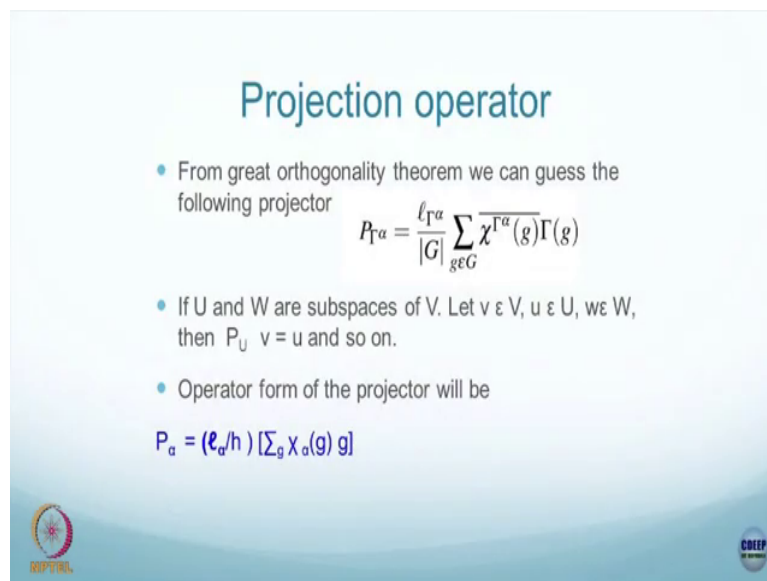


Group Theory Methods in Physics
Prof. P. Ramadevi
Department of Physics
Indian Institute of Technology, Bombay

Lecture – 25
Tensor Product and Projection Operator with the Example

(Refer Slide Time: 00:17)





Projection operator

- From great orthogonality theorem we can guess the following projector

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

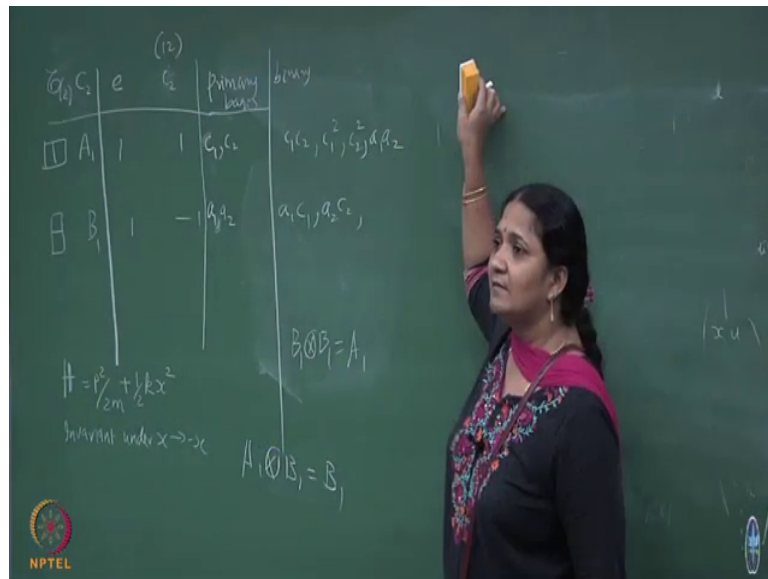
- If U and W are subspaces of V. Let $v \in V$, $u \in U$, $w \in W$, then $P_U v = u$ and so on.
- Operator form of the projector will be

$$P_{\alpha} = (\ell_{\alpha}/h) [\sum_g \chi_{\alpha}(g) g]$$

This can continue ok.

(Refer Slide Time: 00:23)



You can find tertiary basis by taking $A_1 B_1 A_1$ and so on. So, many that is the way you get your tensors which have which are you know 3 index object, moment of inertia has 2 indexed object, quadrupole moment has 2 index object. So, if you want to get a 2 index object it has to belong to a binary basis, if you want to get 3 indexed object it has to belong to a tertiary basis. And, how to construct the tertiary basis is to take tensor product of primary basis number of times, apply a projection operator and find out the basis ok. In this case it was trivial because they are all 1 dimensions, but we will do a non-trivial C 3 v now.

