# Symmetry and Group Theory
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## Lecture – 28
## Irreducible Representations and Great Orthogonality Theorem

Recipe of how to generate unitary representations right, so what I suggest is please workout a few matrices yourself, take some matrix that is nonunitary, do not have to take an entire representation, no you have to take an entire representation, how will it work, how will you get h okay. So please try to work this out by yourselves, workout a few examples right. Next, yes oops you should have said that earlier, the problem is I can see it, so fine.

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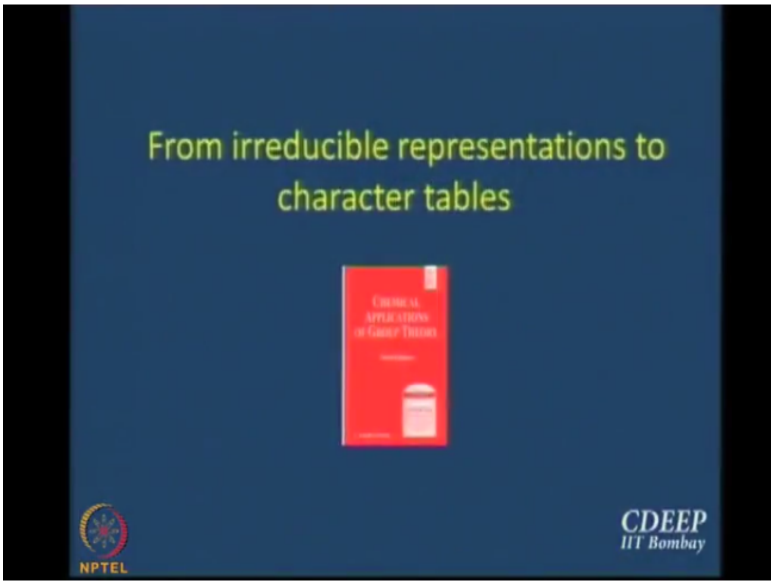


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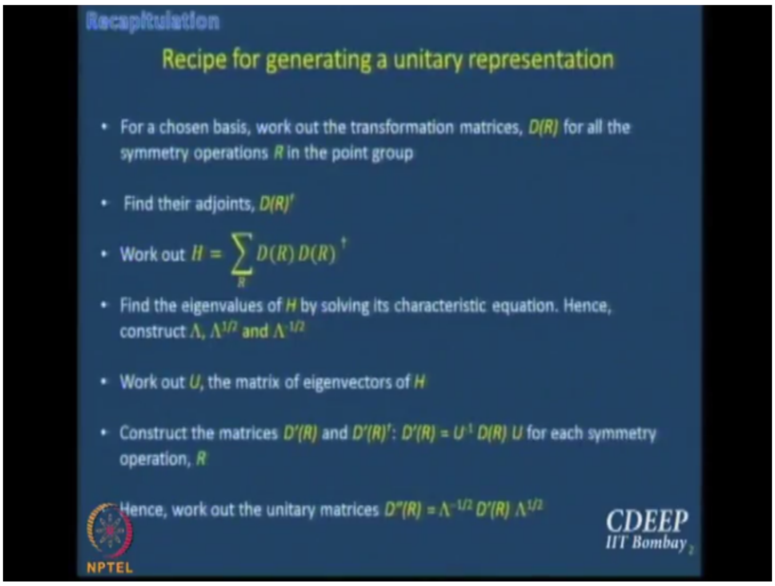

So this is what we are going to talk about today. This is what we are discussing right and whatever also discussed today was a part of this recipe of how to generate unitary representation. So what I suggest is please take nonunitary representations, try to generate unitary representations by yourselves then only you will understand okay.

Recipe per say when you did this it does not seem very difficult, it is not very difficult and then when you read this go back and read the derivation again, learning is always synergistic, you do not really grasp the whole thing at one go okay, you have to keep going back to it. So please do that and I think will be all fine.

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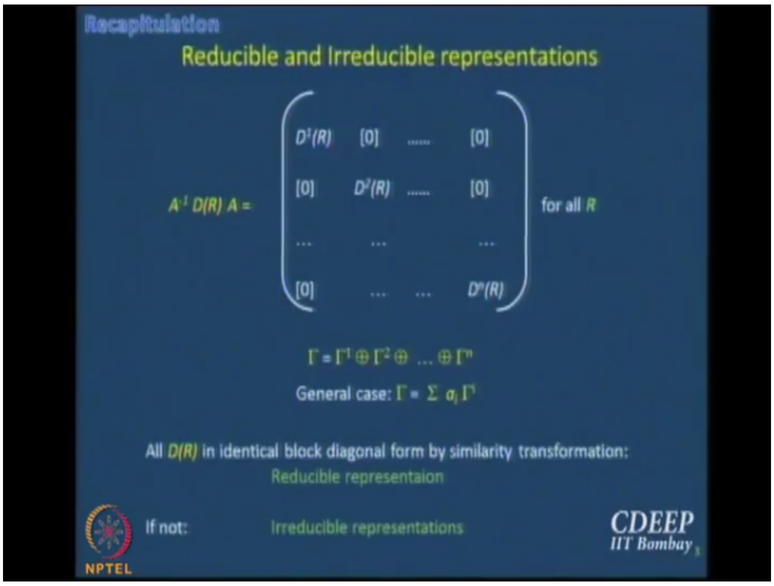


