Group Theory Methods in Physics
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Lecture – 20
Great Orthogonality Theorem and Character Table – II

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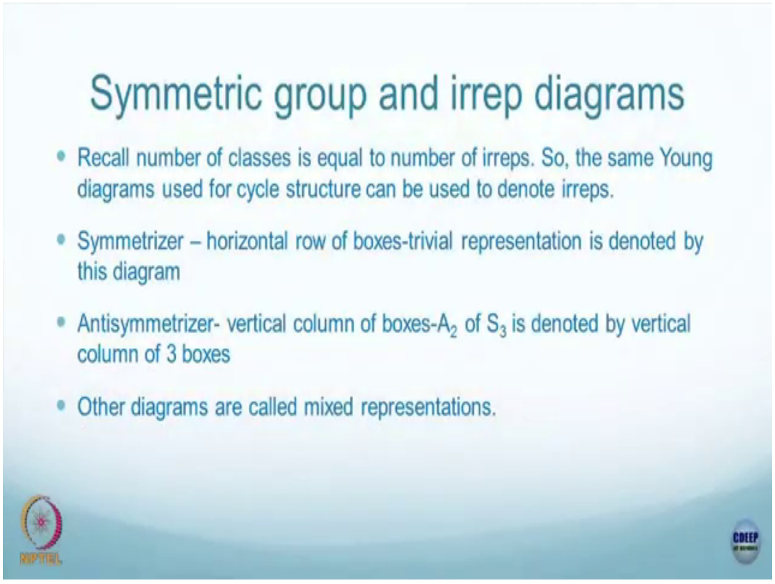

So, recall the number of classes, number of irreps. So, the same Young diagrams which we use for the cycle structure can be used for symmetric groups to denote irreps. Symmetrizer is a horizontal row of boxes; there is only a trivial representation that will also be the unit representation ok. Antisymmetrizer is a vertical column of boxes which is denoted by vertical column of 3 box for the symmetric group of degree 3. Other diagrams are mixed representations ok.

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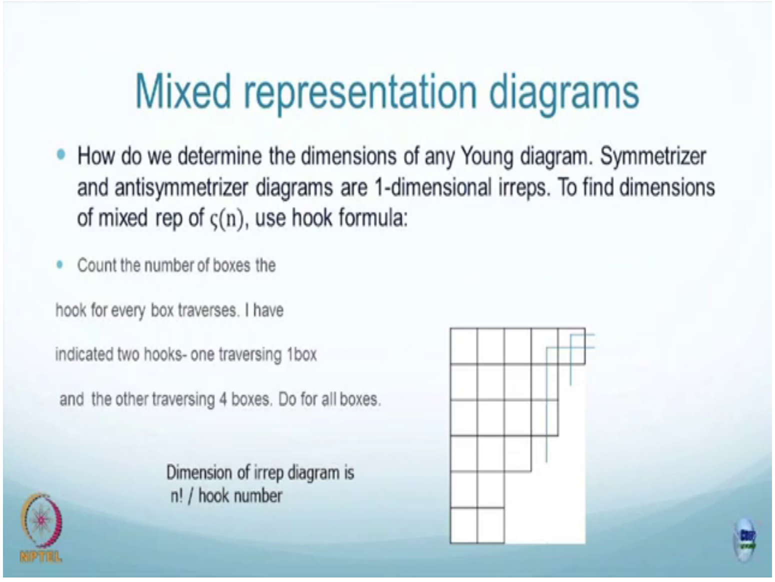

So, I have given you a general diagram here, I have introduced hooks in the diagram ok. The last box the hook is going only through the last box. If you take the this second in the first row the last, but one box I have to make put a hook where it traverses 1, 2, 3 and 4 boxes, is that clear? There are 4 boxes the second hook has to traverse to touch the that box that particular box which I am showing now.

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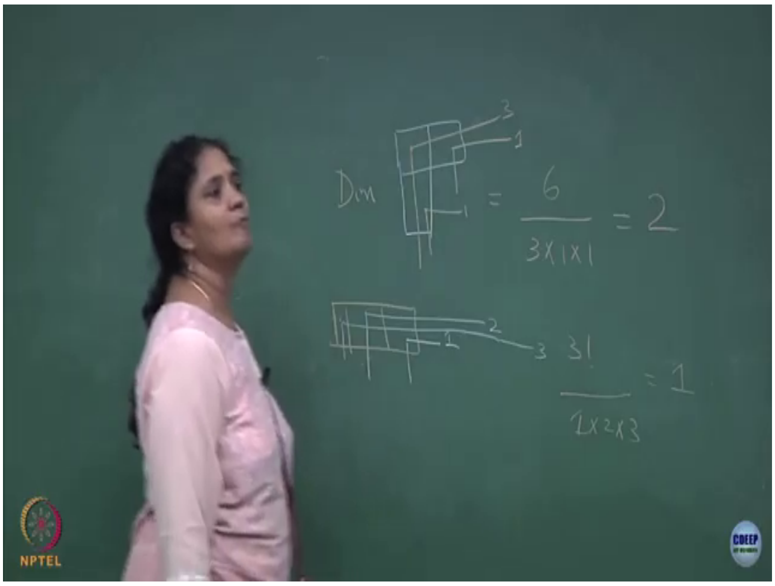

So, let us do this for this example. So, let us take this; this particular box has one hook, this box has another hook, this box has this hook ok. So, this number is 1, this number is 1, 2 and 3 and this one is again 1. So, the formula is dimension of this representation will be n factorial. So, n factorial is this belongs to the symmetric group of degree 3. So, there are 3 factorial which is 6 is the numerator divided by the hook number. So, the hook number is there are 3 boxes, so, there will be 3 hook numbers, you multiply those hook numbers and whatever you get is the dimension.

You can do it for this particular diagram. What are the hook numbers? This one is 1, this one is 2, this one is 3 right. So, what happens? You have 3 factorial in the numerator, but 1 into 2 into 3 which is 1 ok.