(Refer Slide Time: 01:31)

$$\hat{P}_{A_1} = \frac{1}{2} \sum_g \overline{\chi_{A_1}(g)} \hat{g}$$

$$\hat{P}_{A_1} \psi(x) = \frac{1}{2} [\psi(x) + \psi(-x)] \rightarrow A_1 \text{ contains } \begin{cases} \text{gnd state,} \\ \text{2nd excited state} \\ \text{4th} \end{cases}$$

$$\hat{P}_{B_1} \psi(x) = \frac{1}{2} [\psi(x) - \psi(-x)] \rightarrow B_1 \text{ contains } \begin{cases} \text{1st excited state} \\ \text{3rd} \end{cases}$$

So, you can write \hat{P}_{A_1} the projection for the irreducible representation as the character for the group elements in the representation A_1 . And, then you can also put the g operator and not worry about the matrix representations for it, because the matrix representations depends on the dimensionality of your vector space; this is also another way of doing it. So, this is where you can apply \hat{P}_{A_1} if you remember in the harmonic oscillator I said that this Hamiltonian is invariant under x going to minus x .

It has a group symmetry which is isomorphic to permutations of 2 objects or the C_2 group, this is something which I said. And, you can see that if we operate it on ψ of x the projection operator for an irrep A_1 on ψ of x using it this is a operator form of it which I am writing ok. So, operators are typically denoted by; so, if you do this then you see that it will give you the plus sign for the C_2 operation, this one anyway is plus 1 identity operator.

And so, this will be your projection operator or any way function it will project you to a subspace which is an even function. Similarly, if you do projection operator of B_1 on ψ of x what will happen? This has to be replaced by B_1 , B_1 character table is 1 and minus 1. So, what will the thing be? First element of course, is for the identity element is plus 1 ok, the g operators and identity operator so, that will remain a ψ of x . The second element character for the B_1 irrep is.

Student: Minus 1.



Minus 1. So, all your which wave functions, ground state, 2nd excited state, 4th excited state and all belongs to which irrep? In the harmonic oscillator. This projector projects it onto a even wave function. So, even wave functions are A_1 is contains ground state, 2nd excited state all even. And, similarly this means B_1 contains 1st excited state, 3rd excited state, all odd excited states.

So, you do see that the just the group symmetry which is a simplest group symmetry C_2 has helped you to say that the wave functions which you are going to find or the solutions with you are going to find has to be to 1 dimensional representations. By 1 dimensions you mean that it is either going to be the A_1 is a 1 dimensional irrep, the projector will give you only a 1 dimensional state. So, it is either even if it is projecting on to an irrep A_1 , if it is projecting to a irrep B_1 it should be an odd wave function ok.

So, now let me come to one non-trivial example, I did this simple 1 cross 1 matrix which is not that important, but it is a warm up. So, let us take this, we have been doing on the C_3 v the 2 cross 2 matrix representations which are nothing, but your rotation matrices right. Rotation matrices σ_v we have written it many times and I also told you that you can do a tensor product. So, this tensor thing is not coming, but this will give you a reducible representation ok. So, I think I have a matrix example here. So, E of the this E refers to the 2 dimensional irreducible representation of C_3 v for the elements C_3 ok.

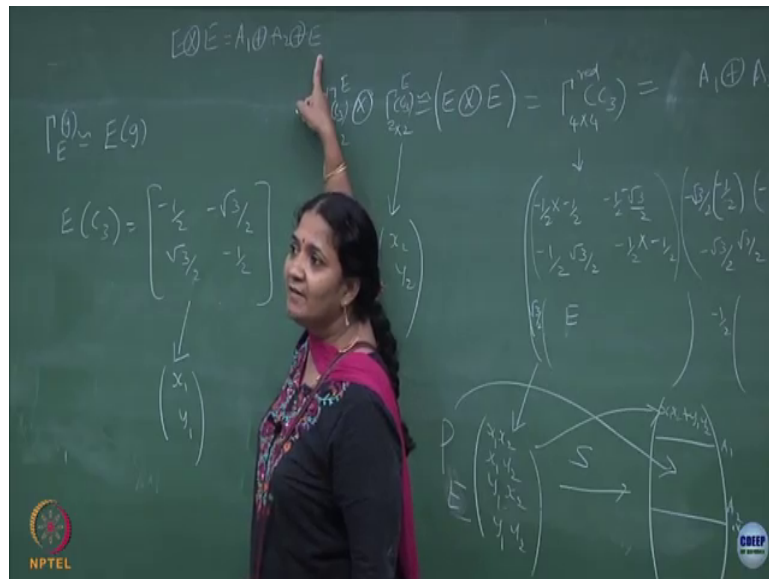
(Refer Slide Time: 06:37)

