Symmetry and Group Theory
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Lecture - 27
Reducible to Irreducible Representation using GOT

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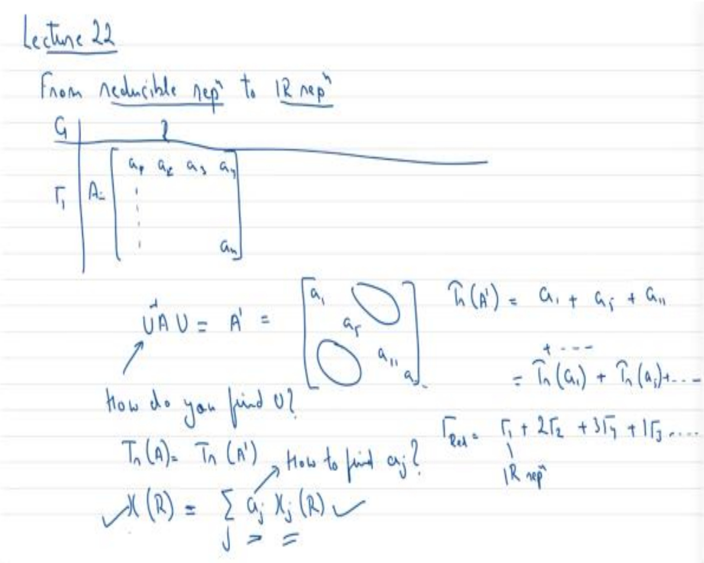

So, in the previous lecture we have seen how to write from scratch, how to use a great orthogonality theorem and use it to write from scratch the irreducible representation all the irreducible representation that constitute the character table of a given point group. So, we have taken example of C2v and C3v point groups and we worked out using that, and I expect that you would do it as a homework assignment to pick up few points groups.

And do it yourself all the calculations to see if you are able to write the character tables given any particular point group. So, now, in this lecture what we will see is how do we go from reducible representation to irreducible representation, so, reducible representation has its own importance and irreducible representation has its own importance, all the properties which lie along the unit vectors, which form a basis for irreducible representation are defined by irreducible representations.

And then we still have to use certain basis sets to actually identify, we will see that later when we discuss the applications that we have to write down reducible representations and then we have to actually reduce it to a IR representation. So, let us see what is the basic idea? So, the idea is let us say if we choose any basis set and matrix under any given symmetry operation are for any given point group or let us say, this is the character table we are writing and then we have any given point group G, and let us say this is tau 1.

So, under any given symmetric operation, we have certain matrix, the order of the matrix will depend on the basis set chosen. So, this can be a diagonalized matrix or non diagonalized matrix. So, this will have matrix elements such as so let us just call it a1, a2, a3, a4 and so on. So, I am not giving you the final dimension, so, it can be any dimension. So, now, we have to diagonalize it to be able to reduce it, and how do we diagonalize it sometimes you will get diagonalized matrix by itself.

But many a times you have to actually diagonalize it. How do you diagonalize it? Let us call this matrix as A. So, to go from A to A prime you have to find a matrix U that we have seen earlier that you can do it and you go to A prime where A prime is a diagonalized matrix, what do you mean by diagonalized matrix? That you will have matrix elements only along a let us say 5, a 11 something. And rest everything here and here will be 0.

So, these are called as diagonalized matrices, which you can obtain by doing a similarity transformation on A, but for that you have to the important point is how do you find A. This is not a trivial thing. How do you find U? How do you find U and U inverse? Which is not trivial, which will give you a diagonalized matrix. So, how do you do that, how do you find this out? The important point here is that trace of A is equal to a trace of A prime that we have seen similarity transformation does not change the trace of the matrix.

And we also know that because this is a diagonalized matrix. So, all the individual matrix elements will actually come from the irreducible representations. So, the trace of A prime as individual matrix elements a1 + a5 + a11 which are nothing but a trace of a 1 matrix it can be 1 cross 1 or 2 cross 2 and so on. But it is an irreducible representation or trace of a5 and so on.

So, this means that I can always say that the character or trace of a given irreducible representation under a symmetry operation is equal to so, this is nothing but trace of A prime. So, this will be equal to linear combination of let us call it as j, a-j and this will be character jth representation under the symmetric representation symmetry operation R. So, now this is a linear combination it can be a1.

