round also, right? So I can write D dashed $ik R Z kj$ sum over $k = 1$ to n .

Are you all comfortable in writing matrix elements like this using the subscripts? Are you all okay with this? I am sorry? Yeah, it is symmetry after all, everything is symmetry. Is this right? What do I do next? Do I know anything about one of these matrices Z or D that can help me with my problem? What do you know about Z ? It is a diagonal matrix, right? Remember what we said. We had said that let $Z = X$ inverse AX be a diagonal matrix.

So given whatever matrix A I have I am going to choose my X in such a way that Z has to be a diagonal matrix, right? So that is what is going to make my life a little easier because Z is a diagonal matrix. And since there is a diagonal matrix, I can write that $Z_{ik} = 0$ unless $i = k$; $k = i$ is what I will write because k is the variable right; i is a constant as far as this step is concerned. And Z_{kj} is also 0 unless $k = j$, right? Right or wrong?

So just put in these values then there is no summation? Summation is gone, right? If I work with one value of i then I am going to add over all i 's, that is a different issue. But for one value of i , the summation signs are going to vanish and I will be left with $Z_{ii} D_{ij} R_{is} = D_{ij} R_{is} Z_{jj}$, right? And see the magic has happened already. What has happened is, on the left hand side, you have D_{ij} . On right hand side also you have D_{ij} is it not?

But on the left hand side you have Z_{ii} , on the right hand side you have Z_{jj} . So let me collect all the terms on the left hand side. I have i th element of D dashed R multiplied by $Z_{ii} - Z_{jj} = 1$, right? 1 or 0? Sure? Okay, I believe you. Now, can this be equal to 0? Why not? What is the meaning of general element? Yeah, but then it may not be equal to 0 when $i = j$. But a better argument is that how did we generate this D dashed matrix?

By the similarity transformation of $D(R)$ right? Now $D(R)$ belongs to irreducible representation and similarity transformation takes you from one representation to another equivalent representation. So you will get another irreducible representation. It will never make it reducible, right? And as we discussed at the beginning of the class, since it is an irreducible representation, you cannot, this cannot have become diagonalized all of a sudden, okay? Fine. So this is not 0.

You cannot say that this is always 0. So then all we are left with is $Z_{ii} = Z_{jj}$. What does that mean? All the diagonal elements are the same; i goes from 1 to n ; j also goes from 1 to n , right? All these are equal to each other or in other words $A = \lambda E$. That is what we wanted to prove. All the diagonal elements are the same and in any case we have performed a similarity transformation that has diagonalized the matrix. Actually, $Z = \lambda E$ is what comes out, right? But then from there it is not very difficult to go to $A = \lambda E$.