Group Theory Methods in Physics

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Lecture – 21
Mulliken Notation, Character Table and Basis

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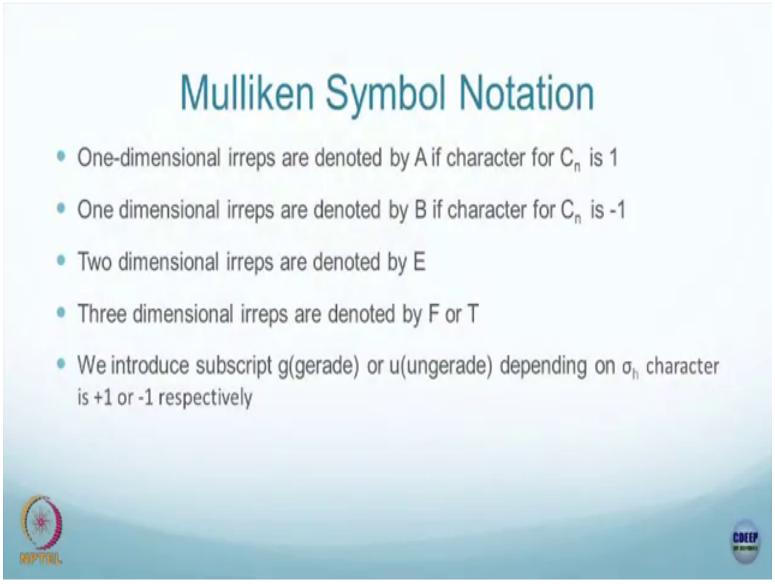

So, just as a warm up what we did discussed in the last weeks lectures the confinement was onto the character table and I said that we will use this Mulliken notation Mulliken symbols to write down the irreps by now should be clear what I mean by irrep. So, that is a short form I am going to use irreducible representation, it is cannot be further broken down into any blog diagonal form by any similarity transmission.

So, those are the irreps and you denote for one dimensional irrep either by a letter A or a letter B, letter A is use if the character of the n fold axis rotation that particular elements C n element if it is plus 1 we use the letter A, if the character is minus 1 you use the letter B.

For two - dimensional irreps we use the letter E, three and three dimensional representation we call it as F or T for all your point groups you do not go beyond three usually it is all the groups which we are studying will be up to three dimensions ok. So, then we also have some more finer details we introduce a subscript g for gerade or u for ungerade depending upon sigma h character is plus 1 or minus 1 respectively.

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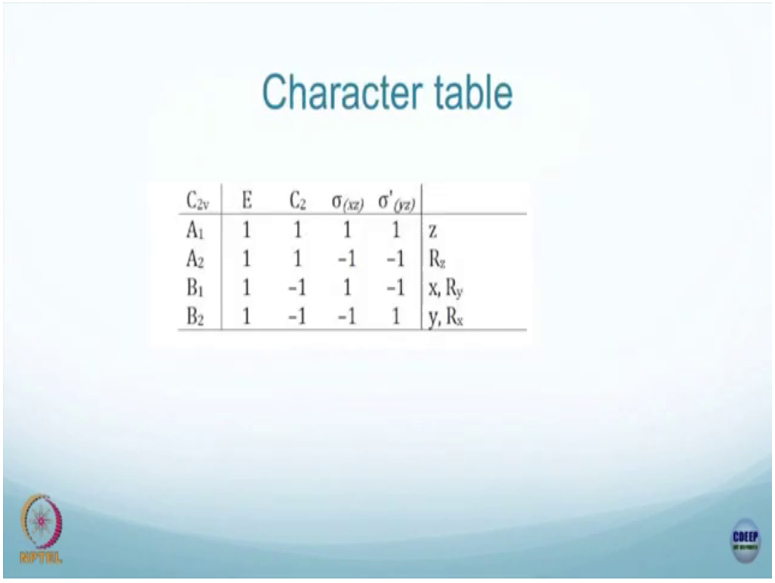

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma'_{(yz)}$	
A_1	1	1	1	1	z
A_2	1	1	-1	-1	R_z
B_1	1	-1	1	-1	x, R_y
B_2	1	-1	-1	1	y, R_x

So, just to give you an example we have done this many times C 2 v the character table we worked it out right E C 2 sigma in the x z plane and the other mirror plane which is also vertical plane both are vertical plane because it has the z coordinate in it the plane contains a z axis ok. So, these A 1 and A 2 are corresponding to they are 2 different one dimensional irrep the first one is the trivial unit representation right.