Now this is where this talk we have started talking about reducible and irreducible representation. By now, I think we all have at least some idea of what reducible and irreducible representations are. To put it very simply, reducible representations are representations that can be reduced and irreducible representations are representations that cannot be reduced.

But then if you make statements like that you are going to get a job in Microsoft right according to that helicopter joke. Guess you do not know the helicopter joke I will tell you after the class but this is the formal definition. Suppose you have a matrix like this which is block factorized, then you can see that it is reducible and you can write this as a block sum block addition of the different blocks.

You write as the addition of different blocks not arithmetic addition, block addition right and in generous some of the blocks may be same. So you can write gamma=sum over ai gamma i. This gamma i may be reducible, may be irreducible, I do not know okay. So the definition is this. If you have a representation in which all the transformation matrices what is DR I hope you have not forgotten.

DRs are the transformation matrices right, transformation matrix for the symmetry operation R. So if all these transformation matrices can be made to take up identical block diagonal form by some similarity transformation then you call it a reducible representation and what I suggest is please get hold of Harris and Bertolucci's book. Harris is very simple name and Bertolucci is not an uncommon name for (()) (03:31) of movies.

There is a well-known film director named Bertolucci but this Bertolucci is not that Bertolucci right. So Harris and Bertolucci's book, they have shown how you can perform symmetry transformation and go from a non-block diagonalised matrix to a block diagonalised matrix, what they have not explained is the logic by which you choose the matrices using which you perform the symmetry transformation okay.

But just as an example you do not have to memorize anything or you do not have to understand anything that as an example just to convince yourself that such kind of similarity transformation can actually be done I suggest that you please go through that section of Harris and Bertolucci's book. What is the name of the book, symmetry and spectroscopy something like that right okay?

Now we learn how we can breakup reducible representations into its consequent irreducible representations without having to do similarity transformation. That we will learn in one of these next few classes right. So if it is possible to change all the matrices into identical block diagonal form by the same similarity transformation, this is x-and x you have to use x- and x everywhere. You cannot use y- and y in some cases and x- and x in some others.

You have to use a same matrix and its inverse. So if you can block diagonalise using that way then such a representation is called a reducible representation and if it is absolutely impossible to do that then you call it an irreducible representation alright.

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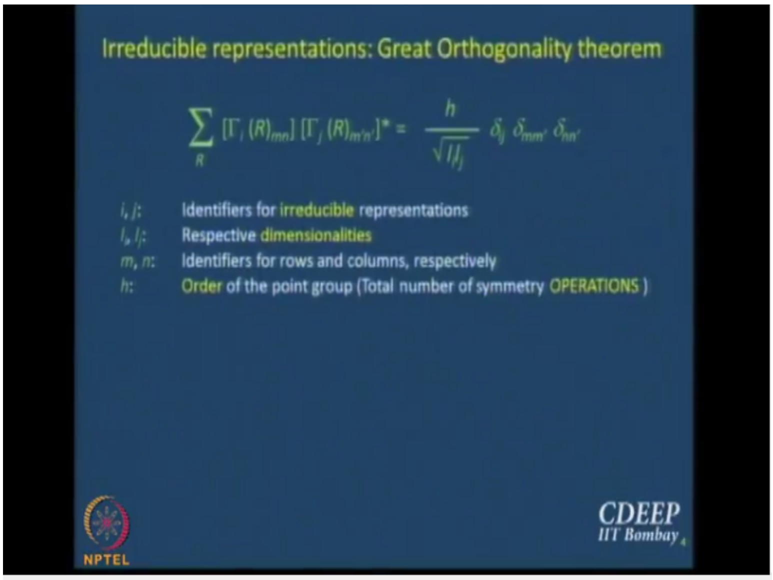


So today what we want to do is we want to talk about irreducible representations and for the time being we want to take great orthogonality theorem (()) (05:30). We are going to derive this also but after midsem. So this is what great orthogonality theorem says just have a look after all our discussions so far I think this is not very scary anymore, still is okay let us see. Sum over R that is not very difficult to understand right.