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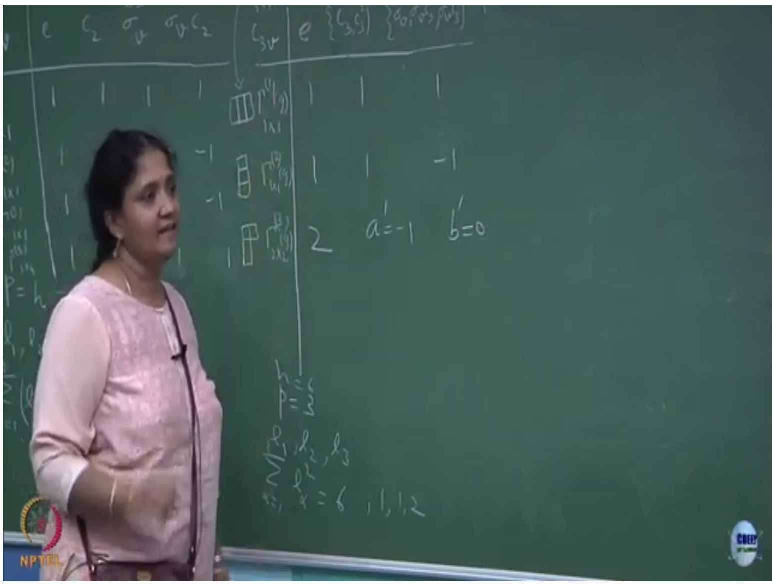

So, this is a compact way of determining the dimension of a irreducible representations for symmetric group which has the same diagrams like the diagrams which we use for the class structure, but the meaning is different. You can determine its dimension of the irreducible representation what are the dimensions of this matrices. So, this diagram will represent the 2 cross 2 irreducible representations of the symmetric group of degree 3 ok.

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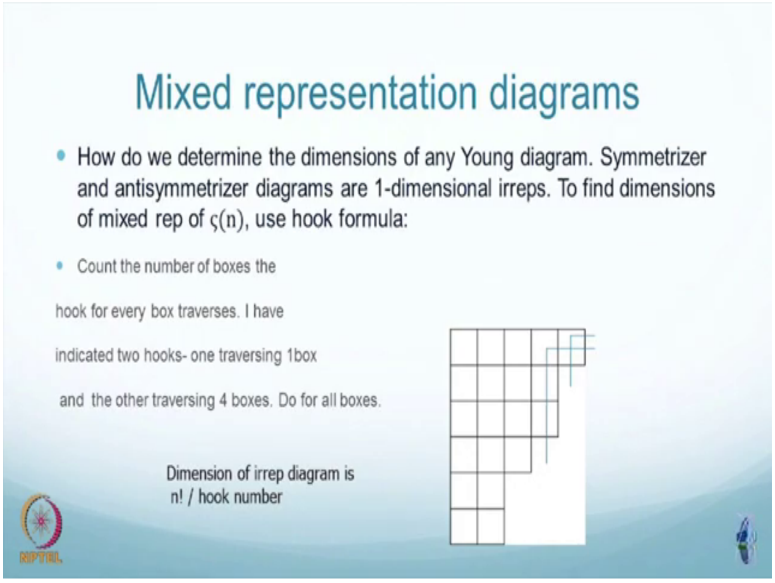

So, I put that hook number here and I said that dimension of the irrep is n factorial divided by the hook number. So, there will be n hook numbers here's which you have to multiply and write the denominator and then figure this out. So, someone can quickly do the other one also and check what I am saying is correct. This will have hook number 1, 2 and 3, again, this is going to be dimension is going to be. So, that is why I said both symmetrizer and antisymmetrizer are one-dimensional objects. This is totally symmetric.

I will come to it why I am calling it totally symmetric and totally antisymmetric by looking at a simple harmonic oscillator. But right now you can see that it is totally symmetric totally antisymmetric is one-dimensions, but what you can get is a mixed representation which is two-dimension ok. So, this is one notation which you have to know in the context of symmetric groups.

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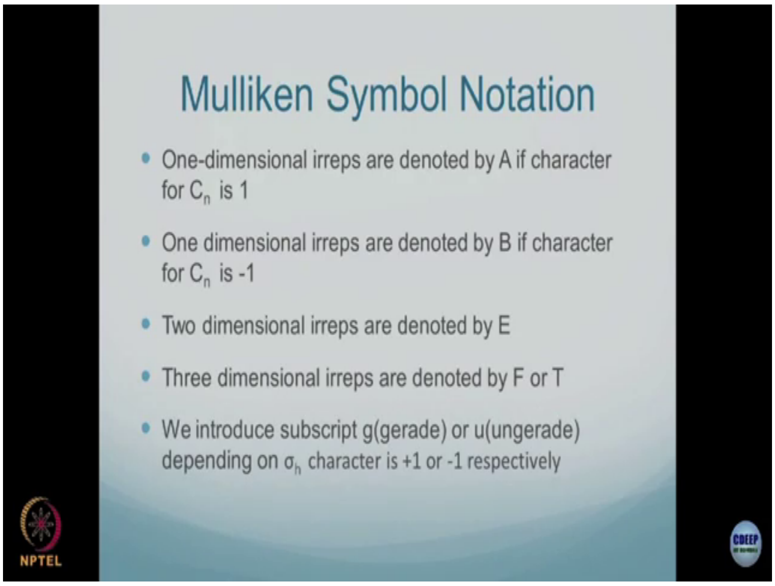

Other one which I want to say is the Mulliken notation which also let me explain in the context of these two examples. One-dimensional irrep is denoted by a character A, so the principal axes here is a two-fold axes ok.

