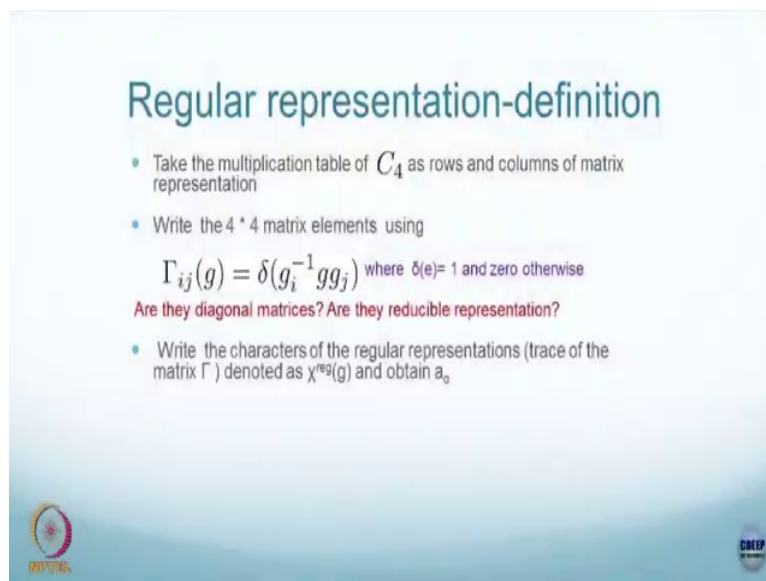


Group Theory Methods in Physics
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Lecture – 23
Tensor Product and Projection Operator – I

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Regular representation-definition

- Take the multiplication table of C_4 as rows and columns of matrix representation
- Write the 4×4 matrix elements using
$$\Gamma_{ij}(g) = \delta(g_i^{-1} g g_j)$$
 where $\delta(e) = 1$ and zero otherwise

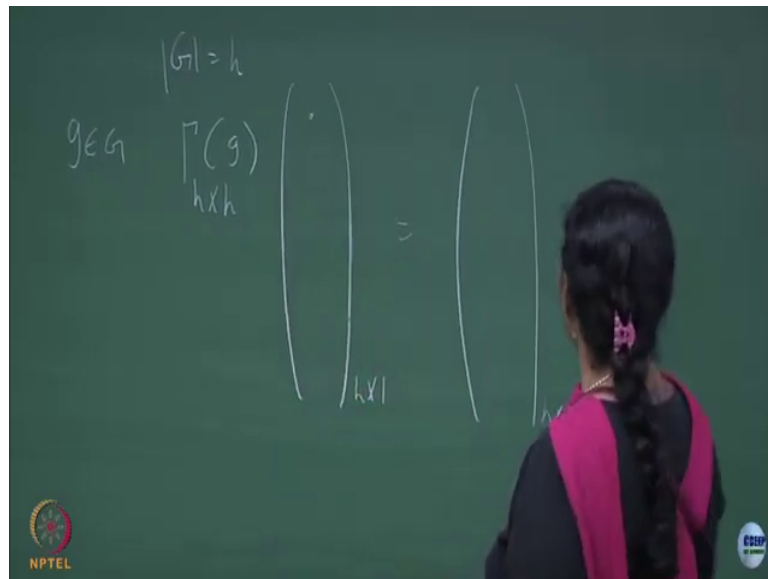
Are they diagonal matrices? Are they reducible representation?

- Write the characters of the regular representations (trace of the matrix Γ) denoted as $\chi^{\text{reg}}(g)$ and obtain a_n

Regular representation is nothing, but typically if you take G group G whose order is which I am calling it as h ok.

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You could write a matrix which is a h cross h matrix; matrix representation whose dimension is also the order of the group. So, for every group element you write a matrix representation. So, how is this matrix elements going to be defined is what I am trying to say the way to see it is that now you can treat whenever you have a matrix which is this dimension it should always operate on a column which is?

Student: (Refer Time: 01:18).