What are we summing over R? A product of two, what is this letter? Gammas, product of 2 gamma, what do we use gamma for, representation. A representation is usually denoted as gamma okay. So gamma i and gamma j, what is gamma i and what is gamma j? ith irreducible representation and jth irreducible representation. Let us say i is 3 and j is 5, they are third irreducible representation and the fifth irreducible representation right.

So first group i and j are the identifiers for irreducible representations. Please remember great orthogonality theorem holds only for irreducible representations not for reducible representations. Now it says is this on the left hand side you have sum over R gamma i R by now you know what R is R is some symmetry operation right and generally we use R for the general symmetry operation, we are summing over R right.

So gamma i Rmn what is that now? Instead of d we are writing gamma. If you want you can continue writing d, I have no issues. In fact, in Bishop's book, they have not used gamma. They have continued writing d even at this stage. If you are more comfortable with d, I have no issue okay as long as you understand what we are talking about.

So gamma i Rmn that means the mnth element, m row and n column, mth row and nth column that element of the, what is gamma i R, the transformation matrix corresponding to the operation R in the ith irreducible representation right. When you multiply this by gamma j Rm dashed n dashed star, now it will not be difficult to understand anymore. The complex conjugate of the m dashed n dashedth element of the transformation matrix corresponding to the same R not in the ith irreducible representation but the jth irreducible representation.

What is a representation? A collection of matrices right, a collection of transformation matrices for all the symmetry operations, different collections have different number. So you multiply this by complex conjugate of that and sum over all R, you get h/square root of li lj. h is the order of the point group; order of the point group means the total number of symmetry operations not elements.

Please remember symmetry operations not elements and will come back to this with a more conflict example right and li and lj are the dimensionalities of the ith and jth representation. What does that mean? What is the meaning of representation of a dimensionality? "**Professor - student conversation starts.**" Yeah, so what kind of matrices are there? In a representation all the matrices will be either 1x1 which is a number or 2x2 or 3x3 or 108x108 something right, something by the same number.

So that is the dimensionality, how much by how much, all square matrices right alright okay with this, fine. "**Professor - student conversation ends**." Multiplied by 3 Kronecker deltas, delta ij, delta mm dashed, delta nn dashed, just looking at this equation are you reminded of something, will derive this of course but just looking at this what is the impression that you get? Do you get any impression? What are you dealing with?

See you are multiplying something with the complex conjugate or something or forget the complex conjugate also for now. You are multiplying something with something else and summing over all possible values and then you get on the right hand side the Kronecker deltas, is not that what you get for a set of orthonormal vectors right and what would h/root over li lj be?

That would be the normal assumed constant, is not it? That is the value to which it is normalized. Now does it make a little sense (()) (10:46) okay not very scary daily, it says that with so many deltas and gammas and sigma's, it might be a little perplexing to start with but once you read it carefully I think you understand. So what is it that are forming this set of orthonormal vectors? Yes, how do you say it is unitary? Actually, what you have said is correct.

In fact, great orthogonality theorem when written in this form holds only for those irreducible representations that are unitary in nature. There is something will learn once again after midsem. If they are not unitary then you are not allowed to write star here, you have to write adjunct, will divide all that okay so this actually you are right, it holds for unitary representations.

But what do we have here, this is a matrix element, this is another matrix element is not it, so what we are saying is that the matrix elements of the transformation matrices in irreducible representations they behave like a set of orthonormal vectors. So okay with what we have written here right. So what are we doing, we are multiplying a matrix element by the complex conjugate of another matrix element essentially right.

I have written down all the possible irreducible representations. I take any arbitrary matrix element from somewhere multiplied by another matrix element but then the second matrix element is not completely arbitrary, it is the matrix element or corresponding to the same symmetry operation. I do not care whether it is 11 or 23 or 58 but it has to be of the same symmetry operation alright and multiply them together.

Actually multiply 1 by the complex conjugate of the other right and do all possible permutations and then add up what I get and then what I see is that this is 0, the sum is 0 unless i=j and m=m dashed and n=n dashed, is not it, this is all Kronecker deltas. So this delta ij is going to be 0 unless i=j, if i=j then this is 1 and once it is 1 it is the multiplication by 1 you do not have to worry about anymore.

When m=m dashed, this delta is 1. When n=n dashed this is=1 right. So when all this is satisfied what do you have on the right hand side you have h/square root of li li actually, square root of li li is what? li, li square, square root of that and then what do you have in the left hand side then sum over R gamma i Rmn right because there is no Kronecker delta mn. Then, you cannot write j anymore you have to write i.

