Symmetry and Group Theory
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Lecture – 32
Reducible to Irreducible Representations

Right, with the same set of matrices, how do I deduce this irreducible representation, hey, do not talk, okay, to do that to learn how to do it, first of all we say that you can do similarly transformation and all that but then it is very difficult to find out exactly which matrices we are going to use to perform the similarity transformation, so, today we learn a very simple formula, very simple relationship, which will let us decompose reducible representations into the constituent irreducible representations, right.

We are going to use great orthogonality theorem for that. So, great orthogonality theorem character table these things well, great orthogonality theorem leads to everything but then we are going to use the character table also, so let us find the characters of these matrices, what are the characters of the matrices? What are the operations, E, C2, sigma v, sigma v dashed, so what is chi R, tell me for this representation?

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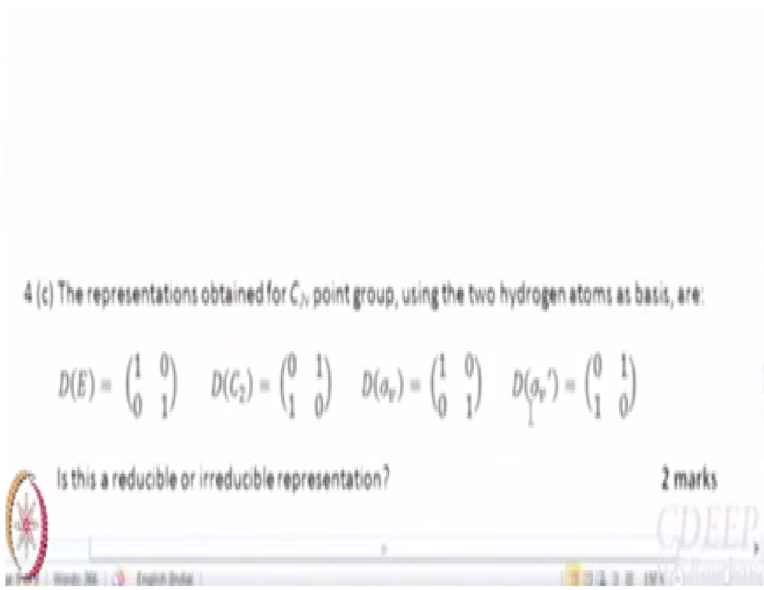

What is chi R for this representation, chi R for E for this representation, what is it? 2; 1 + 1, 2, I am just writing this down, I will show you in a minute, what is chi R for C2, 0, what is chi R for sigma v, 0 or 2, do not get carried away, add and give me the answer, 2, what is chi R for sigma v dash, 0 all right.

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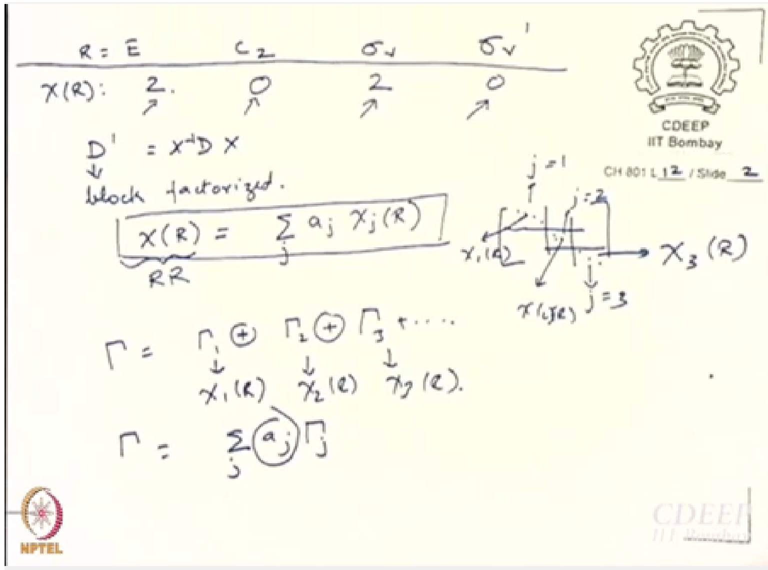

This is all it is, right, 2 0, 2 0, now we are going to learn how to decompose representation into its constituent representations; constituent irreducible representation, now will be it fairly easily. So, see this is a reducible representation, fine, now as you told correctly it is not block factorised but as we also discussed, it is possible to block factorise it by performing some suitable similarity transformation, right.