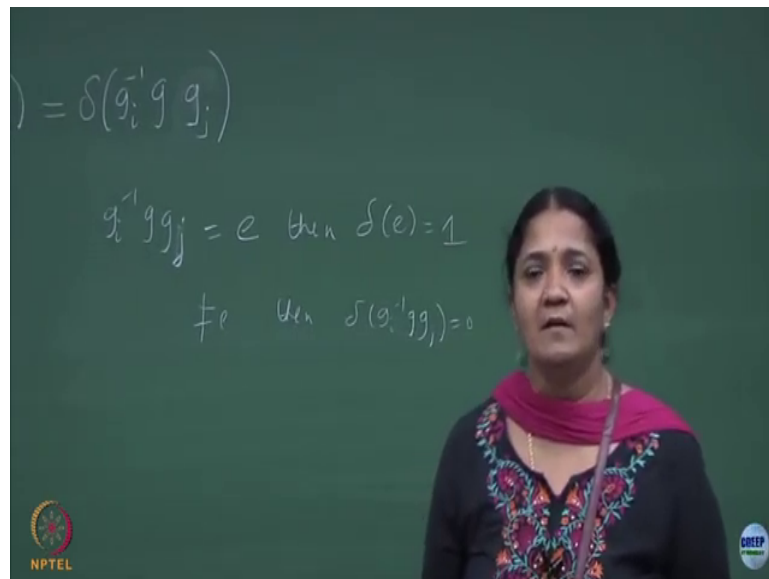
Louder.

Student: h cross 1 .

H cross 1, right. So, it will be. So, you could put the elements here also as if it is each entry here corresponds to one of the elements of the group and so on ok. And, gamma g where it operates on the h elements the order of the group is h there will be h elements in this discrete group it is going to shuffle or give you something it is going to give you some permuted combination right depending on how this matrix is operated. So, that is the idea. So, this will also be h cross 1.

And, you will see that the matrix whose dimensions is exactly the order of the group that acts on a vector space which is also going to be h dimensional vector space. So, these matrices with this additional property so, how do I find the matrix elements?

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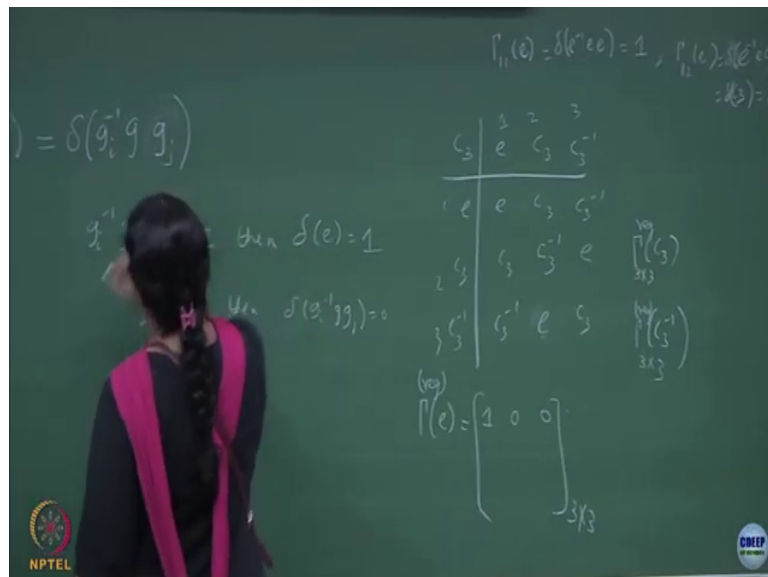


So, matrix elements if I want to find I want to find what is gamma ij element because this will be h cross h matrix I want to find the ij th element for a particular element g ok. So, that you

are given these representations the matrix elements are written by this is the way we are going to write. What is the meaning of this delta? Sorry, I have given it as $g_i^{-1} g_j$ it does not matter, but you follow one notation ok. So, $g_i^{-1} g_j$.

So, this whole thing if it becomes an identity element if this product $g_i^{-1} g_j$ if this is identity, then delta of e is 1 ok. If it is else otherwise not equal to identity if this product can give you any element in the group g if it is not equal to identity then you substitute delta of that element equal to 0 ok. So, that is a definition by which you can determine the elements of the $h \times h$ matrix representation for the group ok. So, you could do this for the C_4 .