Gamma i R then what do I write again, mn star of that if it is a complex quantity right. Shantanu question, is this okay h shape is all the same, you cannot make of whether it is okay or whether it is the other way round understood. So that is the normalization constant right but then if i is not equal to j then what happens to the right hand side, it becomes 0, no matter what the others are.

If m is != m dashed, if n is!=n dashed right hand side just becomes 0 which means that this quantity let me call it a and let me calling b to avoid the complication of saying gamma i mn all the time. So this is a, this is b let us say a and b star, does not mean that a and b they form a set of orthonormal vectors right. There is a condition for orthonormality is not it. Any other question? Fine.

So today we are avoiding the derivations. We are not really deriving anything except for something that is very simple, no matrix algebra.

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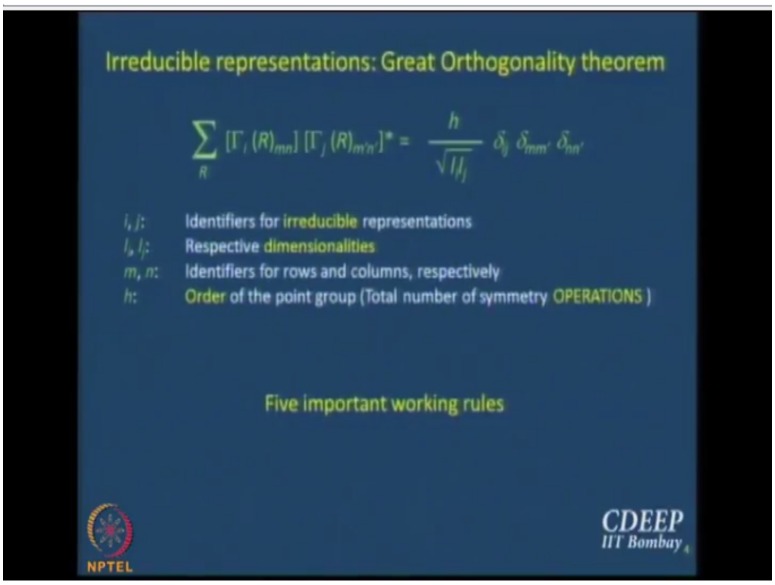


What we want to learn really is we want to learn 5 important working rules that arise at least 4 of them arise from great orthogonality theorem and you already know the fifth.

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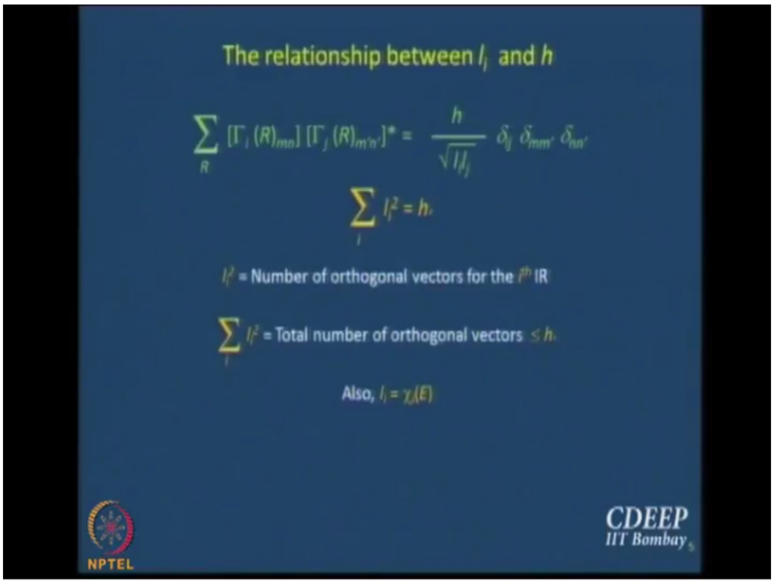


So let us try and learn. The first one is the relationship between li and h. I think it is bad idea to write li's, li is enough otherwise you might think that s is something like li and h. So the relationship between li and h. What is li? Dimensionality of the ith irreducible representation okay. I am making you say it out like school children because if you miss one word here then that is also like Kronecker delta, one word missing delta=0 okay.

So what is this relationship between the dimensionality of the matrices and what is h? Order, it is the total number of symmetry operations. This is the relationship to cut a long story short. Sum over i li square=h okay. We might derive this also later on but this is basically how the derivation comes. Do you agree with me that li square is the number of orthogonal vectors that I get for the ith IR?

The matrix is li by li so li square, there are total number of matrix elements, so the issue is that if you take a sum of that then that will give you the total number of orthogonal vectors and from the property of orthogonal vectors, it is not going to difficult the show that that total number has to less than or equal to h. So h is really the upper bound on sum over i li square but in this case at least we can show that sum over li square is=h.