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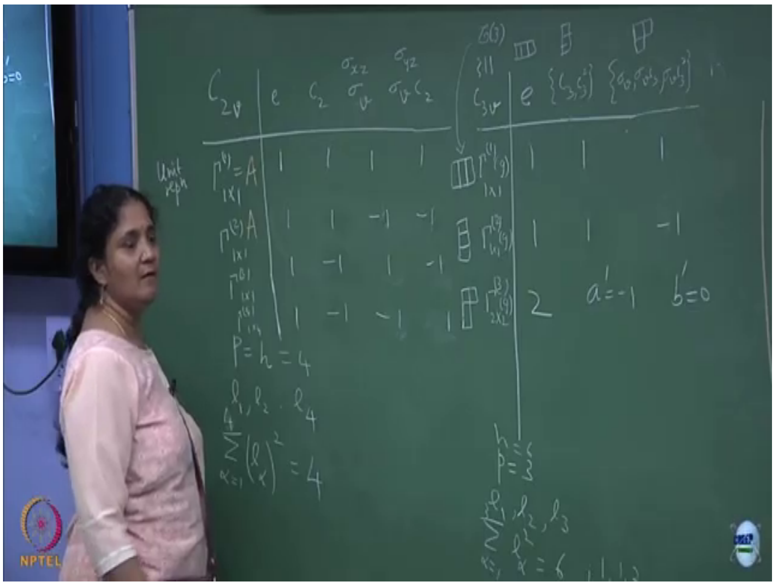

The twofold axes if the character is positive one, then you introduce a Mulliken symbol similar to this diagram there is a Mulliken symbol any chemistry book or any of these books on point groups they use Mulliken symbol and they use the letter A; both these twofold axes have positive.

So, both should have a Mulliken symbol A; you can call one as A 1 and A 2 to distinguish that these two are two different irreps, but with the principal axes character being plus 1. If the principal axes character is minus 1, you call it by a symbol B. So, B 1 and B 2 is one way of writing the symbols.

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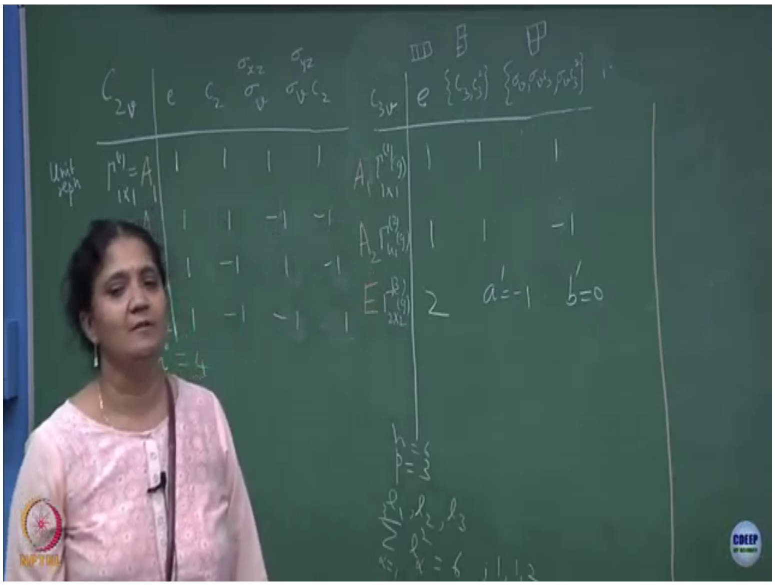
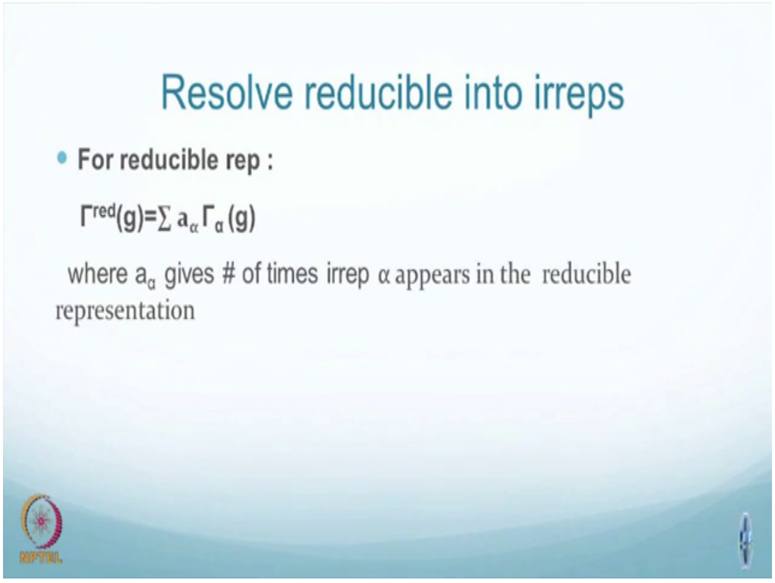


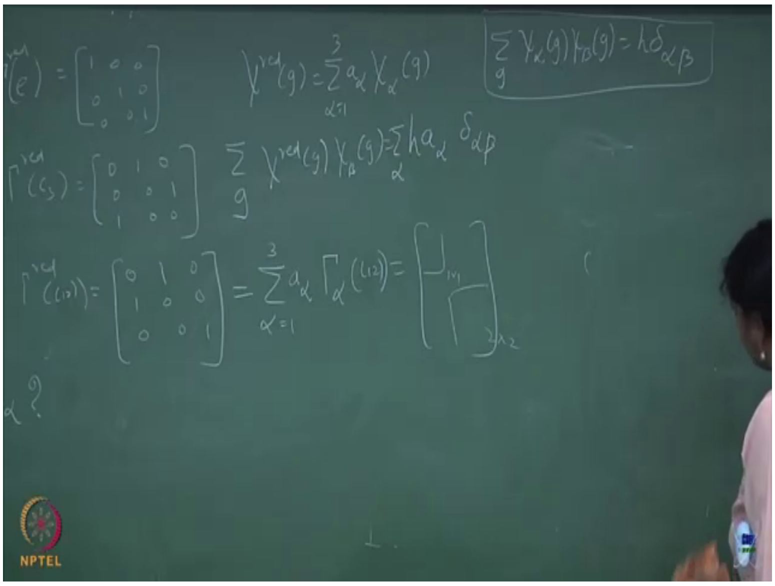
So, here also A 1 let me now remove the symmetric group. So, this one will be A 1, what will this be? Principal axes is threefold axes that also has a plus 1, so this will be again A. And two-dimensional representations are denoted by capital E do not confuse this with the identity element, this is the Mulliken notation and if you have 3 then you will have represent, suppose you have 3 then you will have we call that as F or T ok.