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So, if you try to write the multiplication table let us do it for C_3 . C_3 multiplication table is, so, you can write the multiplication table to help you with playing around. So, this will be for

the identity element. Let us write out what will happen. So, let us first write the multiplication table is that right this is the multiplication table.

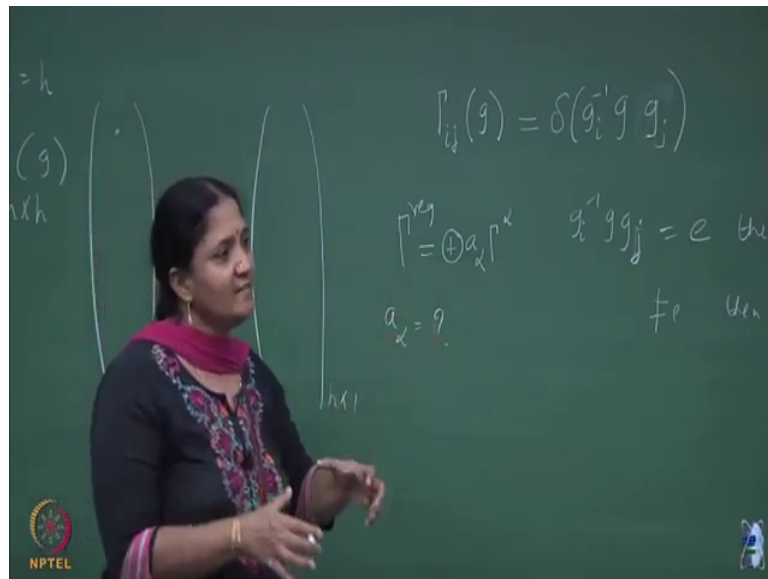
So, let us do γ_{11} of e . So, I am going to call this as 1, 2 and 3; 1 2 and 3 in the multiplication. So, I want to find the 11 element of a 3 cross 3 matrix for the identity element e . So, this is going to be just $e^{-1} e e$ is that right. So, that is going to be 1. If you do γ_{12} of e then it is δ of $e^{-1} e c_3$. What is that? That is δ of c_3 which is 0 by this definition anything which is normal.

So, if you put in all these things you will find all the matrix elements associated with the identity element and you can write the 3 cross 3 matrix for e . So, the first element was 1, second element is 0, do the other things and you can even do not need to write everything you can check by using this that this will also be 0 and so on. So, it will be a 3 cross 3 matrix because it is the order of the group is 3. Clear?

The next question is that whether it will be reducible or irreducible. Answer? It is an Abelian group. Abelian group has irreps which are 1-dimensional. If you have a 3-dimensional representation character table allows only 1-dimensional representation. So, it is going to be reducible. Once it is reducible, what do you have to? So, I have written it only for the identity element. Please do this for γ of c_3 γ of c_3^{-1} ok. All of them will be a 3 cross 3 matrix. Please write it out.

I have done three elements in the identity element, but you can work it out and see. What you have done here will give you a reducible representation. All of them are regular representations that is the definition of the regular representations. So and regular representation order of the group defines the dimensions of those matrices and what you can try and figure it out is that how many irreps with what multiplicity is contained in the regular representation right.

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So, what is the meaning of that? Gamma regular should be a direct sum of a alpha times gamma alpha and you need to determine what is a alpha ok. I will leave it you a similar question can be done for c 4 and this is the way to figure out the representations for the group, but the dimensionality of the representation is like the order h cross h matrices.

Those are regular representation which are reducible and you find number of times each of the irreps appear in this ok. So, this I am not going to do. We have done this elaborately for the one of the groups of c 3 v one of the representation, but this representation I will give it you to check and do the c 4 also ok.

Student: (Refer Time: 09:30).

So, this is a matrix.

Student: Yeah.