So, what I can do is; let us say these matrices are D matrices, I can perform some kind of a similarity transformation. I do not know what x is to get is D dash matrices which are block factorised, okay, I do not what they are but then if I block factorise, I can write down the matrices that I will get, can I write down the matrices that I will get if I block factorise, can I write down the matrices that I get, no, what can I write down?

You have started with these 4 matrices whose characters are 20, 20, I performed a same similarity transformation on all these 4 matrices of these representation and I have got another representation consisting of D dash matrices. What can I say about this D dash matrices, okay let us see we can say 2, 3 things, first is that this representation will also be a 2 dimensional, right, what else can I say?

Yes, there would be block factorise that means they are going to be all diagonal matrices, correct, what else, which is another way of saying that it is going to be there going to be all diagonal matrices, can we think these something was discussed earlier in class, we are divide, same cases, right, same cases right, so even for b dashed, b dashed star, the characters are going to be 2020.

Remember, if I perform a similarity transformation, the conjugates of the same cases, we have proved that earlier, is not it, at that time, we are said that matrices in the same class have these same cases but then after all matrices in the same class are nothing but conjugate to each other, they are similarity transformations to each other, so no matter, what similarity transform I perform, the trace is not going to change, the characters is not going to change.

I hope you are not forgotten, what is trace, what is character, right, okay, everybody comfortable with that. So, I think you all agree that even though I have performed this similarity transformation, whereas these matrices are become diagonal matrices there is no reason why the cases will change, the cases are still 2020, I can still work with these same cases, 2020, okay. Now, let me write these, now, if you know of block factorise matrices, then will you allow me to write things like this.

Chi R; chi of R is the character of the transformation matrix corresponding to R in the reducible representation, this is for, I will just RR, RR means reducible representation; these are the characters of the reducible representation. Will you allow me to write that chi R; chi of R = sum over aj chi j R, sum over j, aj chi j R, a is the coefficient, the question is what is j? J is a number of blocks; let us say this is the block diagonalised matrix, right.

So, for this block j = 1, for this j = 2, for this j = 3, all right and for each block, I can get the chi's so this is chi 1 R, this is chi 2 R, making a mess of it, this is chi 3 R, got it. What are these blocks? These blocks are the matrices of the constituent irreducible representations, remember we are written something like this, gamma = gamma 1 + gamma 2 + gamma 3 and so on, block addition, we have done block addition, where the subscripts 1, 2, 3 are the different blocks.

What I am saying is I am working out the characters of each block for each matrix chi 1R, chi 2R, chi 3 R and it is possible that we have some degeneracy, some blocks are same, that is why we have written okay, we have written this equation like this also, right, some over j, aj gamma j, so chi is just the character corresponding to each operation in the jth block, are you okay with this, are you okay for write it like this.

Chi of R = sum over j aj chi j of R, okay, the character of symmetry operation is in the reducible representation is weighted some of the characters of all the nonstudents in reducible representation. What was that? Aj is the coefficient, so you have written aj here also, the point is basically in gamma 1 + gamma 2 + gamma 3 + gamma 4, sometimes it may be possible that gamma 2 = gamma 4, so it does not make sense writing gamma 2, gamma 4 separately.

I will just write 2 gamma 2, j is the number of; yeah, number of blocks, right, so, number of distinct blocks, so if these are irreducible representation, there will be distinct that is right, okay, and we go ahead.

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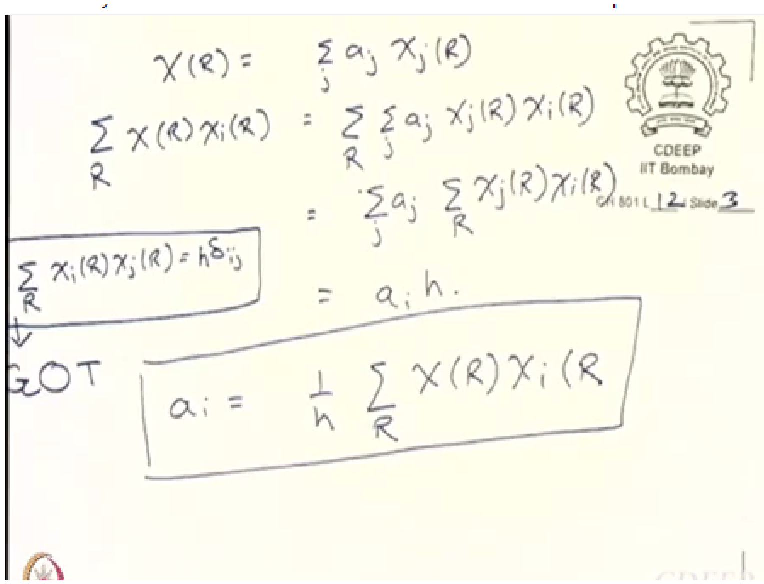