So, for example, this number can appear twice here same number can appear twice. So, what I mean is that you have tau let us say a reducible tau can be tau1 + 2tau2 + 3tau4 + 1tau3 and so on. So, these are individual IR representations so, tau reducible is composed of several IR representations. So, tau reducible is a linear combination with some coefficients because we do not know how many times tau 1 will appear in tau reducible, how many times tau 2 will appear in tau reducible so, that is defined by this coefficient a-j.

And this is the character of jth irreducible representation under symmetry operation R. So, this is very clear that any irreducible representation can be broken down into a linear combination of irreducible representations. Now, the problem is we do not know how to find a-j. So, we do not know this. We know how to write it from scratch how to write irreducible representation from scratch.

So, this we know we know how to write a reducible representation given under any basis set, we know this. So, we can find out the trace of any matrix under any reducible representation. So, this is also okay this is also okay but we do not know how to find a-j. So, let us see if we can actually do this maths.

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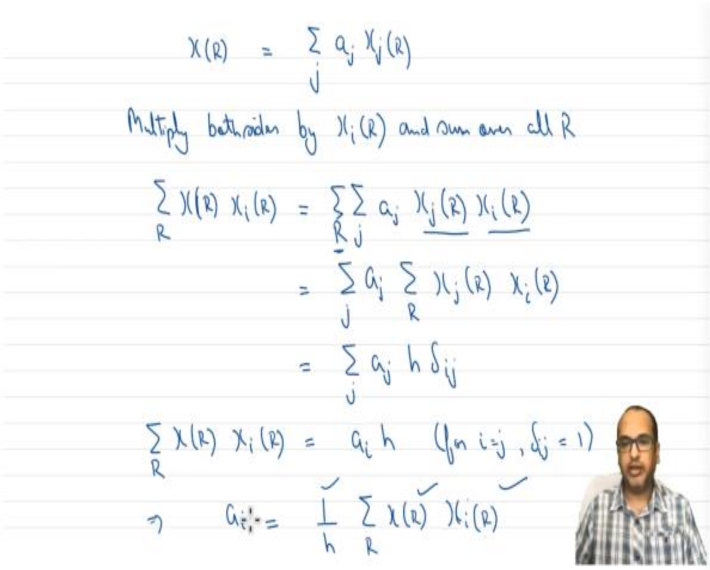

And write down this again so, chi R is equal to summation over all j, a-j chi jth representation and chi. Alright, so now, let us say if we multiply both sides by chi i R and sum over all R. So, if we do this, what do we get on the left-hand side? We get chi R chi i R summation over all R and what do we get on the right-hand side? Summation j summation R a-j chi j R chi i R now, let us see what do we have here.

So, we have this term, we have this term and we have this. We can always take a-j out of the summation of R. So, I can say summation over j, a-j summation over R chi j R chi i R. Now this is a familiar figure from third property of GOT, which we have discussed already this amounts to h delta ij. Character under any given symmetry operation product of 2 different characters for 2 different IR representations under a given symmetry operation and summation over all symmetry operations would give you order of the group multiplied by delta ij so, this is there.

Now, we have summation over j summation over j means that all the values of j we have to take, but the only value of j that will survive which is equal to i, all other summations here will go to 0 because we have delta ij down here. So, this means that the only j value that is equal to i will survive. So, now that summation is expanded so I do not have to write the summation.

So, what we have to do is now j becomes i, and what we are left with is h because for i = j, delta ij = 1 for all other j values, this goes to 0. So, we are left with a-i h and here we have summation R chi R chi i R. Now this problem is very simplified here, we want it, how do we get a and we have got it. So, 1 over h summation over all R characters under reducible representation character under irreducible representation. So, we know this, we know this, we know the order of the group, so we can calculate a-i. Now let us take an example to see whether we can do it or not.

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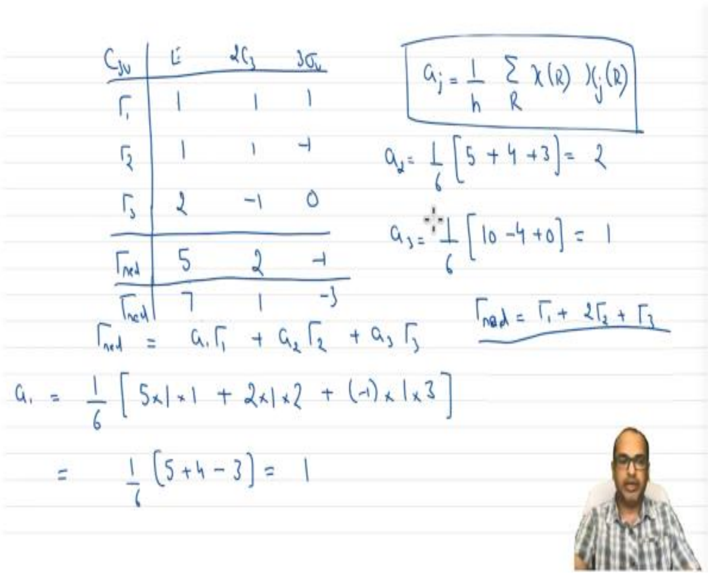