We call it unit representation and the C 2 element the C 2 is the principle axis here that element is plus 1 here that is why we calling it as A these 2 and the C 2 element for the B s are minus 1. So, the last 2 characters we call it as minus 1 and we have already seen that if you had 4 conjugacy class, you will have 4 irreps and by using those postulates as a consequence of great orthogonality theorem there will be 4 one dimensional irrep for the abelian group of order (Refer Time: 03:23) ok.

A question for you if instead of C 2 v if I replace it by C 4 if I replace it by C 4 then can this character table be used or can we have another character table ok, think about it and Thursday we can discuss. So, C 4 and C 2 v character table are they same or there is something which you need to work on. There is a slight difference right C 4 has C 4 times C 4 squared a C 4 cubed there is some certainty is there.

So, you need to worry about that certainty and see whether the character table you can also look up the literature and see how the C 4 table is written ok. C 2 h is again principle axis is 2 fold and then you have a mirror which is in the xy plane ok. So, if you take that then you see that the E C 2 sigma h and I if you look at the sigma h eigen value the sigma h eigen values plus here.

So that is why the subscript g is written, if it is minus then you rewrite it as ungerade and this A and B nomenclature is with respect to the principle axis if these 2 are plus then it is A and the subscript depends on the sigma h value. So, it is g for this and u for this and similarly this one is B both of them are B because the C 2 is minus 1 are you all with me are you all able to see and if you look at the sigma h eigen value you call that as g or call that as u.

So, this is the nomenclature and I will come back to this basis we have already seen that the z axis rotation about z axis does not alter any of these elements. So, the unit representation the basis is z axis ok. So, when it comes here there will be some certainties because when you do z axis what happens sigma h will take it is in x y plane it takes z 2 minus z.

So, your trivial representation or unit representation cannot have z axis as the basis. So, it should be a vector in a x y planes right cross product of a vector in a x y plane having components x and y, that is what we call it as a axial vector you all know what is an axial vector.

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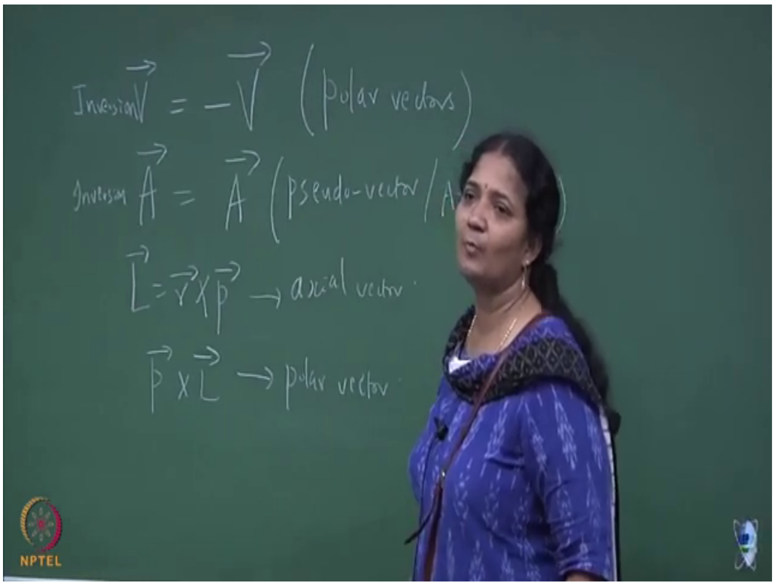

A general vector when you do an inversion if you took a vector when you do an inversion what happens? It becomes.

