

Symmetry and Group Theory
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Lecture - 68

Derivation: Great Orthogonality Theorem - III

Okay, got it? He got it. It is got right? Got is got, alright. Now I will write great orthogonality theorem for you and then I expect some comment, right? I will just write it down.

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GOT

$$\sum_R D_{ik}^\mu(R) D_{mj}^\nu(R^{-1}) = \frac{g}{n\mu} \delta_{\mu\nu} \delta_{ij} \delta_{km}$$

(i) $A = \sum_S D(S) \times D(S^{-1})$

To prove: $A \cdot D(R) = D(R) \cdot A$ for all R .

$A = \lambda E$

Sum over R $D_{ik}^\mu(R) D_{mj}^\nu(R^{-1}) = \frac{g}{n\mu} \delta_{\mu\nu} \delta_{ij} \delta_{km}$. it is a little different from what we have written earlier is it not, right? So my question to you is not now, try and work out whether they are equivalent or one is a subset of the other? What do you think? What we have written here is it going to be the same as what we have written earlier or is it going to be a subset or a superset. Which one is a superset?

This is a subset, right because here we are talking about R and R inverse. There we had talked about all Rs. So now my question to you and this is a homework problem is can you get from here to there? So everybody has studied second law of thermodynamics, right? There are two statements is it not? Kelvin-Planck statement and Clausius statement and it is very common to ask can we prove that these two statements are equivalent to each other. Sujitha is amused.

See here also I want you to figure out by yourself, I am not going to help you in this, whether they are equivalent or not, okay, fine. Let me see how far we can go in proving this. I suspect that I am going to run out of patience towards the end and then run through it quickly, at least let us begin, okay. What are these? μ and ν once again are two different nonequivalent IRs. Yes, what had we written earlier? H by l_i , right?

Earlier we had written that the order of the order is H and l_i is dimensionality. So n_μ , it is not just n . n subscript μ . It is just that my handwriting is not great. So g is the order and μ is the dimensionality, okay. So let us see. Of course there are many deltas and all, but do not be afraid. How do you think we are going to reach the deltas? Can anybody make a guess? We have been talking so much about matrices, how do you think we are going to reach the delta?

Yes, think of unit matrix to start with. So is it not unit matrix made up of Kronecker delta, right? δ_{ij} is it not. When $i = j$ then it is 1. When i is not equal to j then it is 0. So that is how. That is how and that is why we needed to develop that concept of A . Why because A , what is A ? $A = \lambda$ into E , right? λ into E means you have something that comprises of deltas everywhere.

Now do you understand the relevance why out of the blue we had to derive all these two lemmas and all. Because we want to formulate our problem in such a way that we are going to have unit matrices. When we have unit matrices then we have a very binary situation 1 or 0 right when $i = j$ then it is going to be 1 otherwise it is going to be 0 and then when you have this 1 0 situation then once again you can relate it very conveniently to a set of orthonormal vectors, okay? That is why we develop this concept of A all this while.

That is what I want you to understand. Rest of the mathematics, you are much better than me to work out, okay? If you have understood this far I might as well step down. Any one of you can come and do the remaining derivation, it is not all that difficult. But it is important to understand why out of the blue we invoke this matrix A which is a constant matrix, okay? Because that is going to lead us to the orthonormal set of vectors, okay?

Now, with that background let us be brave and tackle the problem. It is not all that difficult any more, okay. Now, so this has to be done in two parts actually. In the first part, I am going to develop this matrix $A = \sum_s D(s) X D(s)^{-1}$ and what I want to prove is that $A D(R) = D(R) A$ for all the symmetry operations. Understand what I am doing?

I am going to write this matrix, $\sum_s D(s) X D(s)^{-1}$ and I am going to prove that this matrix commutes with all the transformation matrices that are there. Understand what I am saying, right? And how is that going to be helpful? If this commutation is there, how is it going to be helpful? Do not have such short memories. What happens when a matrix commutes with all the transformation matrices in an irreducible representation?

Then that matrix is a constant matrix no? Why do you think I have written A? Is the same A, otherwise I would have written x or p or q or z, okay? This A is going to be λI and the moment we reach E, see what I have, this A itself is a summation, right? Summation over all symmetry operations. I am summing over all symmetry operations, okay. So that is going to be something like 0 1 orthonormal vectors, okay?

But let us first prove whether this is correct or not. What I want to prove is A commutes with all the $D(R)$ s. Do not forget what A is. It is $\sum_s D(s) X D(s)^{-1}$.