So, I have just explained it on the screen that one-dimensional irreps are denoted by A if character for C n is 1. One-dimensional irreps are denoted by letter B if character for C n is minus 1. Two-dimensional irreps are denoted by E there they do not care and then three-dimensional irreps are denoted by either letter F or letter T. This is the notation which is being followed for point groups.

So, what have I done so far? I have tried to tell you the notations in the context of symmetric groups, what is the way you represent the irreps, what is the letters you use for the irreps in the context of point groups. There is also one more slight additional subscript called g gerade and ungerade, but this depends on whether sigma h is plus 1 or minus 1 and so on. So, we will come to it as and when we do some examples. I will give you some more problems in the assignment sheet and we could discuss that ok. (Refer Slide Time: 09:18)



So, this is if you have a sigma h element you could put it to be plus 1 or minus 1 respectively ok. So, I am going to come to reducible representations and see how to find out the a alpha's for it ok. (Refer Slide Time: 09:41)



So, one of the reducible representation in the class last yesterday. What was I writing? I said like take the objects as 1, 2 and 3 and do the operation. So, you can have identity element. On gamma reducible for sigma v I am writing only one candidate in every representation, one candidate in the conjugacy class because I feel that trace anyway when I do the characters it does not really matter right.

So, C 3 belongs to one of the conjugacy class, sigma v belongs to the other conjugacy class. What will that be? Somebody can tell me sigma v is equivalent to 12 cycle right suppose. So, now I want to find out that I am claiming that each of these elements I should be able to write it as alpha is 1 to 1 to 3 a alpha gamma alpha of g. So, in this case it is 12, you can do that for every case. These integers will not change, this will be the corresponding for a different element right. This is what we want to find and determine what is a alpha and we determine a alpha for this case. Is the problem clear?

It is a 3 cross 3 matrix representation, this matrix representation I have taken only sample elements from the conjugacy class. They satisfy the group properties; they satisfy the group properties of the symmetric group of degree 3 or even C 3 v it just that you have to call this as sigma v right, but what we know is that the character table did not have a 3 cross 3 matrix. So, you can even blindly say that the 3 cross 3 matrices better be reducible ok you can have only 2 cross 2 or 1 cross 1.

If you had a 3 cross 3 blindly we can say it should be reducible and it should be reduced as a linear combination of the irreducible components and our aim is to determine what are those irreducible components or can I write it in a block diagonal form. It is a 3 cross 3 matrix, maximum it could be a 1 cross 1 under 2 cross 2 or the 3 1 cross 1 and which one will be repeating, which one will not be repeating I do not know now, but we can determine. And, to determine this we are going to exploit the great orthogonality theorem and their properties ok.

So, let me just go over the steps now. So, this we have already seen one of the properties. Now, I am going to exploit this property on the traces of these matrices which means they are characters; characters will also have these properties right. If I write the character for the reducible for an element g it is nothing, but it is not going to change. So, this character which I am finding it to be 0, we should take the irreps in such a way that the character should add up to be 0. This character is turning out to be 1 and so on, clear?

So, the characters will still satisfy that property and we will invoke once I write it this way I can try to do the chi reduced of g with chi beta of g summation over g I can do this. Substitute chi reducible I say alpha chi alpha, then chi alpha chi beta you know what to do right you will get a alpha times. Am I right? Just using the property which I wrote. What is the property? I am just using this property to simplify by multiplying this I am using this. So, there is an a alpha times h times.

Student: (Refer Time: 15:45).

Where is the summation over alpha? Yeah, thank you, good. So, summation over alpha will be there, here is fine good point.

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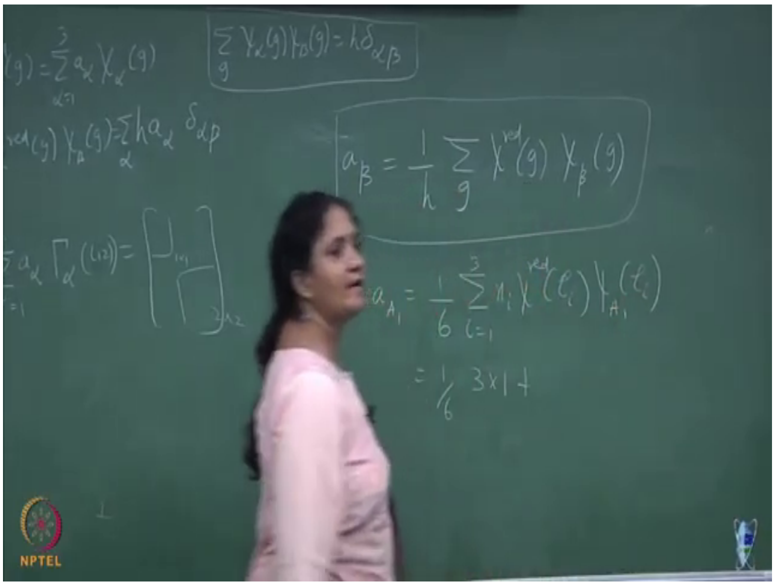

And, then it is going to be 0, for all the alphas other than only the beta. So, from here you can derive. So, a beta will be 1 over h summation over g character for the reducible representation multiplied with the irrep character, irrep beta character. So, this will determine for you the number of times. So, let us determine what is a alpha for this representation which I have written. Can we do that? a for trivial representation which I am calling it as 1 or according to that I am writing it as A 1 according to Mulliken notation I will call it as A 1. Can you tell me how much it is? 1 over 6; 6 because 6 is the order of that group and we are doing it for the symmetric group of degree 3 only right. So, that is why I am doing this. Summation over g can be replaced by summation over classes 1 to 3 n i chi reducible for an element of that class chi beta for that class, allowed.