So, let us take again C3v point group example. So, now I am assuming that you are able to write all the irreducible representations by yourself using the rules of GOT. So, you have E, 2C3, 3 sigma v, again, because I am writing only the traces, so I am combining the class elements here, because class elements will be same. So we have tau 1 as 1, 1, 1 tau 2 as 1, 1, -1 we have seen this earlier and tau 3 is 2, -1, 0 there are 3 reducible representation, because there are 3 classes.

Now, let us say I have chosen certain basis set, where I get a reducible representation as well, I do not know to start with whether it is a reducible or irreducible. So, you can always test it as we tested for water example, whether this will be a reducible representation or irreducible representation, again, using rules of GOT. So that also, I am assuming that you know, how to distinguish between whether it is a reducible or irreducible representation.

So now, once you have written the character table, and you have written the reducible representation under certain basis set, that is it some basic set. So now, as per this rule, so we should have a1 tau 1, a2 tau 2, this is what we defined earlier a3 tau 3. So now our job is to determine what is a1, a2 and a3? So that we can break down this tau reducible into linear combination of the irreducible representations so let us determine a1 first. So, for a1, we have to write 1 over h, what is h here, h is 6, 6 elements, so h is 6.

Now you have to take summation over all R and we have to multiply the trace under tau 1 to the corresponding value of tau, which is basically what I am saying is a-j = 1 over h summation over all R character under reducible representation and character under irreducible representation. This is what we are going to use. So, what I am going to do is I am going to pick up 5 and multiply it with 1, then pick up 2, multiply it with 1, and then pick up - 1, multiply it with 1, and then summation.

And I am also going to tell you one more point here that the class sizes also have to be multiplied here. So let us just see that class sizes have to be multiplied with this multiplication because each class element has same trace. So instead of repeating that, we will just multiply it with 2. So, we will see that so 5, which comes from here, then you have 1 which comes from here into class size, which is 1 over here, then 2 into 1 into class size.

So, this is very important that you multiply it with class size, plus - 1 into 1 into 3. Remember, we have to take summation over all symmetry operations, and if we do not multiply it with class size that means we are not taking summation over all symmetry operations because then we will leave out C3 square or we will leave out sigma v2 and sigma v3. So, we have to include all of this so, that is why this multiplication with class size is important. Now, what do we get here? This is 5 + 4 - 3 / 6.

So, what do we have here 1 so, a1 is 1 that means contribution of tau 1 into this reducible representation is 1 times. So, we can, ok let us go ahead and do for a2 so let us do it here. So a2 again this will be 1 / 6 and then I will just do this 5 + 2 into 1 into 2 that is 4 - 1 into - 1 into 3 that is + 3 this gives me a2 as 2, and then a3. And now, to test whether your calculation is correct or not, these numbers have to be natural numbers or whole numbers 0 can also come, whole numbers.

So, because this cannot be in fraction contribution of any given irreducible representation cannot be in fraction for a reducible representation so again so 5 into 2, 10, - 4, and then 0. So, what do we have here 1, so, that way I can say that tau reducible is equal to tau 1 + 2 tau 2 + tau 3. So, this is a very, very important result that now we are able to write any given reducible representation into a linear combination of irreducible representations, we will see that how important this is when we will get down to applications.

So, for home assignments today, so, let us take this example and try to reduce this; another tau reducible will be; which is 7, 1 and - 3 so, try to work it out. See if you can find out the linear combination of tau 1, tau 2, tau 3 here so, that is all for this lecture. So, that now, we have learnt how to write down a reducible representation, we already knew how to write down a reducible representation.

We already knew that how to write an irreducible representation from scratch without worrying about what the basis, elements are? Or what the basis sets are? And what the effect of symmetry operations are and so on entirely using GOT. And now, we have seen how to convert a reducible representation into irreducible representations, linear combination of irreducible representations.

So, that ends the great orthogonality theorem discussion, and next class we will be discussing the character table how to, like what are the different portions of character table what is it constituted by what are the important regions, where are the basis sets identified and so on so forth. So, that will be done in next class. Thank you.