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$$\begin{aligned}
 D(R)A &= \sum_s \underbrace{D(R) D(s)}_{D(T)} X \underbrace{D(s)^{-1} D(R)^{-1}}_{D(T^{-1})} D(R) \\
 &= \left\{ \sum_T D(T) X D(T^{-1}) \right\} D(R) \\
 &= A \cdot D(R) \\
 \boxed{A} &= \lambda E \\
 X &= \begin{pmatrix} 0 & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots & & \vdots \\ 0 & 0 & \dots & 1 & \dots & 0 \\ \vdots & \vdots & & \vdots & & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 \end{pmatrix}
 \end{aligned}$$

$X_{ij} = 0$
 unless
 $i = k$
 $j \geq m$
 $X_{km} = \lambda$

So let us see. What is $D(R)A$? Can someone help me? Expand. Write down the expression of A and tell me. I will help you a little bit. Sum over s . That is easy. What is A ? What was the definition of A . Sum over s $D(s) X D(s)$ inverse and I am left multiplying it by $D(R)$. So what should I get? Opposite? No, do not expect such fast results. What is the expansion, c'mon that is easy. Yeah. And this is a course in symmetry. No, R is not equal to s . S is a general identifier.

R is a specific identifier so far at least, okay. So there is going to be s that is not equal to R also. What I am saying is since it is a course in symmetry and since de Broglie had said that nature loves symmetry we also love symmetry. We are not unnatural beings. Yeah. Exactly. R is a particular one. So what I will do is I have $D(R) D(s)$ and then I have X . I cannot do anything about x , x is x . But then I have $D(s)$ inverse.

So it will look kind of nice if I write $D(R)$ inverse here, symmetry; like inversion symmetry. But of course it is not enough if I write $D(R)$ inverse and stop there. So I better write $D(R)$ as well, right, agreed? What I have here is $D(R) D(s)$. What I have here is $D(s)$ inverse, $D(R)$ inverse. What is $D(R) D(s)$? Now we are using a group theory. The symmetry operations form a group, right? So a product of two symmetry operations is also another symmetry operation, right?

Symmetry operation No. 1 symmetry operation No. 2 and then third symmetry operation right. third starts with t so I am going to call it T . Not really, I just made that up. I will call it T . What is T ? $T = SR$, alright? $T = SR$ and $D(T)$ is a transformation matrix corresponding to the symmetry operation T and the reason why T is a symmetry operation is which property of the groups tells us that T has to be a symmetry operation also? Yes? Closure. Yes, closure.

Understand what I am saying? So instead of writing $D(R) D(S)$ I am justified in writing $D(T)$ right where T is another symmetry operation which corresponds to operating R and S one after the other, okay? Will you allow me to write this as $D(T)$ inverse? Just multiply together and see for yourself, $D(R) D(S)$, $D(S)$ inverse $D(R)$ inverse. Is that not E ? $D(R) D(S)$, $D(S)$ inverse forget this X . Think that this X is multiplication. $D(R) D(S)$, $D(S)$ inverse $D(R)$ inverse.

So first forget these two. $D(S) D(S)^{-1}$ is E . Then you have $D(R) E D(R)^{-1}$, right? so what I am saying is $D(S)^{-1} D(R)^{-1}$ is nothing but the transformation matrix corresponding to the operation T^{-1} . Anchal, comfortable, okay good. So how do I write this now? I can write this as $\sum_T D(T) X D(T)^{-1} D(R)$. Mehak does this look familiar? $\sum_T D(T) X D(T)^{-1}$.

That is A . It is just that instead of S we are calling it T . But as Shakespeare had said what is in a name, right? It is still a generic symmetry operation, fine, right? So it is $A = D(R)$. Commutation is proved, right? So if commutation is proved then we know already from Schur's Lemma I that $A = \lambda E$. What determines the value of λ ? Value of λ is determined by the matrix X , right? Because $A = \lambda E$.

Now if X is some matrix and then X is another matrix you are going to get different values of λ that is all. The general form is not going to be the same. The general form is going to be the same, sorry, an extra not, okay? The general form is going to be the same but value of λ will depend on which X matrix you are using, okay? So now what we have done so far is that we have developed a perfectly general theory, okay.

Now let us try to make it a little more specific so that we can actually get to great orthogonality theorem. So what I am going to say is that X is of this form. Let us say this is the m th column and let us say, very bad at drawing, completely unsymmetric. Let us say this is the k th row. What I am saying is I can choose an X . X can be anything, right? In the earlier derivation, we did not say X has to be this, X has to be that, X has to be unitary nothing, right? Anything.