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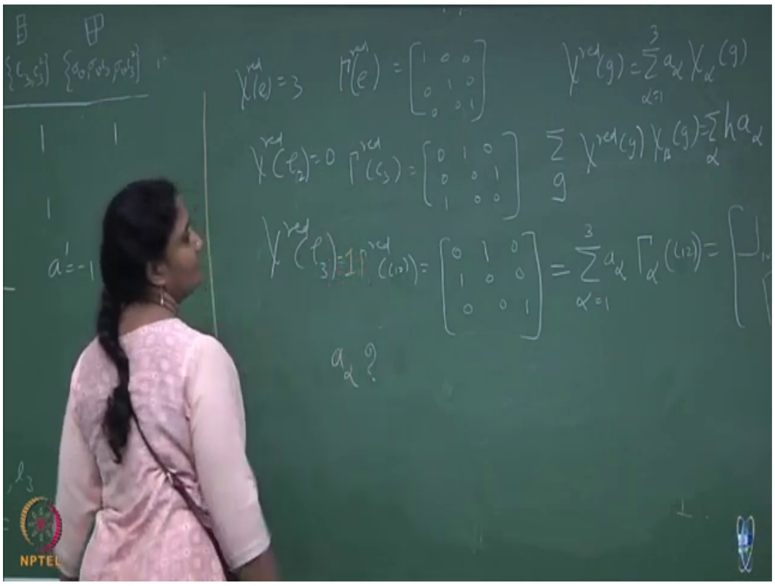

Now, tell me what happens? We have written the can write the characters for them for class 1 element or class 2; this is class 1, this is class 2. What is that? It is 0, class 3 that is 1. So, use that here and tell me what you get for this that is 3; 3 into 1 beta is taken to be the a 1 ok. So, then I have to replace beta by a 1 character for the irrep a 1; a 1 is the unit representation or a trivial representation.

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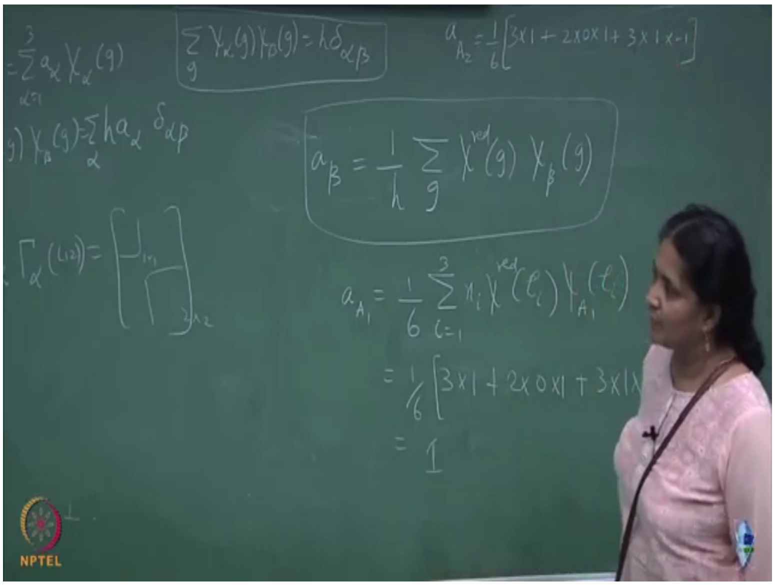

Somebody? Then the second one is 0 2 into 0 into 1 plus 3 into 1 into 1, it is 1. What about a A 2? a A 2 will be 1 over 6, 3 into 1, identity element has no change, 2 into 0 into again a 1 plus 3 into 1 into minus 1 because minus 1 is the character for the A 2 irreps. Are you all with me?

I am putting instead of a 1 I am going to do the same thing for A 2. A 2 character is 1; character is 1 for the second conjugacy class and then the third conjugacy class has minus 1 which has three elements. So, what is this answer? 0. If dimensions are matching you should get e to be 1 a e to be 1. Can you check? Any problem? Should ask if I am. What is the confusion?

Student: In the first class (Refer Time: 20:54).

First class?

Student: 3.

This one? 3 is the reducible for the class I can call this as c 1, that is 3, c 2 is 0, c 3 is 1 right it is clear from here. I have taken 2 element in each class and here is here there is only 1 element. Here there are 2 elements I do not care, characters are same and if you come to the 1 2 element there are also three elements 1 2, 1 3, and 2 3 cycles. So, I am just taking one of them and looking at them right and then I am substituting.

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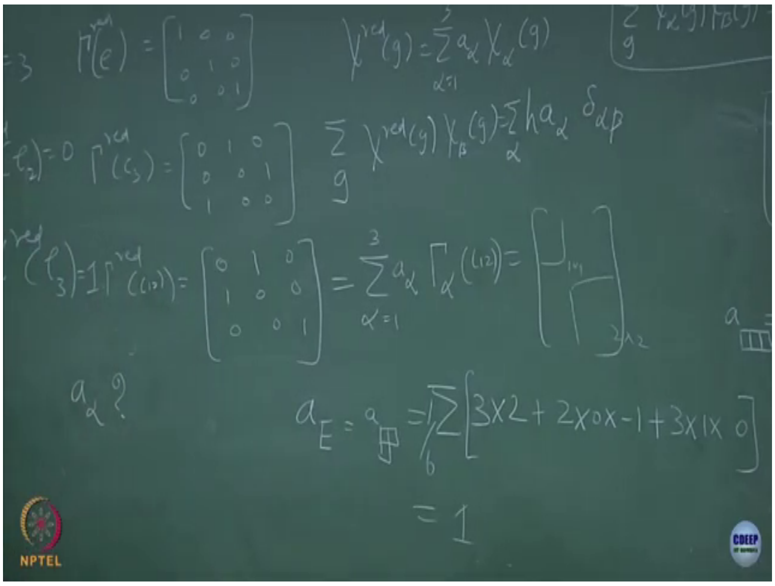

Can you check what you get for a E? Somebody can do that? a E; E is the 2 dimensional representation. If you are trying to write for symmetric group of degree 3 instead of this you could also write it like it corresponds to this diagram. If you are writing it for symmetric group and not C 3 we can say that this corresponds to this diagram and this one will be this you cannot do always. The a 1, a 2 you can do always, but when it comes to symmetric groups only you can do that symmetric diagrams if it involves n factorial elements not for the subgroups of the symmetric groups.