Let us write it again, chi of R = sum over j aj chi j of R, what can I do now, what do I want to do? I wanted to break it down into constituent representations, okay. So, one thing I can do is; let us write, multiplied by say chi iR, where I is one of the j's, I is the specific value of j, so I can be 1, 2, 3 whatever it is, okay, will be = sum over j aj chi j of R multiplied by chi I of R, what should I do next to simplify the right hand side?

You are dealing with irreducible representations, right hand side only has the irreducible representation, right, so what is the relationship between the chi's, yes, delta j means what happens, if I sum over all the symmetry operations, then that Kronecker delta will come, right, so what I can do is; on left hand side, let us say sum over R or right hand side also will put sum over R, all right.

So, I can perhaps write it like this, so what will the right hand side simplify into? Sum over chi a sum over j, so what should I do next, what does great orthogonality theorem tell us; does it not say sum over R chi i of r chi j of R = delta j, is this not a consequence of; do not insert an A before the T, what happens if you insert A before the T, instead of a theorem, you get an animal, right.

So, great orthogonality theorem tells us this, right, right or wrong? Right, is not it, so what I will do is I will just put it like this sum over j let us say aj and sum over R chi j R chi I R, this is not delta aj, what is this? H delta aj, do not forget that okay, H delta aj. Now, so what does the right hand side become? See each one is a specific, I is a specific value, j is the variable, okay, so j is going to go for 1, 2, 3, 4, 5, 6 and I is something.

So, what are the terms that will survive? Only chi i of R, only that will survive, which coefficient will survive, only ai, right, so will you allow me to write it like this, ai * h, right that is a nice relation, so what is ai then? 1/h sum over R, left hand side does not change, chi of R chi I R, okay, so this is the relationship that I want you to remember even if I barge into a room in the middle of the day, wake you up, I need not say night, day, wake you up.

And ask you what is the relationship is, all right, we will use this very frequently. So, what does that means, so that means the coefficient is 1/h sum over R chi of R chi I R, then what you do, you have these 4 chi's, right, 20 20, you take each, multiply it by the character that you have for whichever irreducible representation you are dealing with, right and sum over all R's, all right, so let us see.

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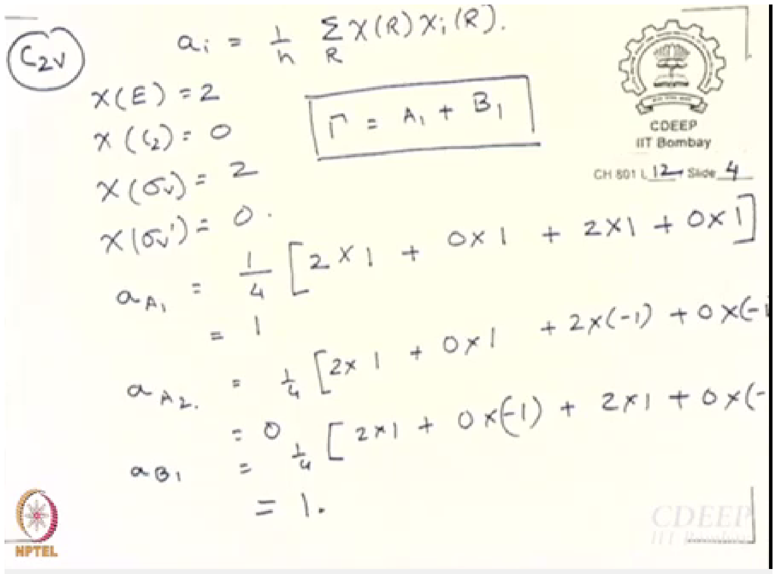

Which point group is this, C2v, visible, yeah, yes, yeah, do not forget that we have class on Thursday at 5:00 pm, for those who came late, we have class on Thursday at 5:00 pm, no class on Friday, then again class on Monday, Tuesday and Thursday next week at 5:00 pm, week after that we have class at 5:00 pm on Monday, I will give you some Pooja homework, Durga Pooja is there from that time, yeah of course, you will get Pooja holidays.

