Symmetry and Group Theory
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Lecture -35
Direct Product

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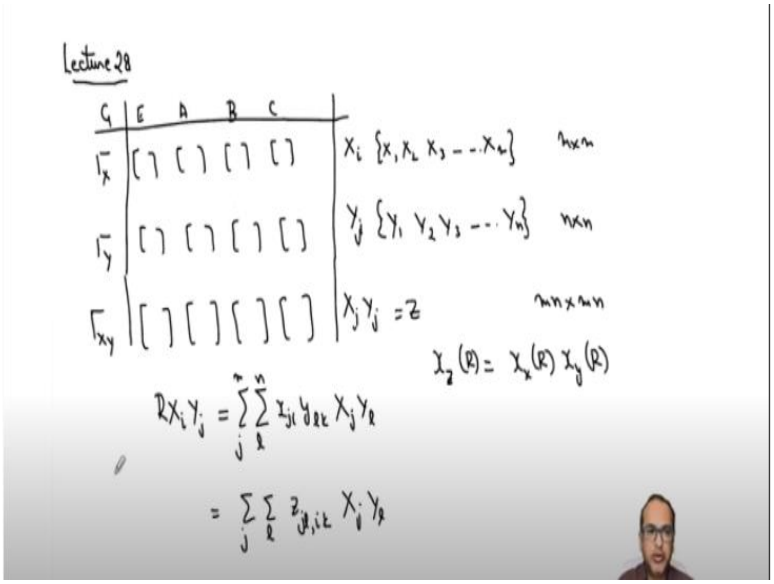

So, in the previous lecture we were discussing direct products. So, let us see what we discussed. So, we saw that if we have a group, point group with these are my symmetry operations and if I have Xi as the linear combination which consists of various functions X 1, X 2, X 3 and let us say X m and another basis is Y j where j varies from 1 to n, Y 2, Y 3 up to Y n. If these two form the basis of the representation then my representation would be written as certain matrices and in this case these are the characters basically.

And if I have the direct product of this also forming which will also form the basis of my symmetry operations then in that case I will have another set of matrices which will form a representation. And I call this representation as tau xy. Now in this case I can always write that R when it is operated on X i Y j then I get summation what we get was x j i and y l k, X j and Y R. So, double summation with j and l going to corresponding values of m and n and then we also saw that we can replace this to a single number.

Because this is a product of numbers simply. So, I can write this and the indices will be written as jl, ik. So, basically this means here is if this is my m cross n matrix and this is my n cross n matrix what I get here is m n cross m n matrix. So, z basically represents the matrix element of m n cross m n. That is if I have a three cross three matrix here two cross two matrix here the direct product matrix will be a 6 cross 6 matrix.

So, writing this and then dealing with such matrices is not straightforward and it is rather cumbersome. So, what we do is we will see what is the trace of these systems. So, basically here what we have shown is that the character under z where z is the product of the two. So, I can write it as z. And under any symmetry operation is the product of the two characters. This we have seen.

Now this means if these numbers are one digit numbers that is 1 cross 1 representation then the characters get multiplied directly. But if these representations are degenerate representations that is m 4 degenerate and n 4 degenerate then the corresponding matrices or the corresponding characters are we have m cross m and n cross n characters. And then we have to take a direct product of those matrices to actually get to the representation of the direct product.

So, now what we will do is we will rather work with traces and we will see why because working with traces actually simplifies the product here.

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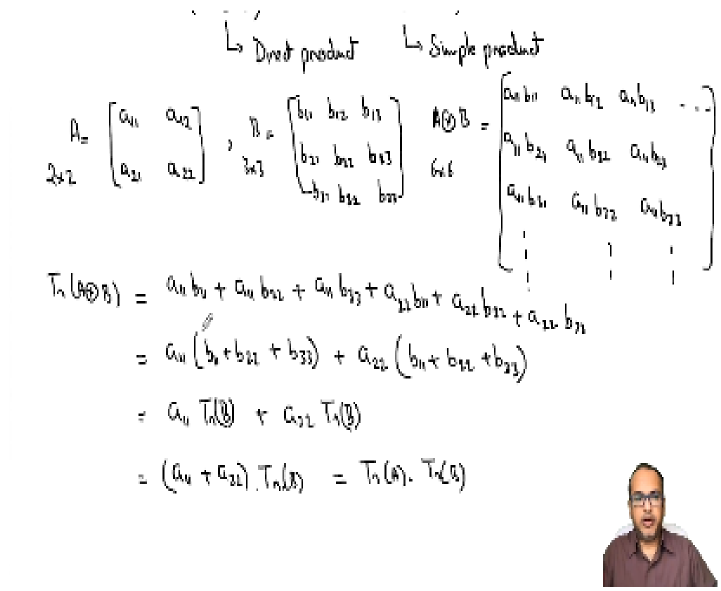