Student: (Refer Time: 34:00)

These are subgroups in general, but for subgroups I cannot draw this diagram that is all I am saying, you have to use the Mulliken notation ok. So, can you work it out this one? This will be 3 into E is 2 character of that is 2 right. E character is 2, are you all with me? And, then 2 into 0 into character is minus 1 and 3 into 1 into character is 0. What happens? 1 over 6.

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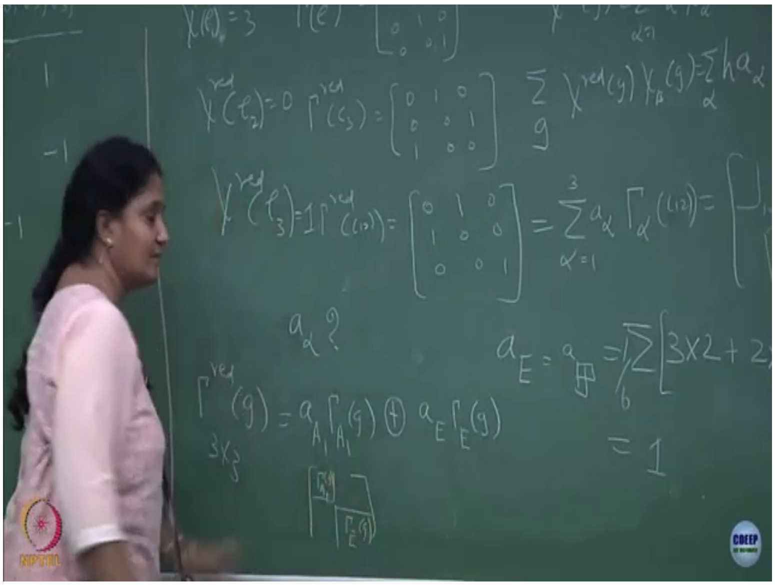

So, what have I shown? The reducible representation for any group element which is a 3 cross 3 matrix which I have here can be written as a A 1 times gamma A 1; someone already pointed it out that I am not just doing a number addition technically it is like putting blocks. So, the symbol for putting blocks is what we call it as a direct sum and this will be a E g for every element you can do this. By this notation I mean that you will have a gamma a 1 irrep and gamma E irrep for every element g. This is the diagram representation matrix diagram representation for writing the symbol.

Student: Ma'am.

Yeah.

Student: We can find out the (Refer Time: 24:51).

In terms of the dimensions of the irreducible.

Student: (Refer Time: 25:00).

I agree, but then you have to make sure that it could be that A 1 is 3 it could be that a A 2 is 1 and a E is 1, how will you distinguish that? To get the 3 you can either get A 1 irrep occur threes thrice, A 2 occur thrice, you can have a 11s and E 1s or a 21s and E 1s, which one this reducible representation breaks to? To know that separation you cannot just only work with dimensions, is that clear? So, in this particular representation which I have given you can say that the representation breaks up a A 1 turned out to be 1.

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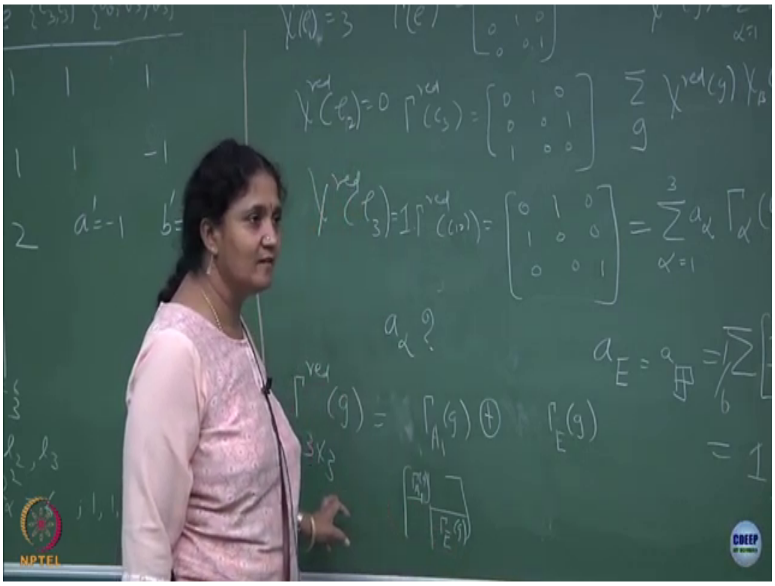

So, I can just replace this by 1 right 1 I do not even need to write and a E also turned out to be 1 and clearly this is 1 cross 1 matrix and 2 cross 2 matrix, they add up to give you the 3 cross 3 matrix which is also consistent and this is the way it will break you can say from great orthogonality theorem. You do not need to find the S you do not need to find the S; you can say that it will break this way with number of times and A 1 irrep will occur is only once, number of times A 2 irreps will occur is 0, number of times the a E the irrep E which will occur is 1. Is that clear?

So, this is what is the formal way of trying to find how a reducible representation can be put in the block form without trying to determine what is the S matrix. And, you can just write that this is the characters a alpha is the number of times the irrep alpha will occur, h is the order of the group. You sum up over all elements the reducible character reducible representation character multiplied with the corresponding irrep alpha. If you sum up over all the group elements you will end up getting the a alpha.