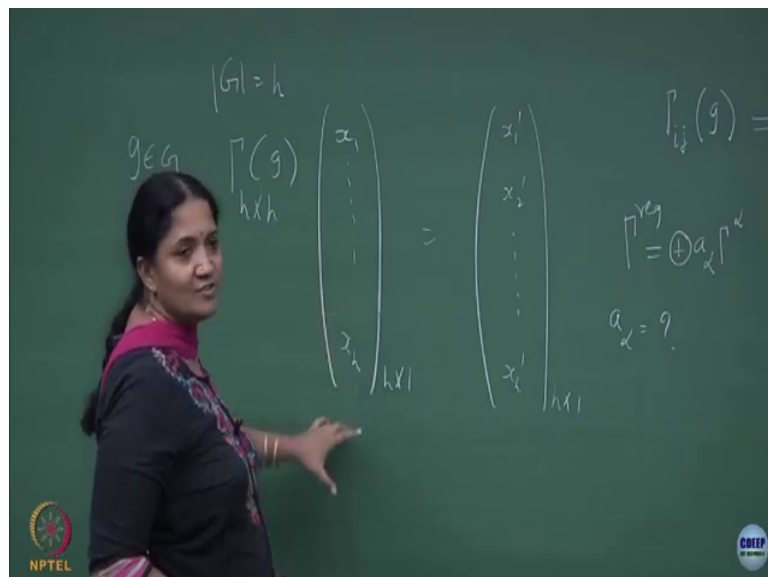
Matrix we will multiply with a column vector.

Student: So, why do we do that?

Huh?

Student: (Refer Time: 09:45).

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So, for every matrix representation linear algebra tells you that it can act on a vector space which is h dimension, that is all I am trying to say. So, this will give you a new column vector. So, technically you could have written it as x_1 up to x_h it will go to x_1' , x_2' and x_h' , but these elements which I am writing here you could also rewrite it as if it is g_1, g_2, g_h these will be some permutations which will happen.

It will become let us say g_1 becomes g_2 so, you could have some permutation depends on the element identity element does nothing and then other elements can do some kind of that is exactly what is happening in your multiplication table. If you operate on c_3 it is taking you the identity element becomes c_3 , then c_3 becomes c_3 in and so.

So, this any row or any column is the permutation order of the elements of the group. That is what the regular representation captures and formally we could say that the regular representation elements can be obtained by using this procedure, it is equivalent.

Student: (Refer Time: 11:14) regular representations are h and the permutations are h factorial. So, it would be subset of those h factorial?



It will be Kelly's theorem tells you that I am looking at a specific group not all the permutation I am going to add it. It is pertinent to a multiplication table right ok. So, this tells you that you can write the characters I am have written the characters I just wrote the matrix representation. You have to take the trace of it because you can determine what is a α from the characters right and obtain a α ok.

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Character table and basis states

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma'_{(yz)}$	
A_1	1	1	1	1	z
A_2	1	1	-1	-1	R_z
B_1	1	-1	1	-1	x, R_y
B_2	1	-1	-1	1	y, R_x

g z= (+1) z is eigenvalue eqn with eigenvalue +1 for all g which are characters of irrep A_1 . Similarly acting on axial vectors and x,y coordinates will show the eigenvalues matching with the other irreps



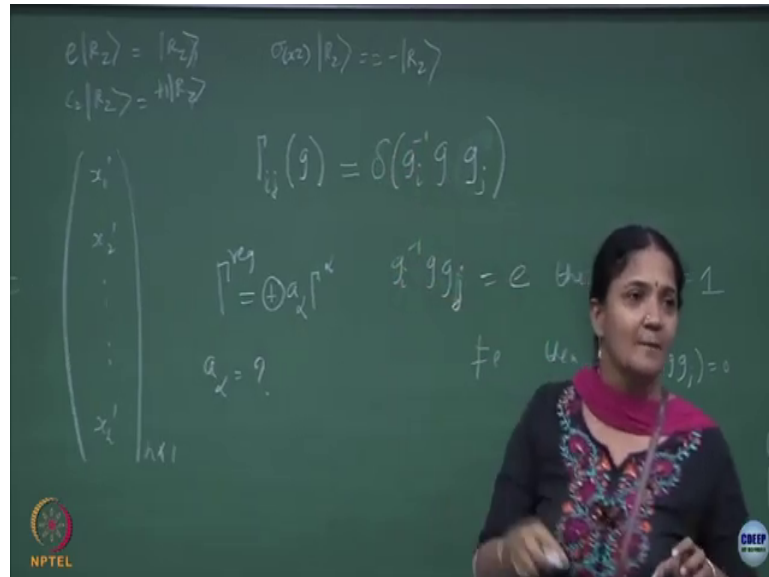
So, this also I have gone through for you the basis column just like I said whenever you have a matrix representation it will act on the corresponding vector space. If the irreducible representation is 1-dimensional, then the basis will be 1-dimensional. What is the right basis in your position coordinate system? In the context of point groups you are going to take principal axis to be along z-axis.