So now I am choosing to my advantage a particular form of X that will help me get to great orthogonality theorem okay and I choose this kind of X . I make everything 0. Of course you make everything 0 then we might as well go home. You get null matrix, right? Everything but one. So I want to work with an X matrix such that $X_{ij} = 0$ unless $i = k, j = m$, and $X_{km} = 1$. You could have made it 5, it does not matter, okay?

It is just 1 is the most convenient number, okay? Do you all agree that even if I write my X this way I do not lose out one bit on the generality of the situation. I am fine, right? See all I care about is that A has to be equal to lamda E and what we have done so far is that it does not matter which form of X you use unless X is a null matrix. A is still going to be equal to lamda E. it is just that the value of lamda will change is it not? I can use any matrix.

So I choose to use this matrix which is really 1 and everything else is 0. So what is the advantage of using this? You are working with a sum is it not? All those terms except 1 is going to become 0 right? When you work with the sum, $A = \sum_S D(S) X D(S)^{-1}$, I do not need a sum anymore is it not? All I have to ensure is that I do not have to in fact worry about anything because I have only one 1 in X. Okay, even then I am not lost on generality. Let us see now.

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Handwritten mathematical derivation on a slide from CDEEP IIT Bombay. The slide shows the derivation of $A = \lambda_{km} E$ from a sum over S of $D(S) X D(S)^{-1}$, where X is a matrix with a single 1 at position (k,m) .

$$X_{km} = 1 \quad A = \lambda_{km} E$$

$$A = \sum_S D(S) X D(S)^{-1}$$

$$A_{ij} = \sum_S \sum_p \sum_q D_{ip}(S) X_{pq} D_{qj}(S^{-1})$$

$X_{pq} = 0$ unless $p = k, q = m$, when $X_{km} = 1$

$$A_{ij} = \sum_S D_{ik}(S) D_{mj}(S^{-1})$$

$$A = \lambda_{km} E \Rightarrow A_{ij} = \lambda_{km} \delta_{ij}$$

$$\sum_S D_{ik}(S) D_{mj}(S^{-1}) = \lambda_{km} \delta_{ij}$$

Okay, now. So far so good? What kind of X are we working with, $X_{km} = 1$; k is specific, m is specific, right? Everything else is 0. All other matrix elements are 0. Diagonal, off diagonal, everything is 0 except one diagonal element, okay. Now, and then I say that A is equal to in any case that A we said that $A = \lambda E$ but lamda is going to depend on X. here we are choosing a very specific kind of X. So this lamda also we call lamda km, okay?

$A = \lambda_{km} E$. that is what we are going to work with. Now let me write the expression of A. A equal to as we wrote earlier, $\sum_S D(S) X D(S)^{-1}$, okay? Now, what is the matrix

element A_{ij} ? A_{ij} then is going to be let us say $D_{ik}(S)$ multiplied by, sorry let me call it $D_{ip}(S)$ multiplied by X_{pq} multiplied by $D_{qj}(S)$ inverse sum over S sum over p sum over q , right? That is the, that is from the straightforward rule of multiplication of matrices, right?

And now the nice thing is $X_{pq} = 0$ unless $p = k$ and $q = m$ when $X_{km} = 1$. What happens then? I still get to write the matrix element on the left hand side but instead of 3 summations, I can work only with one summation, right? Sum over S is the only thing that I need to bother about. What I do is I write D_{ip} has to be equal to k , so I write $D_{ik}(S)$ multiplied by D_{qj} , $D_{mj} S$ inverse.

I do not have to write anything in X anyway because the only nonzero element is 1, okay. So I am left with a very simple summation, right? So do not forget that $A = \lambda_{km}$ multiplied by E and now we introduce our Kronecker delta. What is A_{ij} ? $A_{ij} = \lambda_{km}$, will you allow me to write δ_{ij} ? See we are getting there. We already have one of the Kronecker deltas. There are 3, we have at least got 1, got it, okay?

I do not need you to remember everything. What I need you to understand is how we get to the deltas. We get to the deltas by getting at unit matrices. We get to unit matrices by using Schur's Lemma commutativity. That is all I need you to remember and understand, okay? Beyond this nothing is required, okay fine. So this is what is A_{ij} . So I hope you will allow me to write sum over $S D_{ik}(S) D_{mj}(S)$ inverse = $\lambda_{km} \delta_{ij}$. I have removed my ruler.

So please bear with my ugly non-straight lines. What is the range of i , what is the range of j ? i goes from 1 to n , j also goes from 1 to n is it not? Okay? So I have got one. Let us see if we can get one more. What are the 3 deltas we had? One was μ_{ν} . Can you guess how we are going to get that delta μ_{ν} or delta ν_{μ} whatever you call it. We are going to get there by using the Schur's Lemma II.