Example continued

$$E(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$
$$\Gamma(C_3) = \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & \frac{3}{4} \\ -\frac{\sqrt{3}}{4} & \frac{1}{4} & -\frac{3}{4} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{3}{4} & \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix}$$


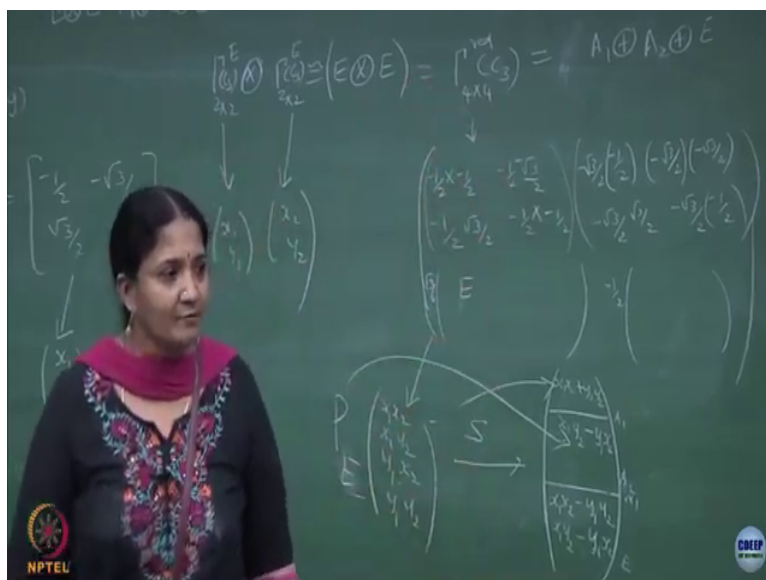
So, that is what that is just a rotation by 120 degrees which you have gone through many times. What is the corresponding vector space? It's just 2 dimensional vector space and we can take the basis to be the x y basis. Is that clear? Are you all with me? So, now you do the tensor product of E cross E, let us do it gamma E I am going to use the shorthand notation as E for g.

(Refer Slide Time: 07:27)



I am going to work it out for C 3 minus or plus ok, it will act on the basis the corresponding basis; let me take it as x 1 y 1 and take a tensor product.

(Refer Slide Time: 08:05)



So, I want to do a tensor product. So, let me write it here which I am going to denote it as E cross E . This is 2 cross 2, this is 2 cross 2, this will be multiplied is going to give me a 4 cross 4 which is reducible and I am confining myself to C^3 . You can do it on every element of C^3 , just for an exercise I am doing it for you here. So, what do you have to do? You have to take this 2 cross 2 matrix, take the first element minus half and multiply with all the 4 elements right.

So, let us write that here that is the first block, second block will be minus root 3 by 2 with minus half minus root 3 by 2; you understand what I am doing right. Are you all with me? So, I have written that 2 by 2 block, right this is one block, this is another block. I need to do the same thing here. What will be the multiplication? It will be this element multiplying with all the 4 elements right. Let me write this as the E ok, you understand what I am saying; the last

one will be a minus half with the same thing; this is what I have simplified here and put it on the screen for you so, that you can check it out ok.

These are the 4 cross 4 matrix representation. What is the basis vector? This one is $x_1 y_1$, let us take for this one $x_1 y_1$, this one as $x_2 y_2$ ok. So, the basis vector for this will be $x_1 x_2$ $x_1 y_2$ then $y_1 x_2$ $y_1 y_2$, is that right? Am I right? Ok. This is a reducible vector space, I want to use the projector to find out what is the irreducible subspace ok, is that fine. Here mechanically we took B_1 times B_1 and said it is A_1 by looking at it. But, technically you should be able to take the reducible representation and break it up and see how many components are there right; so, you can do that here.