So, the z coordinate is a good basis for the reducible representation A_1 right. We did this many times. Unit representations of most of the point group will have z as the basis, we saw. The next one is A_2 is another irrep. The Mulliken notation tells you that A is used whenever the principal axis character is plus 1 in the 1-dimension representation.

So, A we use the symbol A and now what you have to do is every element of A_2 , when it operates on the axial vector; so, if you operate identity element on the axial vector, this will

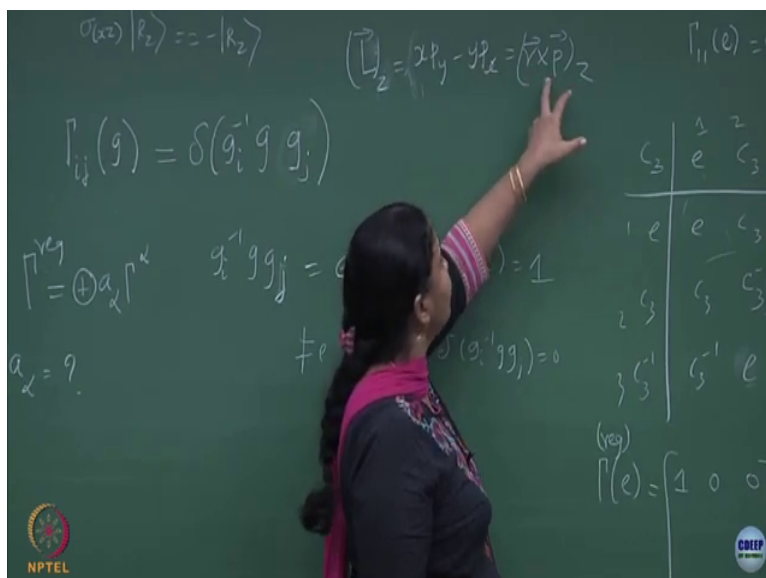
be axial vector right if you operate C 2 on the axial vector what happens? X will change sign, y will change sign.

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So, axial vector will not change sign right plus 1 times the axial vector and if you do sigma xz on the axial vector, what happens? Y we will change sign. So, it will go to minus of R z. The axial vectors z component is something like x cross x.

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So, you can write this R_z as if it is like your angular momentum component. So, you could write it as $xp_y - yp_x$ for example, the L_z component it is an axial vector. So, whenever I do the σ_{xz} on x nothing will happen; σ_{xz} on p_y , what happens? Y component changes sign. So, there will be a negative sign. Similarly, here y coordinate will change sign, but p_x which is the momentum x component will not change sign.

So, essentially you will get a negative sign on the other side and that is exactly what you have here minus 1 is the number which you have to get whenever you operate σ_{xz} element on the A_2 irrep. Similarly, if I operate σ_{yz} again it will be minus by the same argument, but instead of your y it will be the x component which will change.

