Symmetry and Group Theory
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Lecture - 67
Derivation: Great Orthogonality Theorem - II (Schurrs Lemma 2)

I am not saying that I will. Do not allow me to mislead you on this last day of class. How did I write 1 earlier? Now again I have created some degeneracy. Now theorem 2 is a little more complicated and what we will do is we will only prove the positive part of it. The negative part you can work out by yourself if you are interested. So what theorem 2 says is that if, what is this, what is this letter? Gamma.

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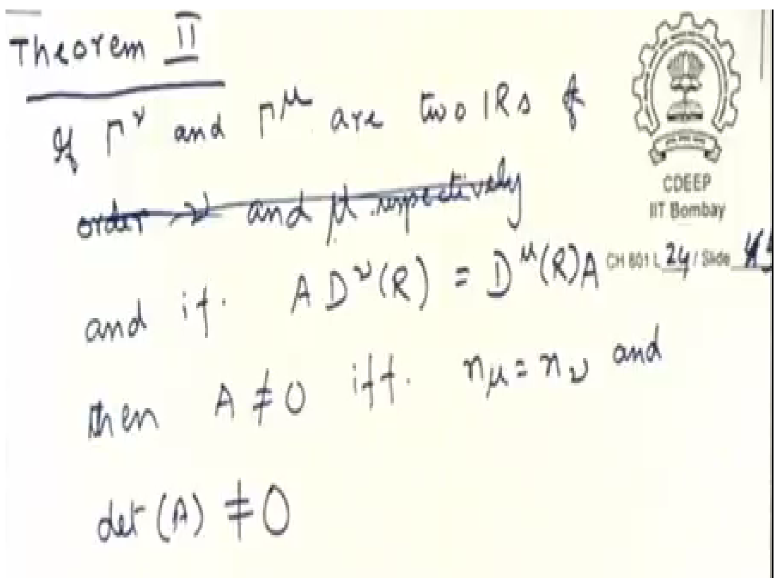

Gamma nu and gamma mu, which kind of reminds me that we have, I know an eminent scientist who used to use, what do we write? We always write sum over ij kl but I know somebody who used to write sum over mu nu delta alpha. Direk also used to do that, okay. Just adds a little more gravity to the situation, okay. What are these, where do you what do we write gamma for usually? Irreducible representation, right?

Let us say these are two irreducible representations of order nu and mu respectively. And the reason why we take the trouble of writing nu and mu and all that is that we are going to use n for something else, okay that is why. And also it looks more serious, okay. So let us say these are two irreducible representations of order nu and mu respectively and let us say you have a matrix A such that A D nu (R) = D mu (R)A. So this is not commutation, right?

This is not commutation. You have taken that matrix, you have left multiplied it, you have used it to left multiply D mu (R) and you get D nu (R) sorry you get D mu (R) right multiplied by A. I am talking about two different representations, irreducible representations. What kind of matrix is A. Is it a row matrix, is it a column matrix, is it a square matrix, what is it? Square matrix? What is it, Kamal? What do you think it is? Triangular matrix, it cannot be.

Rectangular matrix, right? Prolong means I think what you meant is rectangular. See it is going to be square only if n nu = n mu, right? the orders are the same. If orders of the two matrices are the same or rather dimensionalities of the two representations are the same, let us put it that way. Order, when it is order we actually mean the whole group. So if the dimensionalities of the two representations are the same, then and then only is A going to be square matrix.

We are very comfortable with square matrix and with row and column matrix, right? We generally do not like to talk about rectangular matrices. But then the point is if these two irreducible representations are of different dimensionalities then A is going to be a rectangular matrix. Understand what I am saying? So the general case is rectangular matrix. Special case is square matrix if the two dimensionalities are the same.

Let me finish writing the theorem. If gamma nu and gamma mu are two IRs of order , actually I should write dimensionality no? Cut, do not write all this. Add two IRs. Nu or mu are identifiers. Gamma 1, gamma 3, something like that okay. And if A D nu (R) = D mu (R)A then this matrix A is going to be nonzero if and only if n mu = n nu and det (A) is nonzero. This is what we are going to prove, okay?

It is a little more complicated than the first one but we will stick to the simple part of it anyway. We have two different irreducible representations gamma nu and gamma mu and let us say there is a matrix such that A D nu (R) = D mu (R)A for all symmetry operations R. You cannot say that it works with one symmetry operation, does not work with another. That is no fun. For all IRs then A is nonzero if and only if the two dimensionalities are the same and det (A) is nonzero, okay?

And since we are writing A here that is the hint that this A also has got something to do with the A that we used earlier, right. This is a little longer than the previous one. To start with let me make an assumption. Of course, once again whoever has done my class earlier would know that when you assume what do you do? You often make an ass of you and me, right? It is there in the spelling itself. When you assume, you make an asset of you and me, okay?