Inequality is actually equality here. We will come back to the derivation after midsem okay. So this is sum, so these are few things that I need you to remember, sum over i li square=h that is point number 1. Now the other thing is will you agree with me if I write that li=chi i E. what is chi? Trace character right.

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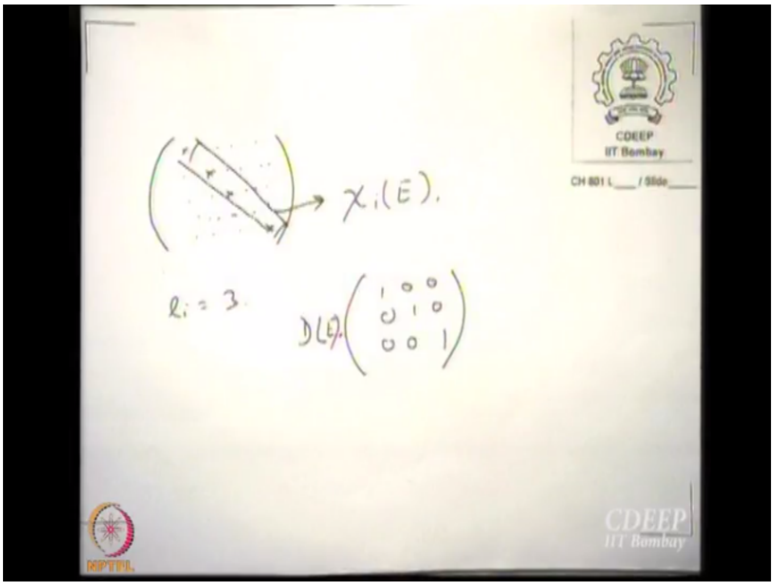


If I add up all this then the quantity that I get is chi right. There is a character or trace whatever you want to call it. Now what is chi i E? Let us say li=3, so then what is the matrix corresponding to E 1 0 0 0 1 0 0 0 1 so what is chi of this matrix? 1+1+1 3 right. Now instead of 3, I say 29, I do not know of any 29 dimensional irreducible representations that is the different issue but let us say it is 29.

Will this still hold or not? That the character of the unit matrix will be equal to the dimensionality it will be 29 in that case is that right okay.

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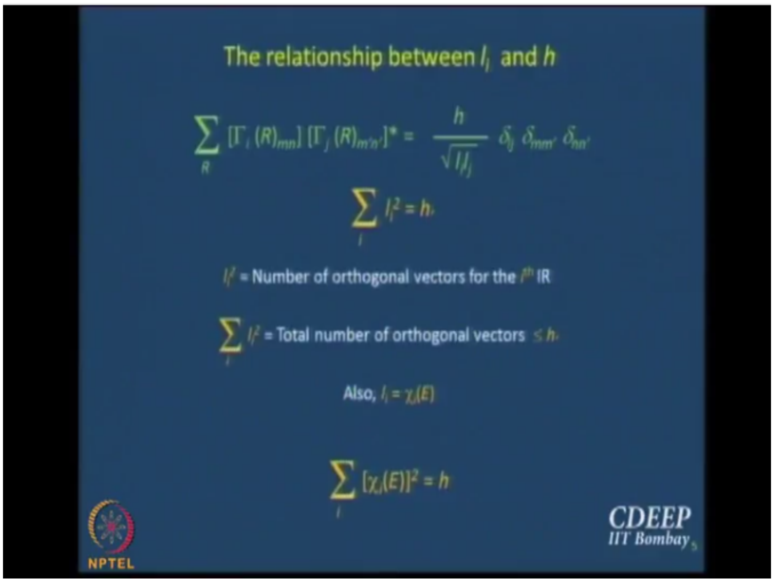


So if li=chi i E then what can I write if li=chi i E and you already know this relationship sum over i li square=h, you just substitute there and this is what I will write, very simple right chi i E square=h fine. So that is our working relationship number 1.