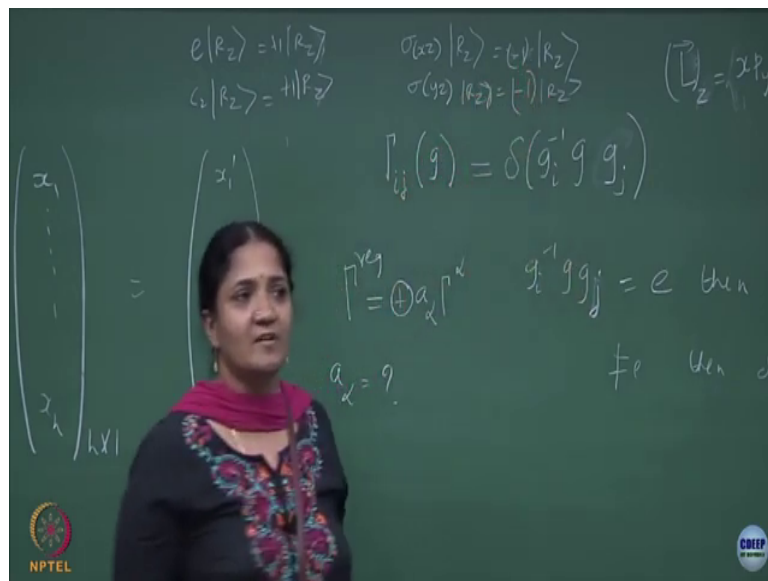
Student: (Refer Time: 15:41).

Which one?

Student: Z (Refer Time: 15:47).

This is $\mathbf{r} \times \mathbf{p}$ know the z component of the L vector it is exactly this ok. So, that is an axial vector. I explained what is an axial vector in the last lecture. When you do an inversion the momentum vector as well as the position vector will change sign, but axial vector components will not change sign that is why it is called as an axial vector. \mathbf{r} is a polar vector, \mathbf{p} is a polar vector, but $\mathbf{r} \times \mathbf{p}$ is an axial vector.

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If you write it in components you can see that, whenever you do this operation $e C 2 \sigma x z$ and $\sigma y z$ on the axial z component you find it to be minus 1 times $R z$ ok. This eigenvalue which you find is what is important. So, you have plus 1, plus 1, minus 1 and

minus 1 in the 1-dimensional representation and that are nothing, but the characters of the A_2 representation.

So, the bases which respects the A_2 representation is not the z component, but the axial component, axial vectors z component. Is this clear? It cannot be z . Why it cannot be z ? If it was z you will get only the A_1 irrep. Mirror reflection on the xz plane will not change it will give you a plus 1 right. If you just did it on z coordinate not at axial z coordinate and this will also be plus 1.

So, the plus 1, plus 1, plus 1, plus 1 will happen for z coordinate plus 1, plus 1, minus 1, minus 1 will happen for the axial vector z component which is denoted by R_z . Is that ok?

Student: (Refer Time: 18:14) on the basis.

So, whenever I am going to write some irreducible representation I have at my back of my mind a matrix representation. Typically matrix should operate on a vector space we should have a basis. If it is if the irrep is 1×1 matrix, the basis should be 1-dimensional and the first easiest one which you would like to look at it is the basis in the position space ok.

You can look at it at abstract vectors also because when you call it as a vector what is the definition of a vector. If it transforms exactly like the components of a position vector you call it as a vector right polar vector to be very specific and then you can give meaning to various other vectors once you have this basis. So, that is the advantage.

Student: (Refer Time: 19:10).

This irrep matrix representations of this irreps will act. Good point. So, all of them in this case C_{2v} is all 1-dimension, it is an Abelian group. It is 1-dimensional. But, we can also look at the C_{3v} where we have 2-dimensional representation right.

So, this is the procedure. You take the group element, operate on a basis find what number you get at least for the 1-dimensional irreps and match for the z it turns out to be the A_1 irrep. So, that is why the basis becomes z and for R_z as I have displayed on the board for you it corresponds to the A_2 irrep eigenvalues ok. It is an eigenvalue equation only for 1-dimension irreps because the vector space is 1-dimension ok.