We have 6 6days of holidays this year I think, okay. Do you have character table with us, I do, so what you do is; please let me write the relationship first, ai = visible right, 1/h, sum over R chi of R, chi i of R, okay and let me also write down what was chi E in all reducible representation, what was chi E, chi of E; 2, what was chi of C2, 0, chi of sigma v, 2, chi of sigma v dashed, 0, right.

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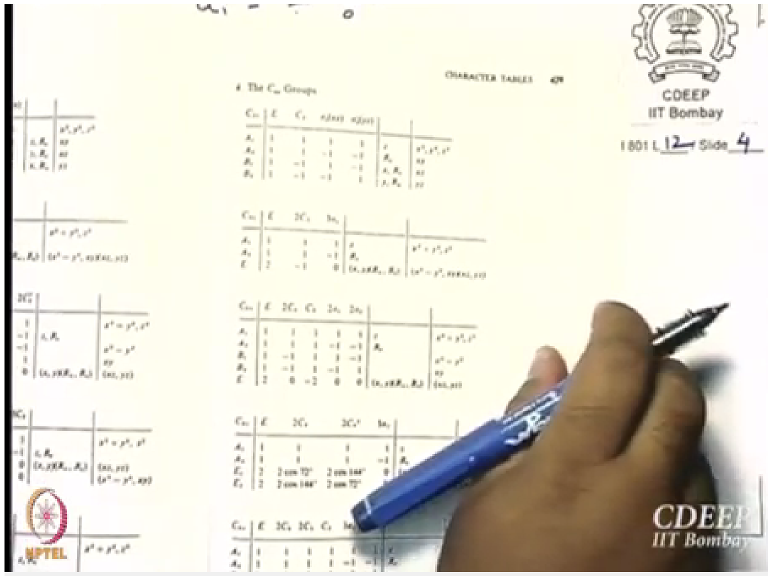

Now, I will show you the character table, here it is, can you read, yes or no, even if you do not you cannot read, you know the first line at least, right, first symmetry species, a1, what are the characters, what are the chi I’s for a1, 1111, totally symmetric representation, right, so what we can do is; I can just try to see what is the coefficient of; I can write it like a, A1, I could also write just small a1, just to make it more obvious will be =; what is h?

4, everybody is convinced, h is 4, multiplied by chi of E is 2, multiplied by chi i of E is 1, right + chi of C2 is 0 multiplied by chi I of C2 is 1 + chi of sigma v is 0, so why fee and why so late, multiplied by chi I of sigma v is 1 + chi sigma v dash is multiplied by chi I sigma v dash is -1, 1, what is the answer? Very difficult to simplification, you might (()) (19:54) can do this, 1, all right.

So, what is the next one, A2, right, what are the characters of A2, even if do not show you, you should able to tell me, 1 1 -1-1, very good, so now let us work this out, a A2 will be = 1/4th 2 multiplied by 1 + 0 multiplied by 1 + 2 multiplied by -1 + 0 multiplied by; does not matter, what is the answer? 0, okay, D1; even if do not show you, you should be able to tell me, $1/4^{th}$; what is it, 1 -1, 1 -1, very good, so 2 multiplied by 1 + 0 multiplied by -1 + 2 multiplied by 1 + 0 multiplied by -1 = 1.

Is there any need to work out, aB2, is there any need for me to work out aB2, there is not because see your reducible representation was 2 dimensional, you have already found that representation is the sum of 2 one dimensional representation, so the fourth representation cannot have any contribution, still if you want to you can work it out, since you do it for the first time? What is B2? 1 -1 -1 1, work it out, what is this aB2.

So, will you allow me to write gamma = A1 + B1, all right, so what have we learnt, so you finally learnt how do you decompose a reducible representation into its constituent irreducible representations and you see you do not have to do any complicated mathematics anymore, we do not have to do stimulated transformation, we do not have to even remember unitary transformation, nothing.

All we need to do is; all that complicated math has given as this (()) (23:01) that is why it is called great orthogonality theorem, this the greatness, you can use it and you can decompose any reducible representation into its constituent irreducible representations, not necessarily, **"Professor – student conversation starts"** why do you say 4, I am sorry, 4 classes, yes, oh, no, no, that was not the character table.

I am not saying that, see what we are saying is; what should the character table look like that we know already that the character table should have 4 but now here, what I have done is; I have given you 4 matrices which make up 1 reducible representation. Exactly, yeah, no, you cannot get 3 1 by 1 matrices, why do you get 3, no, no, it depends on the dimensionality of a bases, the dimensionality of the bases will determine the dimensionality of the representation.