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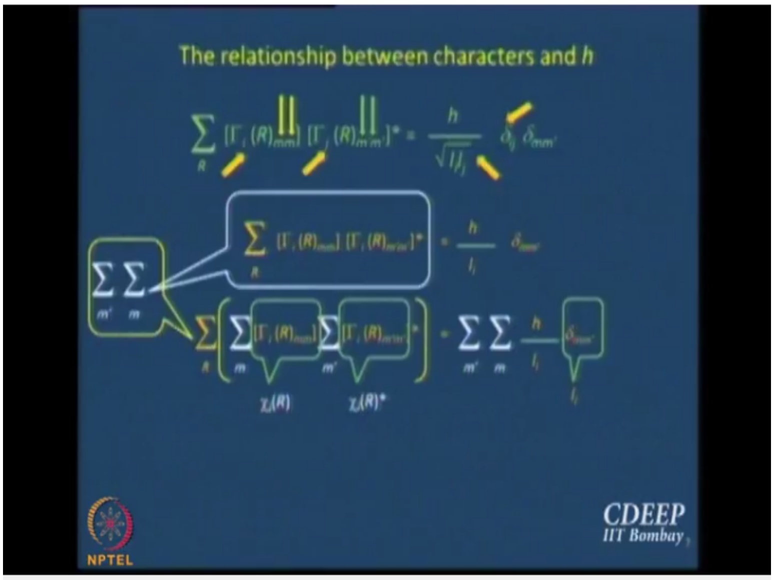


Number 2, this was the relationship between the dimensionality and order now we want to see what is the relationship between the characters of all the symmetry operations and order. We already know one right in the bottom, what about the others, you start from here what you need to do if you want to work with characters then will you agree with me that m has to be=n right.

Similarly, m dashed has to be=n dashed, so what is the advantage of that, the advantage is that I do not have to worry about n's anymore, I do not have to worry about that Kronecker delta at all right. So I have lost one Kronecker delta fine. Next, let us to get i and j, what will happen if i is !=j, 0 so i has to be = j and when i=j you have already told me that square root of li lj that is=li right, delta ij=1.

So this is what you get right, sum over R gamma i Rmm gamma i Rm dashed m dashed star=h/li delta mm dashed. "**Professor - student conversation starts**" see here what I am saying is I want to work only with characters, so I am only worried about the diagonal element, I do not care about the off-diagonal elements, so only when m=n and m dashed=n dashed those are the only elements that I am working with, I throw the others okay "**Professor - student conversation ends**."

So this is how it becomes, now what I want to get rid of n so it makes sense if I sum over all m's and all m dashed then it will not be dependent on m anymore. So if I want to do that then it makes sense for me to write it like this, take the sum over R outside because what do you have here, you have these two quantities right, one is in mm, the other is in m dashed m dashed and you are summing once over m, once over m dashed.

So if I just take the sum over R outside then I can write it like this sum over m gamma i Rmm*sum over m dashed gamma i R m dashed m dashed star okay. Now what is this first thing, gamma i R mm, you are very sure that it is the character right but before that right hand side also has to be summed over m and m dashed fine. So this is the character right. What is the second one? That is also the character, it is just the complex conjugate of character fine.

What is the right hand side now? Left hand side what I have got is I have got sum over R chi i R chi i R star and if you are working with real matrices, the real representation then it is simply sum over R chi i R whole square. What do I have on the right hand side? If I sum over m as well as m dashed is perhaps easier to think out like this.

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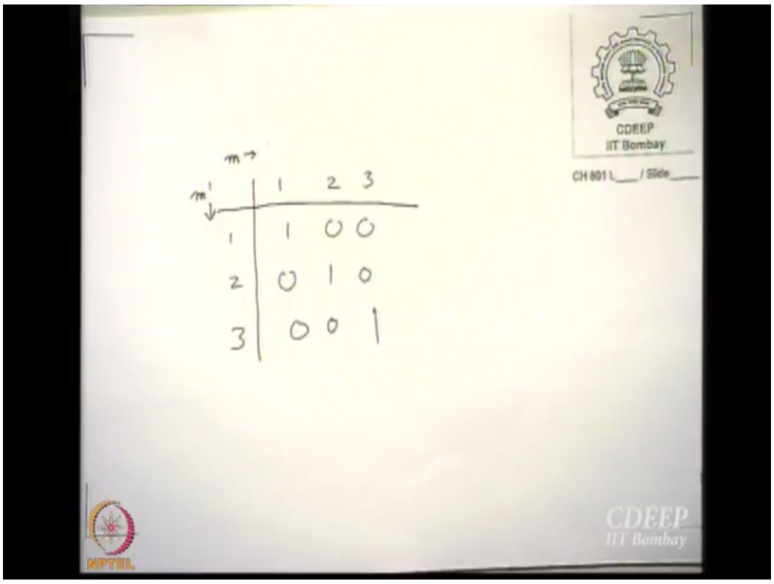


Let us say I will write all the m values here and I will write all the m dashed values here and once again I want to work with 3 values of m let us say li=3, 1, 2, 3, so m=1 2 3, m dashed=1 2 3. So first I want to work out the products and then I write them, it is easier for me to do it if I look at it in a table. So what is this product 1*1? When m=1 m dashed also=1 then what is Kronecker delta, 1 0 0 0 1 0 0 0 1 right.