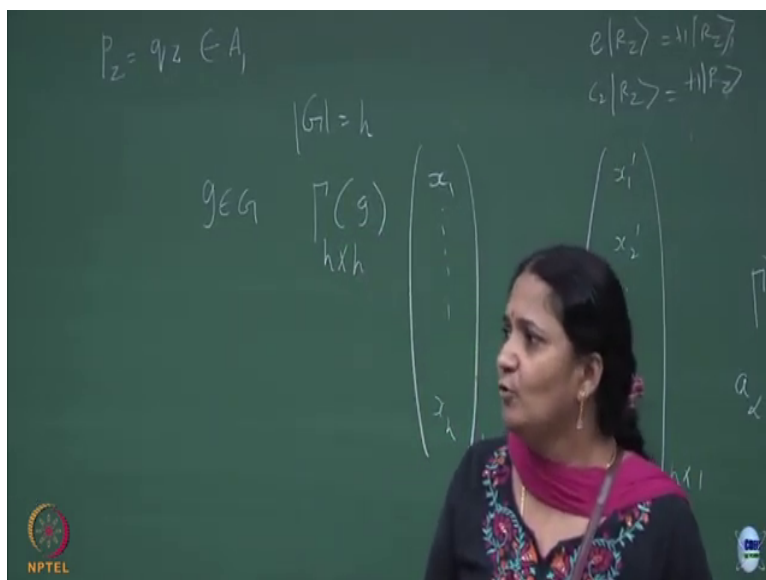
So, similarly acting on axial vectors I have not done the other things x coordinate, y coordinate, R_y and R_x . Please check it out that you will see that the corresponding eigenvalue the set of four eigenvalues which you get when you operate these group elements like the way I did it do it for x , do it for R_y .

So, these two are two independent basis. You can either work with the basis which is the x component or it can be R_y which is a axial y component ok. These two are there are two different bases which you can use for the same irrep it is all I am writing do not confuse that to be a 2-dimensional basis. It is two independent 1-dimensional bases, either you can use a x component as a basis or you can use the y component axial vector as a basis. Is this clear?.

That is a way to fix the closest basis which is in your position space. The reason why we are doing all these things is that all the operators or observables in nature can be either treated to be a vector or tensors right. You know that you have electric dipole moment; electric dipole moment is what? It is a vector right then you also have something called as a quadrupole moment tensor right. These are things which are objects which are observables in nature.

Whenever I am going to look at observables, suppose, I look at the electric dipole moment and I am going to look at only the z component of the electric dipole moment which is the right irrep for that operator if I asked I look at this table, look at this basis vector for position coordinate z it is the A_1 irrep.

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So, I will say that the z component of the dipole moment operator right, this is the notation for the dipole moment operator. This should be belonging to the A 1 irrep that is the way I will write. This is another reason why I need to know the basis because we are going to do electric dipole moment transition interaction which can lead you to a transition from one energy level to another energy level and then we need to play around are these observables belonging to which irreps.

Then you have to resort to looking at the character table and the basis states and it will help us to see which irreps it belongs. If I ask for the x component of the dipole moment vector then the corresponding irreducible representation to which it will belong will be the B 1 ok. Is that clear? So, that is where this basis state will play a crucial role in getting.

So, the and also the basis states will change when you go from one group to another group, that also you should remember. If I start with a system with certain symmetry you first draw the character table. After you draw the character table you write the character table you write the basis then the operators will belong to one of those irreps that is a next step.

So, we will come to this a systematically, but as of now I assume you understand now how one frames the primary basis. Why primary? It is not involving any quadratic powers of these coordinates and the primary base is column which I have written is these possibilities for the A 1, A 2, B 1, B 2. Is this clear to you?.

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Tensor product of representations

- $\Gamma^\alpha(g) \times \Gamma^\beta(g)$ is a reducible representation which are $t_\alpha t_\beta \times t_\alpha t_\beta$ matrices
- Characters of tensor product representation will be product of characters

$$\chi^{\Gamma=\Gamma_1 \otimes \Gamma_2}(g) = \chi^{\Gamma_1}(g) \chi^{\Gamma_2}(g)$$

$$\Gamma = \bigoplus_{\alpha=1}^r m_\alpha \Gamma^\alpha$$

$$m_\alpha = \frac{1}{|G|} \sum_{g \in G} \chi^\Gamma(g) \overline{\chi^{\Gamma^\alpha}(g)}$$