Student: Ma'am.

Yeah.

Student: Why do we want to take x_1 is through (Refer Time: 11:49) because these are the same representation (Refer Time: 11:51).

Which same no no its a same representation, but one is acting on particular 1 another one is acting on particle 2 or one is acting on the position space, one is acting on the momentum space. So, you can take it like that. You can also do it on the same particle twice that is a different thing, then you will have quadratic powers that is what I wrote here like you can do $C_1 C_2 C_1$ squared is like on the same basis, but this is on a two different spaces that is why that. So, all those finer details can be worked depending upon whether both are same space or different spaces.

Right now, I am taking it as like let us take a this is something which you have been doing mechanically. I am sure your all been doing two spin half particles, you combine and then you find the irreducible sub space. Now, I am trying to tell you that this is purely from this projection, purely from multiplicity when you take the tensor product what are the irreps, how

many times it occurs. And, then the projection operator will tell you what are the sub spaces ok.

This one which I have written is a reducible space, what I am going to show is that that S matrix will break it up into a piece which is $x_1 \times x_2$ plus $y_1 \times y_2$ that is one piece. Then you will have a another piece which belongs to A_2 and then another piece which belongs to E which are all binary basis. The binary basis is nothing, but the dot product of 2 vectors belongs to your trivial representation. This is like taking dot product of $x_1 \times y_1$ with $x_2 \times y_2$ and you will get it naturally. How will you get this? If you do a projection operator A_1 , it has to give you this.



If you do a projection operator A_2 , it has to give me this which is also 1×1 , if you do a projection operator E, if you do a projection operator E; the projection operator should be; what should be the rank of this projection operator? It is a 2 dimensional projection operator or it will give you two independent basis which means its rank is 2, it is a rank 2 projection operator. And, the rank 2 prediction operator will give you these two basis. And why have I said $A_1 \ A_2$ and E? I have not really done it here, but if you try to work this out you will find it is a direct sum of A_1 plus A_2 plus E ok.

I have not really worked it out, but this breaking is using that multiplicity argument; you can check this out, I have not done it here. So, basically I am trying to say that $E \times E$ in the shorthand notation which I am using will turn out to be A_1 plus A_2 plus E ok. So, this is what? This is 2 dimension, this is 2 dimension, it is 4 dimension; this one is 1 dimension, this one is 1 dimension, this is 2 dimension; it breaks up into irreducible subspaces which is 1×1 , 1×1 and a 2×1 .

The corresponding matrices will be block diagonal ok; the corresponding matrices will be block diagonal with first block diagonal as 1×1 , the next one is 1×1 , but it belongs to the irrep which is different. If it is 1×1 you can look at the character table and see that it is A_2 characters entries and then the last one will be the conventional 2 dimensional irrep ok. So, this is what I am trying to show on the screen here.

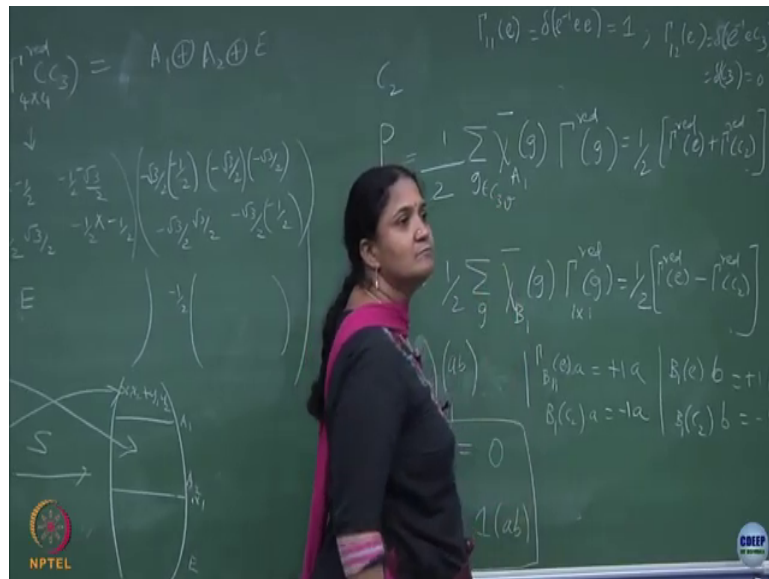
(Refer Slide Time: 16:01)