This is essentially like the unit matrix. So now if I add everything up 1+0+0+0+1+0+0+0+1 that is 3 right.

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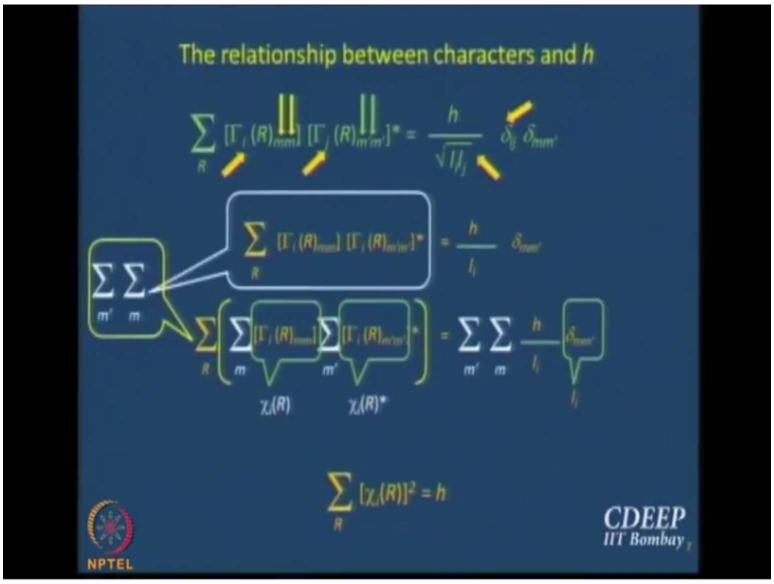


So if I did that for li=5, what would the answer be? 5, for li=283 without getting carried away too much the answer is li and there is a nice situation, li in the numerator, li in the denominator, li and li cancel, you are left with h. So this is the answer, actually I have written the complex conjugate right. It is really mod square alright. So this is our relationship number 2 right.

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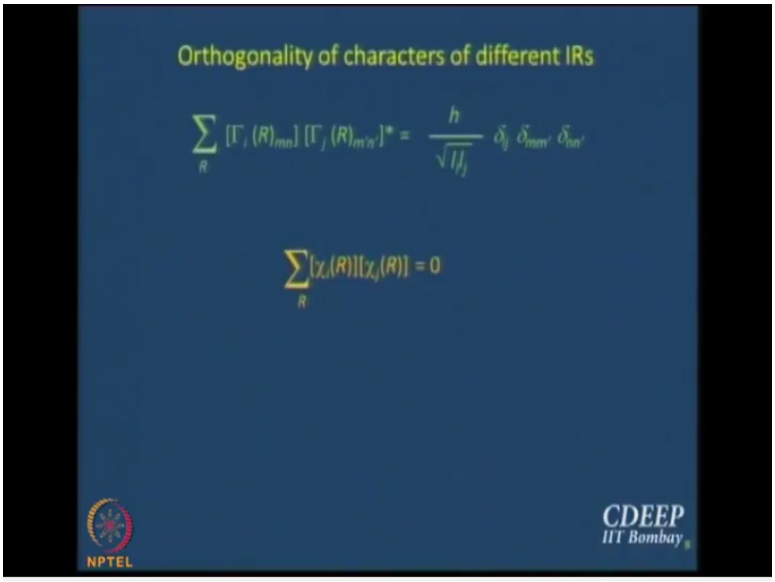


Now number 3 is the orthogonality of characters of different IRs. Once again you go back to great orthogonality theorem and then we will see after midsem how in fact even now we can do it, I want to get somewhere so I do not want to spend too much of time here at the moment, so you can prove that sum over R chi i R chi j R that is going to be=0, will divide this more formally when we come back after midsem.

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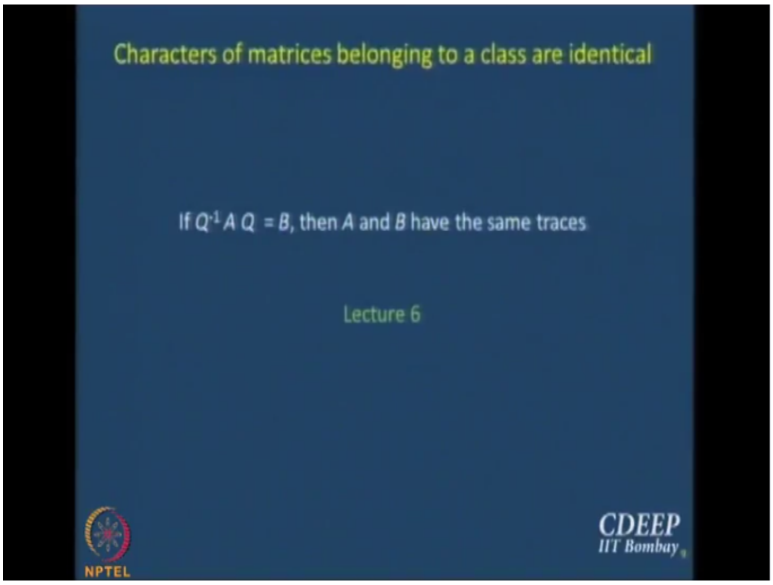