So, what we will show here is the trace of a direct product of two matrices so which is basically here. So, this is the direct product of two matrices here this matrix. This set of matrices is equal to product of trace of matrices. That is very good point now let us say. So, what we are saying here is that if we take a trace and multiply these two what we will get is we will get a trace of this. Trace is basically sum of the diagonal elements where trace is you can say sum of the diagonal elements.

So, carrying out the multiplication of the two matrices to obtain a direct product is not as trivial and then working with traces is much better, because we will show that trace of a direct product of two matrices that is trace of this matrix is equal to product of the two traces. Now let us see how to get that. Let us say mathematically what we can write. We can write this statement as trace of A cross B.

Now the direct product is denoted by this symbol. So, this means direct product. So, we are saying that the trace of direct product of two matrices, matrix A and matrix B is equal to product of trace of A into trace of B. So, now notice that this multiplication is a simple product. This is a simple product. Because these are just the numbers. So, numbers can always have only the simple product whereas the two matrices have a normal matrix multiplication or a direct product.

So, this is a direct product. So, now let us write the two matrices with different dimensions just to make it general. So, let us call it as 2 cross 2 matrix or let us call it as 2 cross 2. So, we will say a 11 and a 12 this is equal to a 21 and a 22. And let us call another matrix which is let us call it as 3 cross 3 matrix. Let us say b 11, b 12, b 13, b 21, b 31, b 22, b 23, b 32, b 33. So, now if we have to take the direct product what we do is A direct product B.

Now if this is 2 cross 2 if this is 3 cross 3 what we will end up is, we will end up in 6 cross 6 matrix. So, that means each of this element will be multiplied by each of this element. Now that gives you a 11 b 11, a 11 b 21, a 11 b 31. So, I have multiplied a 11 first, I picked up this a 11 over here and multiplied with all the matrix elements here like this. So, a 11, b 12, a 11, b 13. Similarly here we will have a 11, b 22, a 11, b 23, a 11, b 32, a 11, b 33.

So, so on you will get 6 cross 6 matrix. I am not going to write the full representation here so full matrix but you got the point. So, next element will be a 21 multiplied with all 9 elements of the b matrix. So, now if we want to calculate the trace of A cross B, A direct product B we will have to take all of these elements and make a summation. So, that means this is a 11 b 11 + a 11 b 22 + a 11 b 33 and the right end 6 elements right the corner will get basically this multiplied by all of this.

So, we will get a 22 b 11, a 22 b 22 + a 22 b 33. This will be the trace because these will be the 6 elements along the diagram. So, now I can say that I can take a 11 common from here and what do I have here is b 11 + b 22 + b 33. And I can take a 22 common from here and I get b 11, b 22, b 33. And this is nothing but trace of B and this is nothing but trace of B. And if I take trace of B common so I get a 11 + a 22 trace of B.

And this is trace of A over here. So, trace of A into trace of B. So, now my life is easier because if I know the trace of this and this, I simply have to multiply the two numbers to get the trace of this matrix. So, that is why working with traces is much more convenient. So, we will be working with traces here. So, now let us take an example over here.

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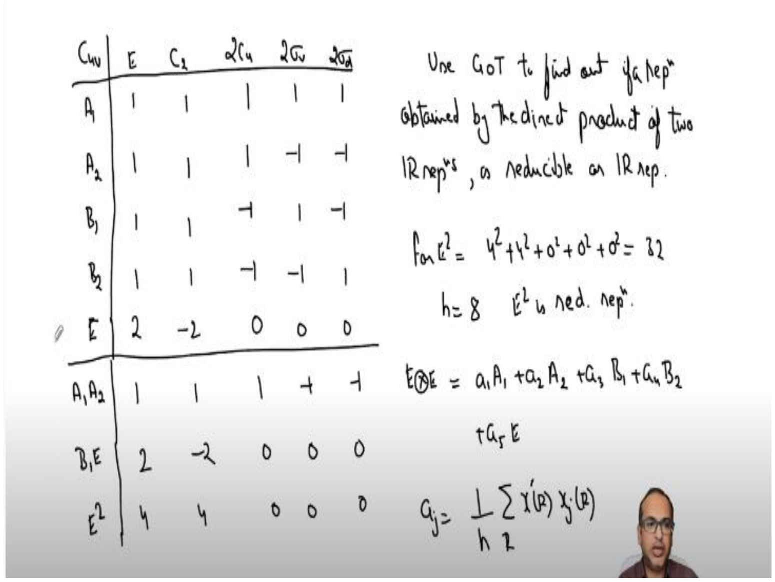