Example continued

$$P_{\Gamma^{\alpha}} = \frac{\ell_{\Gamma^{\alpha}}}{|G|} \sum_{g \in G} \overline{\chi^{\Gamma^{\alpha}}(g)} \Gamma(g)$$
$$P_{A_1} = \frac{1}{6} [\Gamma(E) + \Gamma(C_3) + \Gamma(C_3^2) + \Gamma(\sigma_v) + \Gamma(C_3\sigma_v) + \Gamma(C_3^2\sigma_v)]$$


So, I have explicitly tried to P A 1 in the case of C 3 v group all the characters are plus 1 using this formula ok, but now you replace it by all the elements of C 3 v and do not worry about this.

(Refer Slide Time: 16:25)



So, this is what I have written it on the screen here, order of the group is 6. The dimension of the matrix dimension of the irrep A 1 is 1 cross 1, 1 dimensional irrep and then the all the characters of this A 1 which is a unit representation is all 1. So, you add up all the matrices. I wrote only 1 matrix, you have to write the matrices for all the elements and add it up. What you get is what do you call it as a projection operator for A 1. So, I have shown that here P A 1 turns out to be this, sorry this is not right is that right yeah it is right. So, this is a 4 cross 4 matrix, write the 4 cross 4 matrix sum it up.



(Refer Slide Time: 17:23)

Example continued

- The projection matrices are

$$P_{A_1} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}, P_E = \begin{pmatrix} \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$
$$P_{A_2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Check the rank of these matrices



And what you get are the projection operator for A_1 , again do it for using the characters of the irrep E ; please check this and the last one. And, you can check that the rank of these matrices are these two are 1 and 1 and this one will have a rank 2 ok.

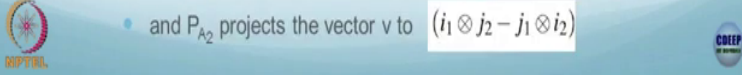
(Refer Slide Time: 17:53)

Example continued

- $P_E v = ?$ What the two binary basis of irrep E?

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \alpha - \delta \\ \beta + \gamma \\ \beta + \gamma \\ -(\alpha - \delta) \end{pmatrix}$$

- $P_E v = \frac{\alpha - \delta}{2}(i_1 \otimes i_2 - j_1 \otimes j_2) + \frac{\beta + \gamma}{2}(i_1 \otimes j_2 + j_1 \otimes i_2)$
- Similarly, P_{A_1} projects the vector v to $(i_1 \otimes i_2 + j_1 \otimes j_2)$
- and P_{A_2} projects the vector v to $(i_1 \otimes j_2 - j_1 \otimes i_2)$



The immediate step after this as you take an arbitrary vector just like I took $x y z$ or $a b c$ take an arbitrary 4 dimensional vector, you know what is the basis state right. I am using here the $i_1 \otimes j_1$ notation, but it is like $x y$ coordinate if you want to take it. So, $i_1 \otimes i_2$ $j_1 \otimes j_2$ $i_1 \otimes j_2$ $j_1 \otimes i_2$ ok. So, what is happening is that if you do the projection operator for each of the irreps on this arbitrary vector, you get this answer especially for P_E I get this answer ok.

What does it mean? I get a linear combination for arbitrary $\alpha \beta \gamma \delta$ so, this means that there are; so, this one will be according to that. It will be $x_1 x_2$ minus $y_1 y_2$ and this one is $x_1 y_2$ minus or plus $y_1 x_2$. This is just basis for the E projection and for the A_1 anyway I have written and A_2 will be the mistake I did, this is minus I have used i_1, i_2 , but it is the same as the i component and the j component.