Student: Minus.

Minus the same vector right so, this is what will happen for polar vectors ok. Axial vectors; axial vectors under inversion will remain as axial vector does not change sum, sometimes called a pseudo vector or axial vector both are means the same. You know what is the example simple example is your angular momentum r cross p cross product of 2 polar vectors will behave like a axial vector right.

So, this is an axial vector, what about p cross L, p is the momentum, L is the angular momentum, p cross L behaves like a polar vector ok. So, this one is behaving like a this is a crucial conventional cross product which you know in your three dimensions. So, in this case when you see the unit representation or the trivial representation in the slide.

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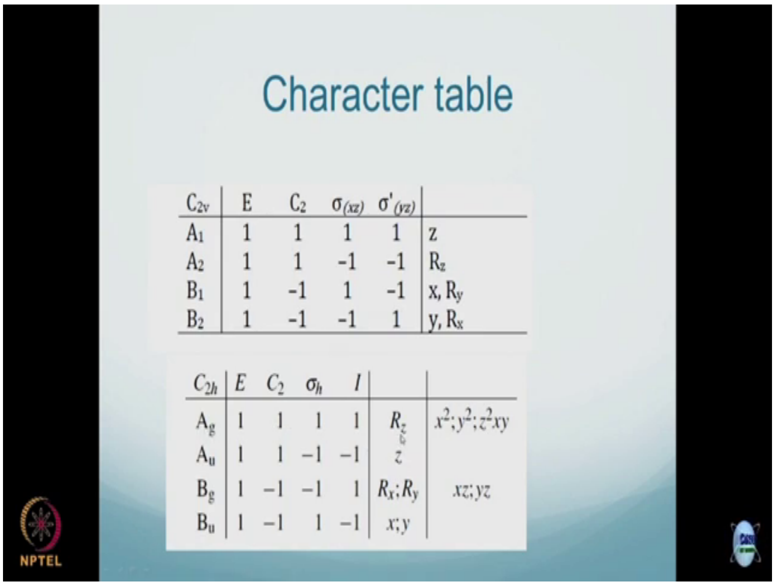

So, this slide shows that sigma h eigen value is plus 1 right, all the eigen values have to be plus 1 which basis will have all the eigen values of plus 1 if you want to look at it you will be able to show that it should be an axial vector only if the z component of the axial vector, roughly you can see that L z if you are taken x will change and under C 2 x p x right.

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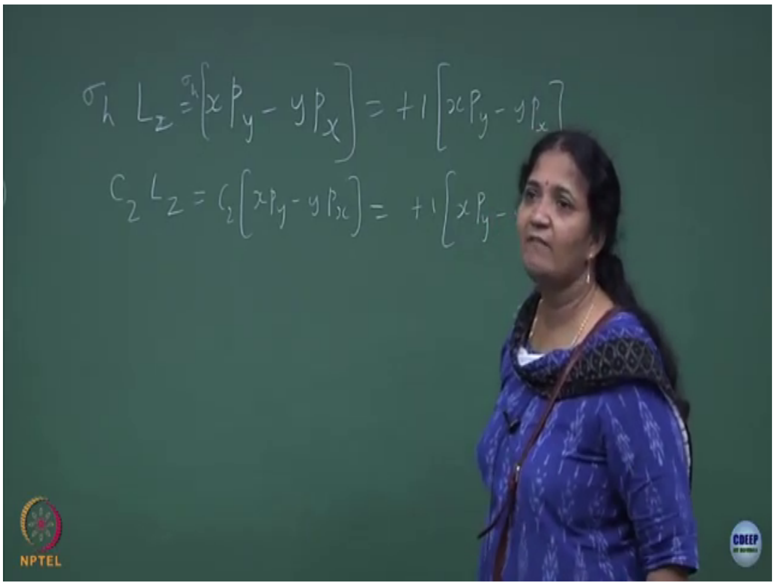

Let us write it L is z is x p y minus y p x right, if you do a sigma h operation on this it should be applicable not only to a position vector it should be applicable to any vector components. So, sigma h on this is in the x y plane right. So, I have to do sigma h on this one. So, what will happen x and y components do not change so, it gives you a plus 1 times ok.