So, let us take an example of C4v and elements are E, C2, 2C4, 2 sigma v, and 2 sigma d. And the representations I have is A1, A2. So, I am writing the symbols now, B1, B2, and E. Let us also do some exercise of what information we can get from symbols. So, A1 that means this is one dimension, one dimension, one dimension, one dimension. This should be two-dimension. So, we can write down the characters.

Now because this is one and two that means the principal axis here will be C4. So, principal axis will be positive here. And replaceable access will be negative here. And then this we cant tell this is C2 polymer with principal axis and then from sigma v we can say that this will be positive because this is A 1 and this will be negative because this is A 2. Similarly positive negative and this also we cannot tell from symbols.

So, we have to look at the notes, minus 1, 1 and the rest of this also we cannot tell 0, 0, 0. But we could still fill a lot of character table by just looking at the Mulliken symbols. So, now let us say if we take a representation for where we have direct product of A1 and A2 so we can write down the product of the two traces and we will get 1, 1, 1, - 1, - 1. Let us take another example. Let us say if we obtain a direct product of B 1 and E so what do we get?

2 - 2 and then we have 0, 0, 0. So, these are all zeroes. We can also do a direct product with self IRs. So, E cross E will be equal to 4, 4, 0, 0, 0. Now whether this A1 and A2 is reducible or

irreducible that you can always use great orthogonality theorem to find out if a representation obtained by the direct product of two IRs, two IR representations is reducible or irreducible. So, for example, if we say A1 A2 this we can directly see that it is a irreducible representation.

Because it is composed of only A2. Similarly, B1 E we can say that this is also irreducible representation because it is only composed of E. E square, however, we can say that it does not belong to any of this so it has to be a reducible representation and we can also test it. So, for E square, for example we can say sum of squares of characters is 4 square + 4 square + 0 square + 0 square + 0 square, this is equal to 32.

Whereas our h is 1, 2, 3, 4, 5, 6, 7, 8. So, since these two numbers are not matching that means E square is a reducible representation. So, that should be very easy to find out. So, now how do we find out the components what constitute E square? So, we can do that also. So, E cross E is equal to we can say a1 A1, a2 A2, a3 B1, a4 B2, and a5 E. So, remember the reduction formula which we use so a j is equal to 1 over h summation over all R chi R and chi j R.

So, this was the reduction formula which we derived earlier so where this is the character under reducible representation, this is the character under irreducible representation. And we can actually find out all the E s corresponding with this. So, let us see for this we will work it out.

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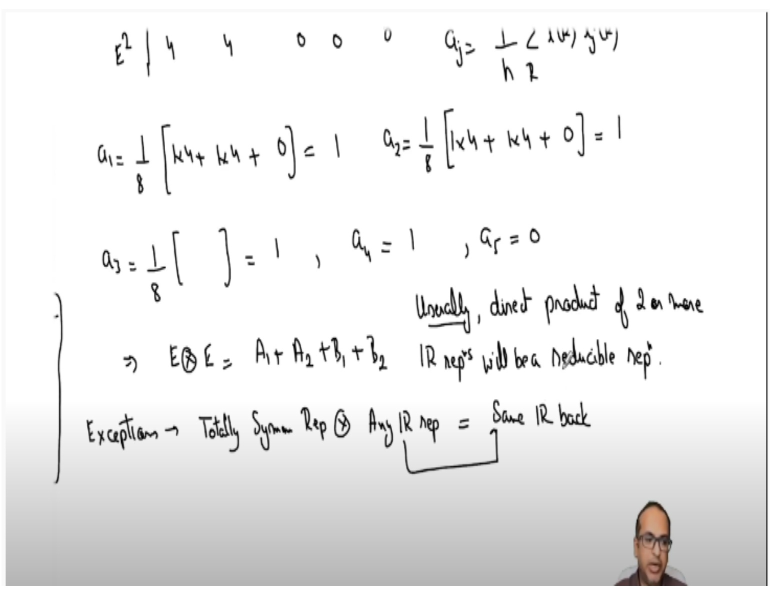