The thing which I want you to do is I will put this on Moodle, please check this algebra; it is just to I have given you the concept today. But, unless you work it out all the 4 cross 4 matrices and substitute and check it out, you will not understand what I am saying. So, I have given you this data, this also you should check. You should also check that the projection operator P_{A_1} when operates on an arbitrary $\alpha \beta \gamma \delta$, it gives you only this subspace whose basis is going to be given by $x_1 x_2$ plus y_1 or I call it as $i_1 i_2$ plus $j_1 j_2$ ok.



And, you can check P_{A_2} will give you this and P_E will give you this. So what does that tell me, that I can start writing binary basis z^2 is a trivial binary basis which will come from $A_1 \otimes A_1$. If you do $A_1 \times A_1$ you will get a z^2 . How were you getting $x^2 + y^2$? It is this one when x_1 and x_2 are taken to be the same x , you get $x^2 + y^2$ that comes from the tensor product of $E \otimes E$ and it belongs to the A_1 irrep ok.

(Refer Slide Time: 21:21)

Recall Character table

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2; z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x,y); (R_x, R_y)$	$xz; yz$

Binary basis emerging from tensor product



And similarly you can work out all the tensor products ok.

(Refer Slide Time: 21:29)

C_2 group

$$P_a = (e_a/h) [\sum_g \chi_a(g) g]$$

For C_2 act the two one-dimensional projection operator on wavefunction $\Psi(x)$ and obtain the projected state.

These projected states are the relevant basis wavefunctions of the irreps A and B of group C_2 -we discussed in class





So, we will anyway this I have already discussed with you.

(Refer Slide Time: 21:35)

Recall Character table

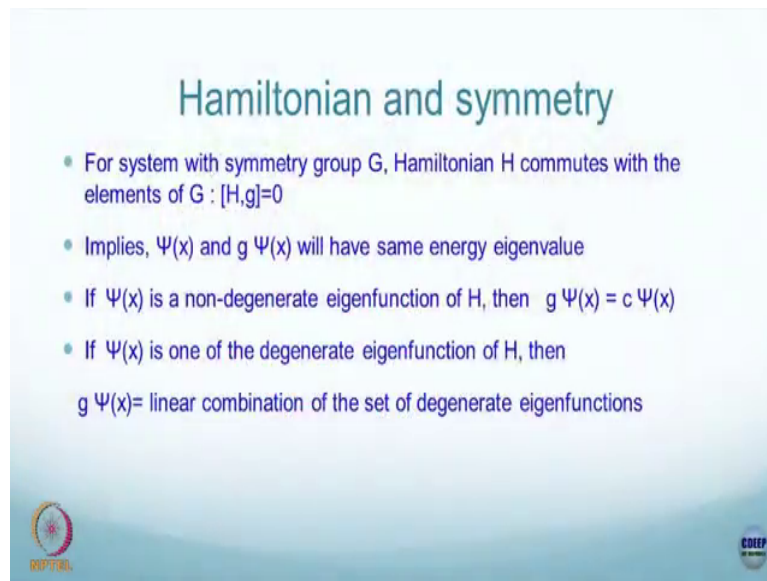
C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2; z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y); (R_x, R_y)$	$xz; yz$

Suppose C_{3v} symmetry of a molecule breaks to a subgroup $C_s \equiv \{E, \sigma_v\}$ due to external perturbation. How does the two-dimensional degenerate level of C_{3v} split with respect to C_s subgroup?



This also I was telling you that typically a system will have a bigger group and then you break it up into a smaller group ok. This you can try it out and there was one more assignment problem which you have supposed to do it and take a look at this. Essentially you will have a system, sudden perturbation will break it up into a lower symmetry system. Once it does whatever irrep in which the system was there it becomes the reducible representation and it will break it up into irrep of the lower group representation ok. So, this is what will happen in nature ok.