And if you remember Schur's Lemma II is what correlates two different irreducible representations right of different dimensionalities also, okay? That is where this μ_{ν} will come from. I do not even want to get that far, I will show you. I will show you the book, you can do it

yourself. But let us do the other one, okay? So to do the other one, what I need to do is first of all I have to get to the deltas one by one. I have to get rid of this one.

If I want to get to the λ_{km} , δ_{km} or δ_{mk} whatever you want to call it, first have to get rid of δ_{ij} then it will become a little simpler. How do I get rid of δ_{ij} ? By setting $i = j$, right? Can you set $i = j$ and see what you get? Just instead of j you write i . What do you get? It is not very different. Sum over S , $D_{ik}(S) D_{mi}(S)^{-1} = \lambda_{km}$ is it not? Okay?

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Setting $i = j$,

$$\sum_S D_{ik}(S) D_{mi}(S)^{-1} = \lambda_{km}$$

Sum over i ,

$$\sum_S \sum_{i=1}^n D_{ik}(S) D_{mi}(S)^{-1} = n \cdot \lambda_{km}$$

$$\sum_S \sum_{i=1}^n \underbrace{D_{mi}(S)^{-1} D_{ik}(S)}_{D_{mk}(S^{-1}S)} = n \lambda_{km}$$

$$\sum_S \sum_{i=1}^n D_{mk}(E) = n \lambda_{km}$$

$$n \lambda_{km} = \sum_S \delta_{mk}$$

$$= g \delta_{mk}$$

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I can write sum over S $D_{ik}(S) D_{mi}(S)^{-1} = \lambda_{km}$. I do not have to write δ_{ij} anymore because I have said $i = j$. So δ_{ij} is 1, okay? Now what do I do? I need to get to this δ_{km} somehow and the only way of getting to it is to do another summation. Let us sum over i . What do you get? I hope you do not mind me writing sum over S outside, it is fine right? they are interchangeable.

Sum over $i = 1$ to n $D_{ik}(S) D_{mi}(S)^{-1}$ is equal to how much? See this left hand side = λ_{km} is true for every value of i is it not? How many values of i are there? N values of i . So I think even my 7-year-old younger son will tell me then that if you sum it over i also then right hand side gets multiplied by n , right or wrong? See does not matter what the value of i is. The value is λ_{km} . Now put $i = 1$ you get λ_{km} . Put $i = 2$ you get another λ_{km} .

Put $i = 235$ if it is required, you get another λ_{km} . So it is n multiplied by λ_{km} ? Okay, now let us see if I can simplify it a little bit. So what I notice is $D_{ik}(S)$ and $D_{mj}(S^{-1})$ inverse. So if I just write it in the opposite sequence it might well be a little more easier to see what that means. So what I am saying is $\sum_S D_{ik}(S) D_{mj}(S^{-1}) = n \lambda_{km}$.

I will just take this forward, I will take this here, $D_{mj}(S^{-1}) D_{ik}(S) = n \lambda_{km}$. What is this? Not the political party. D_{mk} of which matrix? This gives me D_{mk} of $S^{-1} S$ a very complicated matrix because you are multiplying a matrix by its inverse. What is $S^{-1} S$, is E . So $\sum_S D_{mk} E = n \lambda_{km}$. So what will that be? How do I write this? $D_{mk} E$. Do I not write it as δ_{mk} ?

I can write it as δ_{mk} is it not? But once again we have got the unit matrix. That is all we need to do here. Get to a unit matrix. And you get your Kronecker delta. So what I can write is, I can write $n \lambda_{km}$ is equal to $\sum_S \delta_{mk}$ right and that is equal to $g \delta_{mk}$. We are summing over S , right?

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$$\sum_S D_{ik}(S) D_{mj}(S^{-1}) = \frac{g}{n} \delta_{ij} \delta_{km}.$$

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So finally the expression that we have got, if we combine the two is $\sum_S D_{ik}(S) D_{mj}(S^{-1}) = \frac{g}{n} \delta_{ij} \delta_{km}$, okay? Now invoke Schur's Lemma I you are going to get the third delta also. So I do not want to go there because some had at least come at 5 o'clock. It is

almost 7. It is the last class. You are going to have end sem very soon. So I stop here, right? It has been a wonderful experience teaching you.

I had a lot of fun. I hope you had some as well. You have done well in mid sem. Do well in end sem as well even though it is (()) (34:13) right. It still feels good, right? That will be all for this course. Thank you.