So, for a 1 let us say 1 over 8 and we will have so this will be 1 into 4 + 1 into 4. So, what I am doing is I am making a product of 1 into 4 + 1 into 4 plus whatever product. It does not matter because it is all 0. So, this will be 4 + 4, 8 so this will be 1. So, that means there will be A1 component present. So, let us do for a2. So, a2 will be 1 over 8 1 into 4 + 1 into 4 plus again this will be all 0.

So, we will have at least one A2 present. Let us move forward. For a3 we have to now multiply with b1 characters. So, 1 over 8 and doing the same thing what you will get? You will get one I have not done the complete calculation here, but what we will get is 1 and a4 also we will get 1. And we can see that a5 will be 0. So, this implies that E direct product E will be equal to A1 + A2 + B1 + B2 and that is all.

So, we can see this. So, if we make a sum of this 1 + 1 + 1 + 1 = 4 and then again 4. Now 1 + 1 - 1 - 1, 0. Again there are two positives, two negatives so 0, two positives two negatives 0. So, it is very clear that this is a reducible representation and it gets reduced to A1 + A2 and B1 + B2. So, that is also very clear. So, we can say here that usually direct product of 2 or more IR representations will be a reducible representation.

So, I use about usually here because there are exceptions. Exceptions are if you are multiplying totally symmetric representation into any IR what you will get is that same IR back. Because totally symmetric representation is all ones. So, multiplying anything with all ones will not change anything and then you will get the same IR back. That is very easy to see. So, let us also see a few more or one more rule.

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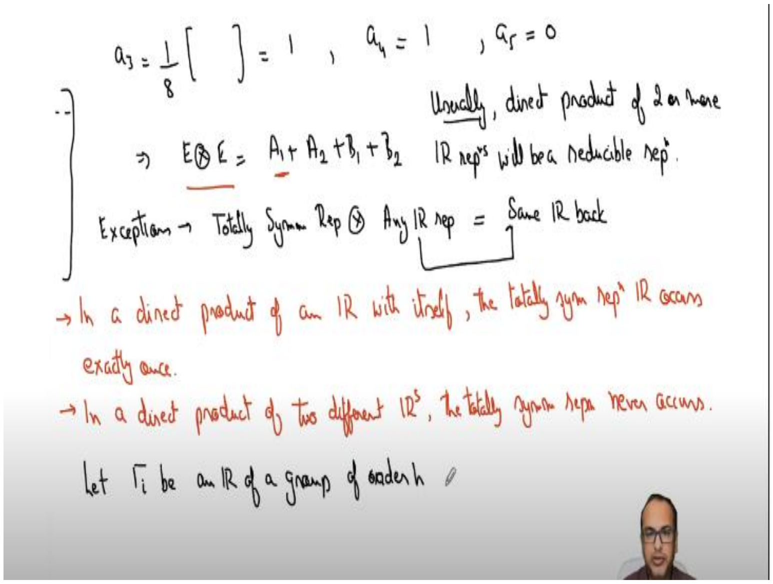

So, this is a rather important rule so pay attention to this. In a direct product of an IR with itself, the totally symmetric representation I am not saying it as A or A1 because in different point groups the nomenclature or molecule symbol for totally symmetric resolutions can be different. Somewhere it can be A, somewhere it can be A1 and so on. But it will always be A or A1 or something similar to that. But here we will use the general term totally symmetric representation IR occurs exactly once.

So, if we take the direct product of an IR with itself, like we took direct product of E with E here in this example over here. So, we saw that A1 comes only once. So, that is the totally symmetric representation will definitely come and it will come only for one time. So, totally symmetric representation occurs exactly once and we will also see that we will show both of these in one go. So, I am just writing it together.