Next, we will use something you know already. The characters of matrices belonging to a class are identical. We discussed this in lecture 6 right. If Q inverse A Q=B then A and B have the same traces, trace and character are one and the same.

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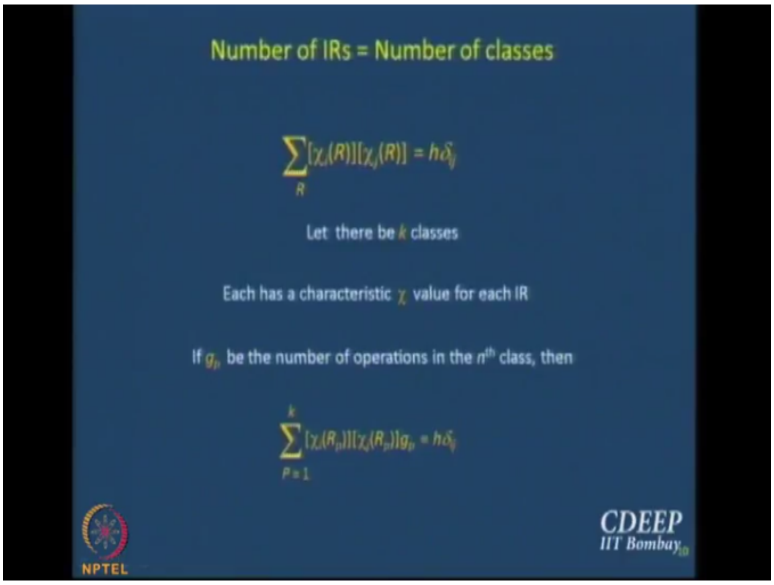


Last is very useful, in fact you see, in our subsequent discussion we will start with this. Remember the question we asked, just before getting into this business of matrices and determinants and all this is how do I know what is the total number of irreducible representations right and this is the answer. The total number of irreducible representations i R here does not mean infrared or any other thing, irreducible representation. Total number of irreducible representations is the number of classes.

Once again we are going to discuss it in little more detail when we come back. This also arises out of the condition that has to be satisfied via set of orthonormal vectors right but the answer that we need to work with is number of IRs is number of classes. So you have five relationships.

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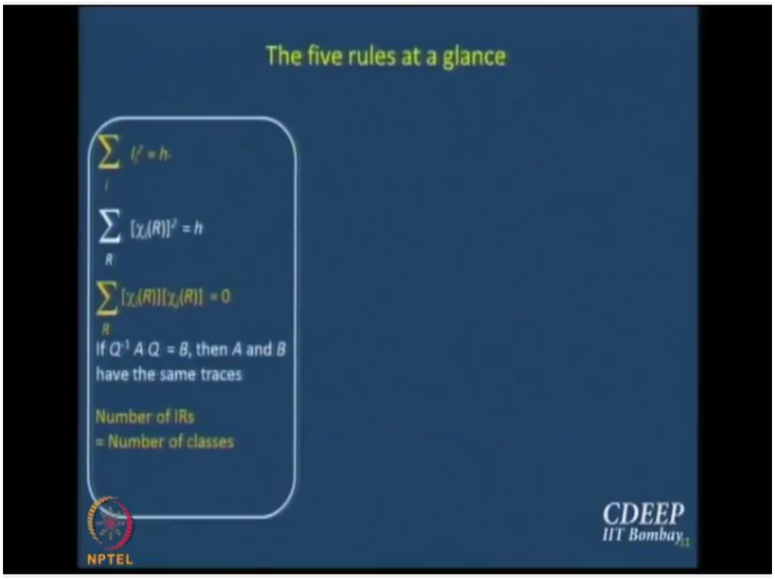


What are the five things that we need to work with these? First is sum over i li square=h, second sum over R chi i R mod square actually remember do not forget that we can have and we will have complex quantities = h, sum over R chi i R chi j R=0, here also you should write the complex, there can be some quantities. Then, same class means same character within the same irreducible representation. Finally, number of irreducible representations = number of classes.