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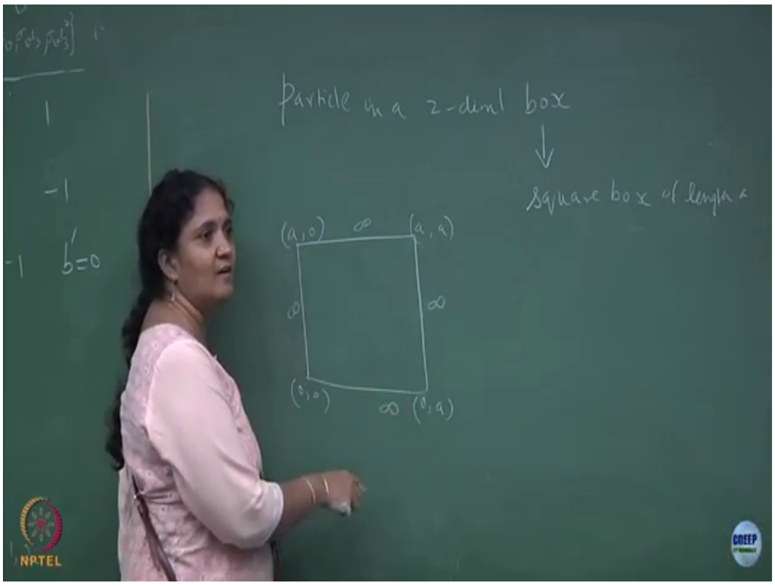

So, particle in a let us take a 2-dimensional box ok. If the box is a square box what is the meaning of it? Let us take the square box of length a ok. What is the meaning of this? You will have a x, y coordinate 0, 0; 0, a; a, a; a, 0 or the other way round, but I am just following.

So, what I am saying is that if I take the particle to sit inside this box in a 2 dimensional plane by saying that it cannot move out of the box the reason is that I am going to put a infinite barrier at all these sides of the box. Potential is going to be infinity that it the particle can never have that much energy to even climb up, even quantum mechanically also is impossible.

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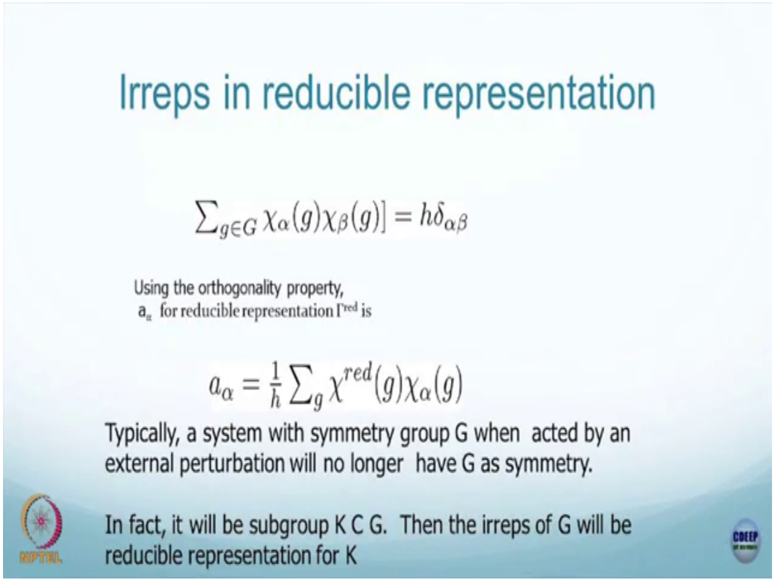

Paneling is possible only when there is a finite potential otherwise it cannot come out. The wave function will vanish at the boundary that is what you see.

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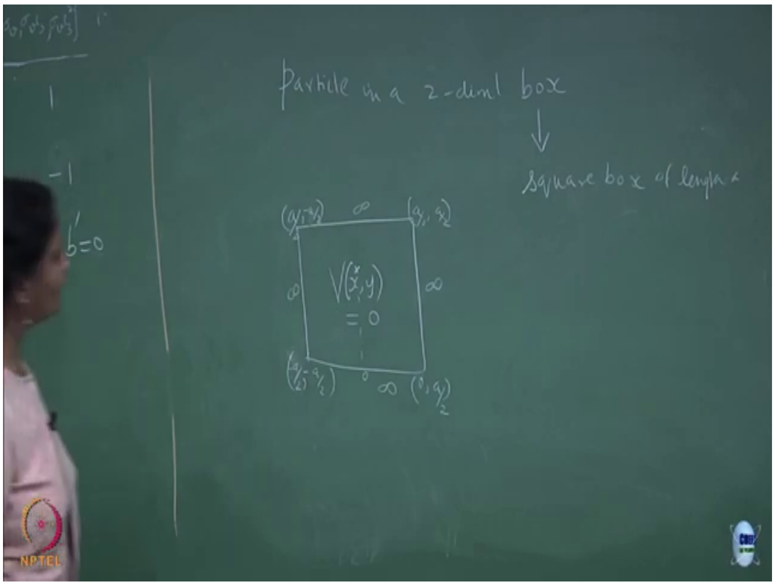

So, this box if I look at the potential, so inside I can call it as potential V of x, y I am usually we take V of x, y to be 0. We say that potential inside the region and 0 it is like a free particle not quite it is constrained to move only inside this box. So, it is not actually free particle. If it was a free particle its energy will be a continuous energy. It is free to move every anywhere. So, it cannot have quantized energies, the quantization is coming because you have constrained it and made the momentum to get quantized. So, energy gets (Refer Time: 29:43) right. So, this is what you have.

We can look at this problem as if you are looking at a symmetry problem ok. You can shift the origin and make the center point as the origin and then you will have a symmetry what kind of symmetries you can have. It is a 2D plane ok. So, let us shift the origin to the center point and then you will have coordinates which are you can play around and see this coordinates.

Only thing is this coordinate and this coordinate this point will be a midpoint 0 ok. So, there will be a minus a by 2 probably plus a by 2 and so on. You understand what I am saying. So, there will be an a by 2, a by 2 and probably this one is also and then this one will be a by 2. So, some shift in the coordinate which you can do.

So, once you do the shift in the coordinate you will see that there is no difference in making x going to minus x or y going to minus y, you do see that the system is having some symmetry what are the symmetries you can start looking at the symmetries you can even do a rotation by 90 degrees right.