It is not change in the character table, we are using the character table to find out what are the constituents of the reducible representation, we are not trying to write the character table again, understand, character table of course, that we have worked out already but while you worked out character table, did you work it out for bases, with bases, no, right, you work it out using great orthogonality theorem, so that is part 1 of the story that is done.

Now, knowing that part 1 of the story, what we are trying to do is; now we are generated some reducible representation using some bases of our choice, it is not necessary that the dimensionality of the bases of our choice has to be the order of the group, it has to be less than the; it can actually as you will see in the next example, it can be more than the order of the group also, it can be anything.

Now, we want to break it up into these constituents that is all, no, you would not, you will get the number of bases, the sum of whose dimensionalities should be equal to the number of elements in the bases. See, what has happened, you are taking xyz, you got 1 dimensional representation earlier and this one we are decomposed into 2 one dimensional representation, right. So, 1 + 1 + 1; 3, as a dimensionality bases were also 3, what was that? How will you get 4?

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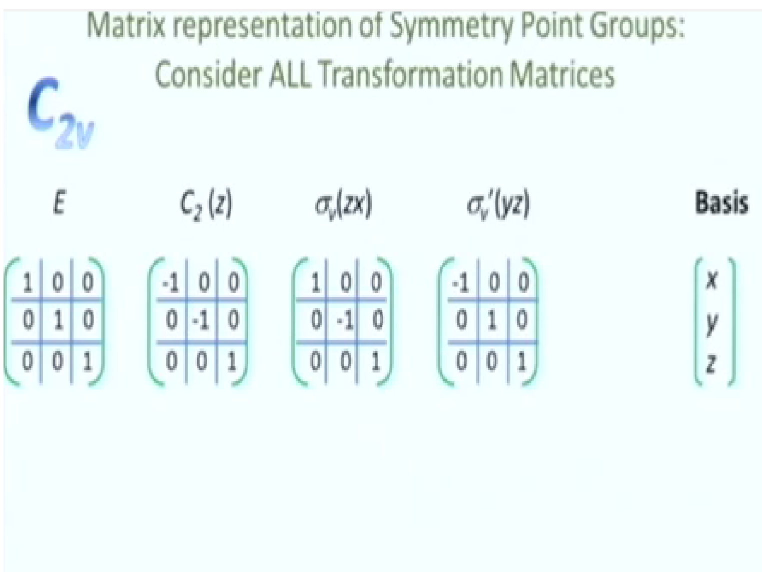

Because the thing is your matrix will always be 3 by 3, know if you take xyz, you cannot get 4 by 4 matrix, is not it, you got 3 by 3 matrices, you did not get 4 by 4 matrices. The good thing about technology is that everything is here, okay, so these are the; this is the bases we worked with hold on a minute, you got 3, right but you need get all 4, okay, convinced but there is an important point that Ocher has made that the dimensionality of the reducible representation has to be the same as the dimensionality of the bases you use.

And it also has to be the same as the linear sum or weighted sum of the dimensionalities of the constituent irreducible representation, are you all okay now? Is there is a question please ask, before we move ahead? So, let us saying is that if you have a bases right, 3 dimension, 4 dimension, let us say 5 dimension bases, so if I have a 5 dimensional bases, can I have a 5 dimensional bases, can you think of an example?

Yes, you say 5, (()) (28:11) D orbitals naturally, so I can use this D orbital as my bases, so I have a 5 dimensional bases that means all the matrices I generate from the transformation matrices there will be all 5 by 5 matrices, right, so this reducible representation that I get by taking a combination of these transformation matrices that irreducible representation is going to have a dimensionality of 5, right.

So, what I am saying is now suppose, you are able to break it up into 2 sets of matrices, okay, 2 irreducible representations, then I am saying that suppose, gamma 1 and gamma 2; 2 irreducible representations are there, then the dimensionality of gamma 1 and the dimensionality of gamma 2 should also adapt to 5 and your book is a good example that is why I took 3 and 2 because in octanited field, you know the D orbitals gets split into 2 groups as you know.

What are the groups? T2g and Eg now that you know the nomenclature, tell me what is Eg, what will be the dimensionality of Eg,, 2, what will be the dimensionality of T2g, 3, what is 2 + 3, 5, so that is what I was talking about, okay, make sense, will be may get reputations, yes but even if it is not more than the order of the group, you can have reputations, right it has to be. **“Professor – student conversation ends.”**