Similarly C 2 on L z will be C 2 on x p y minus y p x C 2 on x will change sign and C 2 on p y will also change sign, the y component will change sign x component is that right, C 2 180 degree rotation about z axis will change both x and y components. So, it is minus into minus which is plus. So, that is why it is going to be plus 1 times x p y minus y p x.

So, if you are given axial vector the z component of the axial vector is the basis for the unit representation of C 2 h, but whereas, if you look at C 2 v the z component itself of a polar vector itself is basis vector. So, I leave it you to check the other basis vectors in the same argument, on the slide if you see C 2 v I have said that the axial z component is the basis what do I mean by this if I do sigma on that R is z ok. So, I need to show that if you had R is z. So, this is 4 C 2 v this I did it for C 2 h if I take C 2.

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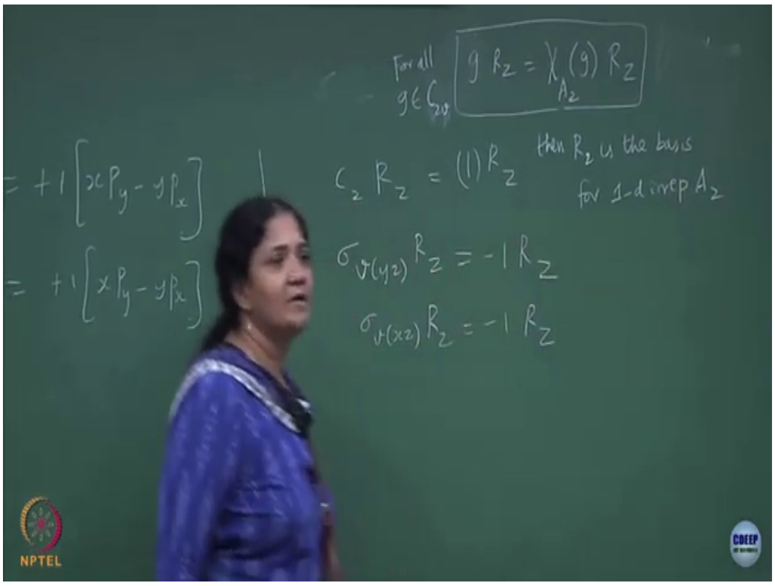

C 2 of course, you have argued here what did we get? It is plus 1 right. So, that is plus 1 sigma v y z component, someone do it on this.

Student: Minus.

And sigma v x is z component and what else we left I did it anyway we know. So, if you see here the character table the R z basis is the right basis because it will be an eigenvalue equation of every group element acting on R is z because one dimension it is also trivelin eiegn value question.

So, every group element the character in the A 2 representation for every group element on R z turns out to be. So, I should say here in the group element, the group element on this is the character on A 2 for the g element on R z is that is this true for all 1 dimensional irreps ok. So, I did this for A 2 you can try and do this for B 1 and B 2 check it out, the x y we have already discussed right.

When we wrote the rotation mattresses we discuss this, but for R y and R x also you can check B 1 there can be 2 possible basis it can be the polar x component or the axial y component it should be 1 diamond basis, similarly if you look at B 2 you can show that it is polar y component or R x.

Student: (Refer Time: 14:26).

This equation is like the group this is what I did know the group element if you apply on R z that is the group element when it picks up the corresponding character times this basis. So, this is like an eigenvalue equation the number which you get should match with your character table number if it is not happening then you have to find out which irrep it is happening it should be for the all gs.

For all gs element of g. In fact, this g is actually C 2 h c 2 h or C 2 v sorry C 2 v this is C 2 v check that this is satisfied then you know that R z is the basis vector for the irreducible representation. So, let me write that also clearly for the 1 d irrep A 2, any questions on this? Same thing I want you to do for the other rows I have done explicitly now for the first row of C 2 h and I have done it for the second row of C 2 v ok.