In a direct product of two different IRs, the totally symmetric representation never occurs. So, that means in the product above if we see here in for example, we did this B1 E. The B1 E this is the product of two different IR representations and in this case B1 E is actually equal to only E. So, there is no other representation. So, that means in B1 E this will never occur. So, similarly if we do A2 into B1 or A2 into B2 or A2 into E or B1 E or B2 E in any of these direct products A1 will never come.

That is what it says. And if we do self-product A1 will come and it will come exactly for once. So, this is what it says that in a direct product of two different IRs the totally symmetric representation never occurs. So, let us try to see, let us try to prove it. Let tau i be an IR of a group of order h.

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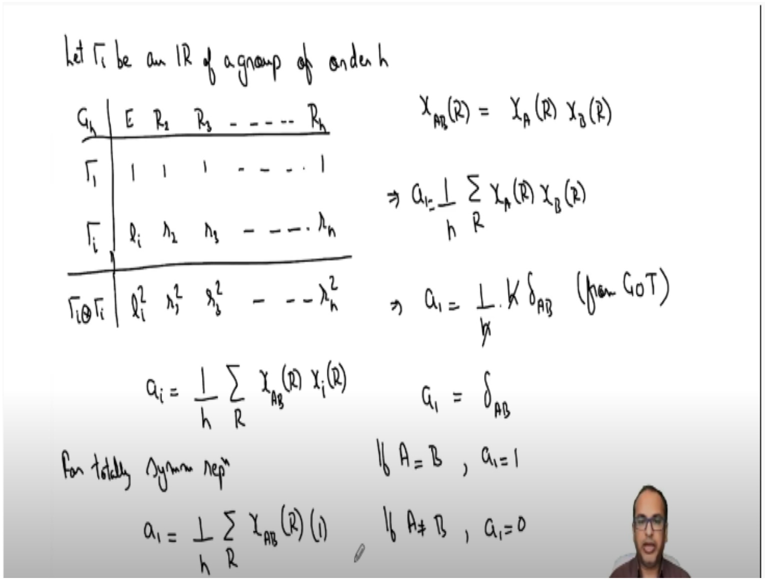

So, what I mean here is that if we have a group of order h, let us call it as G h, then I can say that this is E, R2, R3 and upto Rh. I am not classifying these as different classes. I am just writing R1, R2, R3, R4, Rh and R1 I am simply writing as E. So, let us say I have a tau 1 which is the totally symmetric representation, so I will have all ones here. And I have a general IR which is tau i. So, that means here it will be li which is the dimension of this.

It can be one or anything and then I will have different characters or matrices depending on the dimension of this r2, r3 and so on rh. Now if I do a direct product of tau i into tau i, what do I get? I get li square then I get r2 square, r3 square, rh square. So, here now if I want to find out the component IRs of this, then I can say that ai is equal to 1 over h summation over all R, this is directly from reduction formula. So, this is character under direct product and this is the character for the corresponding irreducible representation.

So, for totally symmetric representation if we want to find out what is the component for totally symmetric representation, we can say that this will be a1 and this will be tau 1 here. So, I can say that a 1 is equal to 1 over h summation over all R chi AB over R and this will be character under any symmetry operation corresponding symmetry operation which will be actually 1. So, that product is not to be written because this will be 1. It will always for all R it will be always 1. So, this implies that I can write my character as chiA R chiB R.

So, I can always use this equation here. So, a 1 is equal to 1 over h summation over all R, chiA R where A and B are two irreducible representations. So, that means I can say that from great orthogonality theorem I can say that this is 1 over h into h delta AB. So, summation over all our character of two IR representations gives you delta. We have learnt this in terms of chi i, chi j and this will be delta i j. Remember so this is directly from GoT properties.

So, if you go back and look at the lectures where property is, five properties of GoT discussed we had discussed this one. So, that means now h is cancelled here, so this is basically delta A B. So, a1 is nothing but delta A B. So, now you can say that if A is equal to B, then a1 is equal to 1. And if A is not equal to B, then a1 is equal to 0. So, now here we have shown the first case which we wanted to show if in the direct product of an IR representation with itself where A will be equal to B basically.

So, a1 is equal to 1, a1 means the totally symmetric representation will come only once and it will always come, it will come only once. If the direct product is of two different IR representations, then a1 or that is the totally symmetric representation will never come. So, that is also easy to see. So, I think that is all for this lecture and now next class we will see how do we use direct products.

So, those examples we will see what is the actual application of direct products in solving some problems of quantum mechanics that we will see in next class. Thank you.