But see science is all about assumptions that do not make an ass of you and me, right? Intelligent assumptions, valid assumptions. So let us try to make an assumption that will simplify the problem but we will not lose out on the generality and one such assumption that we can make is that let us work only with unitary matrices.

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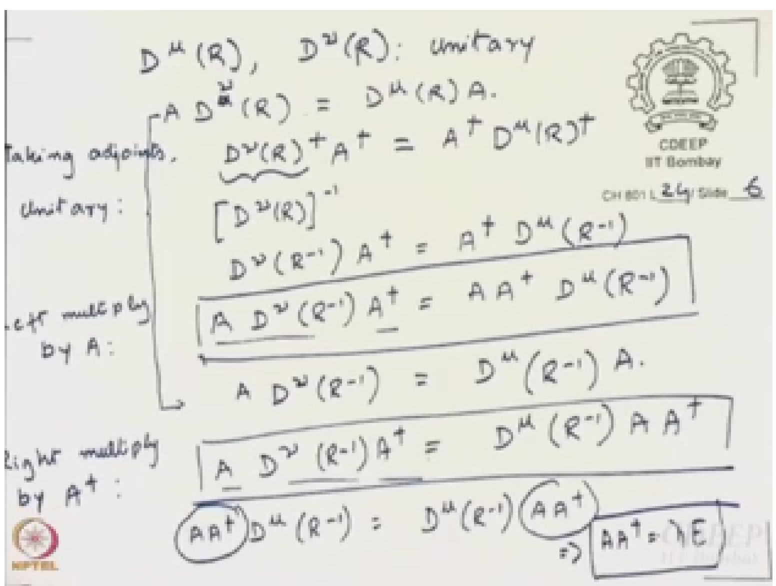

Suppose I say I am going to only work with one by one matrices. Then of course the meaning of the word assume is what I said already. We are not saying that. I am saying that let us say that these matrices are unitary. Am I allowed to make that assumption? And this in case it does not ring a bell yet was our mid sem question. Mid sem question, yeah. Unitary transformation can be done, right?

It does not matter, you take any representation and you can make a unitary transformation and generate unitary matrices. And then it is easier to work with them and also when you are talking about irreducible representations you are going to work with these orthonormal basis and then the transformation matrix is going to be unitary anyway, remember? So I think we are fine if we make this assumption that d mu R and d nu R are unitary and we will see in a while how that makes our life a little easier, okay. Let us go ahead.

So what we have said already is A D mu (R) = D, I think we said A D nu (R) = D mu (R) A, okay? That is a definition of A anyway. Starting with this if I want to simplify, what we do is first of all let us take advantage of the fact that it is unitary. If I want to take advantage of the fact that these matrices are unitary, what should I do? Whenever you have matrices you somehow want to get to the inverse, right? Because matrix multiplied by inverse is any case E.

And in case of unitary matrix what is the inverse. What is the inverse of a unitary matrix? Transpose is going to get you maybe two out of five, adjoint. Transpose and then take complex conjugate or complex conjugate and then take transpose whatever; adjoint, right? So whatever we would like to do is let us generate the adjoints because eventually we want to do similarity transformation. For that you need the invoices and here the invoice is just the adjoint.

So let us take adjoints. I can write D nu (R) adjoint A adjoint = A adjoint D mu (R) adjoint. I think we have encountered this earlier just before mid sem when we did that unitary transformation discussion is it not? You take an adjoint of the products, they get interchanged, okay? Now, these are all unitary matrices right? since these are unitary matrices this D nu (R) adjoint is the inverse of D nu (R) right?

This is D nu (R) inverse of that, right and are these any kind of unitary matrices under the sun? No. Right. Now they would not write R. What kind of matrices are you working with? Transformation matrices, right? So now you tell me what is the inverse of a transformation matrix. Now you go from mathematics to chemistry. Inverse of transformation matrix is the transformation matrix of the inverse symmetry operation. Is it not?

Inverse of the transformation matrix has to be the transformation matrix corresponding to the inverse symmetry operation. C 3v, C 3 and C 3 square are inverse of each other. So inverse matrix of the transformation matrix of C 3 is the transformation matrix of C 3 square, remember? Because when you multiply them you must get the unitary matrix, unit matrix, right? So I can write d nu (R) inverse A dagger = A dagger D mu (R) inverse, alright?

And then I want some kind of a similarity transformation. For that I can either right multiply or left multiply. I choose to left multiply so that I am going to do a similarity transformation of the left hand side. So what you want to do is left multiply by what should I left multiply by so that this left hand side becomes a similarity transformation? A, B, X, C, D, P, Q what? A, right because this is the inverse of A. Not necessarily.

Not necessary but this look at least something like a similarity transformation. A D nu (R) inverse A dagger = A, A is not inverse sorry my mistake. It looks something like a similarity transformation, not actually. A A dagger D mu (R) inverse. It will help us eliminate some things. So this is where we have reached. We have to remember this. A D nu (R) inverse A dagger = A, A dagger D mu (R) inverse, okay?