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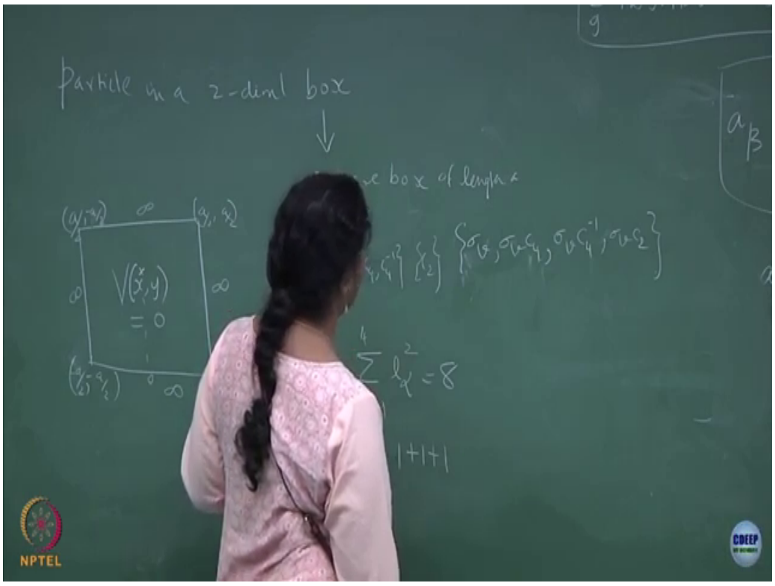

So, you will see that it has a symmetry with the fourfold axes, you can also do a mirror. So, technically it will become like a C 4 v symmetry. Again, you can start writing the character table for C 4 ok. So, if you start writing the character table what is the order of the group? It is 8 right; order of the group is 8 and now how many classes will be there? So, typically you know that identity is there one class as C 4, C 4 inverse, one class as C 2 and when you have a sigma v C 4 C 4 inverse and a C 2 right sigma v sigma 1, you understand?

So, let me write it clearly. So, this will be sigma v, sigma v C 4, sigma v C 4 inverse, sigma v C 4 square which is C 2. How many classes are there? 1, 2, 3 and 4 classes. So, you can write summation over alpha 1 to 4 l alpha squared to be 8. What are the dimensions possible, someone can help me out? Is there 4 classes or have I said anything wrong?

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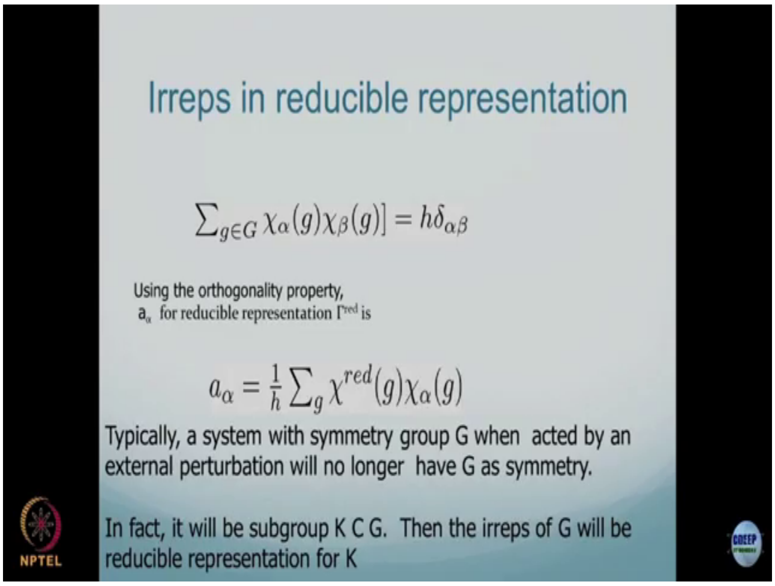

Anyway so you try it out we will we will discuss this, but this is the way to go about it. C 4 v is a symmetry of it and then suppose some perturbation happens some kind of a storm happens that this square box starts you know either shrinking not uniformly; not uniformly completely it becomes rectangular let us say. Then what is the symmetry?

If it will become C 2 E right it goes to a lower symmetry group ok. From C 4 v box it goes to a lower symmetry group; the symmetry group is definitely having less number of elements as symmetry elements are also very less compared to fourfold symmetry twofold is the less symmetry.

Such a thing happens to start with you might have an irrep for C 4 v, but that irrep of C 4 v will not continue to be any irrep of C 2. This is what I am meaning by saying that typically a system; typically a system with symmetric group g in acted by some external perturbation will no longer have a group g asymmetry in fact, it will become a subgroup of G. In fact, C 2 v you can show it to be like a subgroup of C right. You can take the C 2 element E C 2 element and sigma v together will become a subgroup.

Student: Ma'am, is it possible that (Refer Time: 35:01)?

That is also possible, but typically the system when you leave it, it does not enhance the symmetry it can create more chaos in some sense. So, it does not really become more orderly. So, in that sense.

Student: (Refer Time: 35:20).

We would like yeah reverse process if it is a reversible process yes, but you have to do it by some methodical perturbation that here I am trying to say that technically some disturbance can actually or some impurity suddenly comes in, it could change the potential to something in such a way that this potential will not have the C 4 v symmetry ok.

So, I am just giving you a simple example, but this things these ideas can be used in complicated examples. Then the irreps of g which you started with in the character table will no longer be a irrep of K, it will be a reducible representation for K and then we start doing this procedure of breaking the reducible representation of a higher group symmetry due to perturbation breaks to lower group and how many times in the lower group that irreducible representation of a higher group which is reducible as far as lower group is concerned you can determine by this process K.

Many of the molecular symmetry initially it might have a tetrahedral symmetry suddenly some impurity can make it into a lower symmetry, like it will have a C 3 v symmetry and not tetrahedral symmetry. And, then what happens is that in the spectral lines they start seeing that something was degenerate some of the lines which were 3-fold degenerate suddenly start splitting you know Zeeman effect right. If I turn on a magnetic field right you start seeing splitting.

Turning on magnetic field is actually breaking the symmetry and once you break the symmetry the things which were degenerate actually starts splitting and how do we understand these things from the group theory point of view is my aim in bringing in this notation. And, we will do some simple example by which you will appreciate what is your view.