(Refer Slide Time: 22:17)



The slide is titled "Hamiltonian and symmetry" in a teal font. It contains four bullet points in blue text. The first bullet point states: "For system with symmetry group G, Hamiltonian H commutes with the elements of G : $[H,g]=0$ ". The second bullet point states: "Implies, $\Psi(x)$ and $g \Psi(x)$ will have same energy eigenvalue". The third bullet point states: "If $\Psi(x)$ is a non-degenerate eigenfunction of H, then $g \Psi(x) = c \Psi(x)$ ". The fourth bullet point states: "If $\Psi(x)$ is one of the degenerate eigenfunction of H, then $g \Psi(x) =$ linear combination of the set of degenerate eigenfunctions". In the bottom left corner, there is a logo for "RIPTAS" featuring a stylized atom. In the bottom right corner, there is a logo for "CDEP" with the text "at IIT Bombay" below it.

So, to sum up what I am trying to tell you, I just wanted to flash this for you since I have done so much. For any system with symmetry group G Hamiltonian H will commute with the elements of G that is the definition of saying that, if suppose the Hamiltonian has a symmetry, Hamiltonian will commute with every element of this C_2 group. The non-trivial element is only the C_2 element, Hamiltonian will commute with that. Once it commutes whenever there is a commutation relation like this in quantum mechanics you allow for you allow for state ψ of x and $g \psi$ of x to have the same energy; you all know that right.



If you have operator A and operator B commuting, you can have a simultaneous eigen states of both operator, the two operators which commute. Here the first operator is Hamiltonian; so, I am saying the energy eigen states have to be degenerate in general. When will it not be degenerate? If g on ψ of x is proportional to ψ of x that is what happens in this harmonic

oscillate, g on ψ of x is proportional to ψ of x then you will get non-degenerate eigen state. How do I see it in this irrep language? How do I see it in this irrep language?

(Refer Slide Time: 24:05)

Character table and degeneracy

- Character table gives the characters and dimensions of the irreducible representations α 's
- $\Gamma_\alpha(g)$ irrep for group G will act on ℓ_α dimensional basis states ξ_i where i takes $1, 2, \dots, \ell_\alpha$.
- $\Gamma_\alpha(g) \xi_i$ will be linear combinations of ξ_i 's
- Both $\Gamma_\alpha(g) \xi_i$ and ξ_i have same energy if H is invariant under the group symmetry G - hence **dimensionality $\ell_\alpha > 1$ of irreps** indicate degenerate eigenfunctions
- Relook at particle in a 2-d square box and its group symmetry which allows 2-fold degenerate wavefunctions

If it was degenerate then you will have g of ψ of x will be a linear combination of the set of degenerate eigen function, this is known in quantum mechanics. Now, in the irrep language look at the character table. So, when you take the character table C_{3v} has two 1 dimensional irrep, one 2 dimensional irrep, C_{2v} has two 1 dimensional irrep. Once you look at this character table, the corresponding matrix representation will have to act on a vector space which will have basis states. So, ξ_i is what I am calling it as a basis states, where i will run from 1 to ℓ_α .

And, what is the meaning whenever there is a group symmetry in the system when I operate this on ξ_i , it will be a linear combination of ξ_i . If it is 1 dimensional vector space, if ℓ_α

is 1 what is the linear combination available? You do not have other linear combination ok. So, γ_g of ψ_i and ψ_i will have to have same energy, if the Hamiltonian had the group symmetry. And, γ_g of ψ_i will give you a linear combinations of basis states of that irrep, if there is only a 1 dimensional irrep, what is the linear combination?

So, it is non-degenerate, if you are looking at 1 dimensional irrep χ_i and you do γ_g on χ_i it better be only proportional to χ_i ; you cannot get anything linear combination. The linear combination will happen only when you go to C_{3v} or other groups with 2 dimensional irreps, where the basis will be 2 dimensional basis or 3 dimensional basis depending on what group symmetry we are looking at ok, is this clear?

So, now with this information you take a relook at the particle in a 2 dimensional box ok, that is why you start getting degeneracies when you go to 2 dimensional box is because of the C_{4v} symmetry. Because, C_{4v} symmetry will allow for a 2 dimensional irrep and then γ_g of ψ_i will be a linear combination that is why you start getting degenerate states for 2D harmonic oscillatory or 2D particle in a box, but not for a 1D harmonic oscillator. 1D harmonic oscillator has to be non-degenerate because the irreps of the character table are only 1 dimensional, you cannot get degenerate energy eigen states, is this clear? Ok. So, let me stop here.