Now we have started from R and we have reached R inverse, right? Another way of doing that would be from here. This R is general is it not? It is any symmetry operation. So I do not think anybody will have any objection if I write A D nu (R) inverse = D mu (R) inverse A is it not? Instead of R I can write R inverse, right? Now what do I do? I want to eliminate something right? I can choose to eliminate this or I can choose to eliminate this.

Let me try and eliminate this one. If I want to eliminate this, I want the same term in the second equation also. What do I have to do? See A D mu R inverse is already there and this is just A D nu R inverse right multiplied by A dagger. So if I right multiply this entire expression by A dagger then the 2 LHS become the same, right? And you get A D nu (R) inverse A dagger = D mu (R) inverse A A dagger, right? So what do I eliminate?

I eliminate this and this and I am going to get A A dagger D mu (R) inverse = D mu (R) inverse A A dagger, right? So what is that? That is commutation is it not? Commutation. A A dagger D mu (R) inverse = D mu (R) inverse A A dagger, right? Okay. Do not forget that a product of two matrices is a matrix in its own right. Just because I have multiplied two matrices you should not think that what I have got is something different. It is a matrix.

Commutation, right? And what was theorem 1? So this A dagger I can call it maybe anything. I can call it alpha. So would you not agree that this alpha matrix is a constant matrix, right? So which implies, not much space left. A A dagger is lamda into E, okay? What is it that we wanted to prove. Let us not forget what we wanted to prove. This is not theorem 1. This is theorem 2.

And theorem 2 is if these are two IRs and if A D nu (R) = D mu (R)A then A is nonzero if and only if n nu = n mu and det (A) is nonzero. That is what we will prove now. Actually we are almost there.

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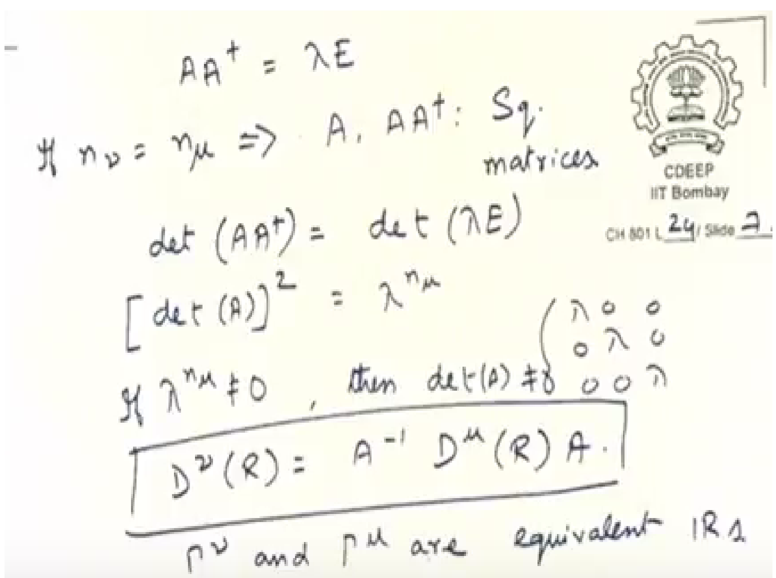

So what have we got? We have got A A dagger. So what happens if n nu = n mu. What kind of matrix will A be? Circular matrix? Square matrix. And what about A A dagger? So it will be square of square matrix, right? So 4 dimensional matrix, is it not? That will also be a square matrix, right? So both A and A A dagger are square matrices, okay? And we know already that A A dagger = lamda E. So what then is det A A dagger? I will make your job a little simpler.

Det lamda E. Let us talk about A two by two matrix. Lamda square. And let us talk about a three by three matrix. Get the point, right? Lamda to the power n, okay. So this is going to be lamda to the power you can write whatever you want. I will write n mu. I might as well have written n nu. It does not matter. What about the left hand side? What is det A A dagger. Will you allow me to write it as det A whole square? Just work it out. Take any matrix. Take it adjoint, right?

Multiply them together. See what the determinant turns out to be. Work with a two by two matrix. It will turn out to be this. So what is det (A) then? Det (A) is square root of lamda to the power n mu, right? So if lamda is nonzero, lamda to the power n mu is nonzero. Then det (A) is also nonzero, right? And it is going to have an inverse and you are going to be able to write D nu (R) = A inverse D mu (R) A. For which value of R? For all values of R.

So that is the relationship between gamma mu and gamma nu then, right? What is the relationship? The corresponding transformation matrices are similarity transformations of each other. Which means that gamma nu and gamma mu are equivalent matrices, equivalent IRs sorry. What is it that we wanted to prove, are two IRs and if this then A is nonzero if and only if n mu = n nu and det (A) is nonzero. We have proved the if part.

We have not proved the and only if part. We said if and only if is it not? So if is proven. Only if, I leave it to yourself. It is not all that difficult. It is worked out here. It is the appendix of chapter 7. Look it up, you can do it yourself. At least you have proved the if part.