Please try it out and make sure that you understand the conventional basis in the position vectors or axial vectors, position vectors are like polar vectors and axial vectors are going to have this pseudo operation under inversion.

Student: (Refer Time: 16:50) axial vectors in x y z are.

That is right correct that is the notation I am going to fall ok.

So, I have added one more column in the C 2 h which well come back to it this is called binary basis x is a basis which you can call it as a primary fundamental basis, you can take powers of those basis and you can start looking at what are the binary basis we will come to it and sometimes it is not always possible to write the basis. So, if you do not find a basis you leave it blank in the convention position vectors ok. So, since I have put this in let me also give you a small example ok. So, C 2 character table ok.

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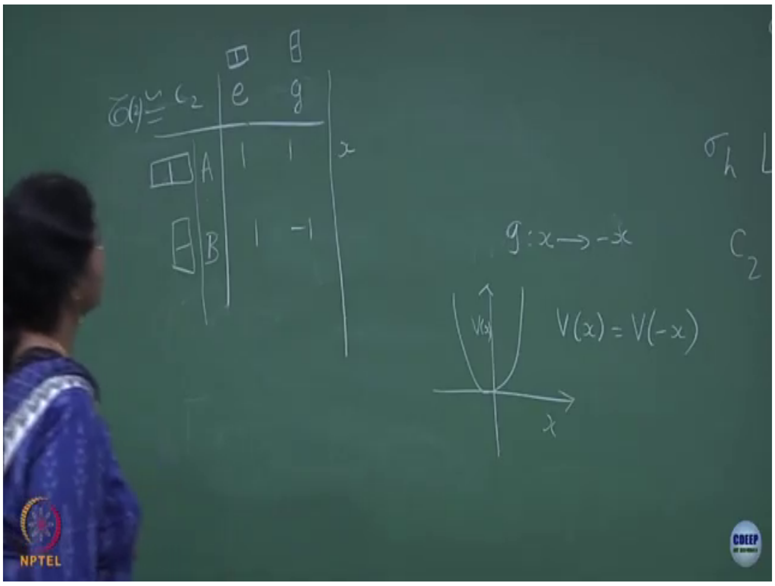

C 2 is isomorphic 2 also the permutation of 2 objects right it is also isomorphic 2 just only mirror and so on. So, C 2 what is the number of elements there is only one element e under C 2 ok, I can even put this to be some g such that g square is e that is the condition order to group.

It all isomorphic, you can treat it like a permutation group or a C 2 group or other mirror groups also e and c v e and sigma v or e and sigma h. This in the permutation group what are the diagrams identity element is 2 1 cycles, how will I draw this way and g is 1 2 cycle the squire of that element is identity right you all with me.

So, in that notation how many irreps are there; how many irreps are there? 2 irreps first irrep will be unit element, second irrep will be 1 minus 1 this cannot change this has to change for orthogonality. According to our thing we will write the unit representation in the permutation group as if it is a symmetrizer and this will be anti symmetrizer, if you are looking at it as a C 2 group what are the index we will use this will be a C 2 element.

Then this will be A and this will be B, there are no A 1 B 1, because there are not more than 1 as 1 irrep with Mulliken notation A 1 irrep with Mulliken notation B correct. So, what are the basis vectors you can ask, you can treat us if you are looking at A 1 dimensional problem let us take our simple harmonic oscillator 1 d harmonic oscillator right. What does the symmetry of this V of x equal to V of minus x I can define a g operation on x takes into minus x, identity operation does not do anything g operation changes to minus x.

So, the x is a good coordinate in fact, y can also be used z can also be used by the same kind of, but I am confining myself to a 1 d problem. So, this is x no that is not x someone this is not x, g has too g on x has to be minus x which one ok? So, this is the character table which will help me to look at the harmonic oscillator problem.

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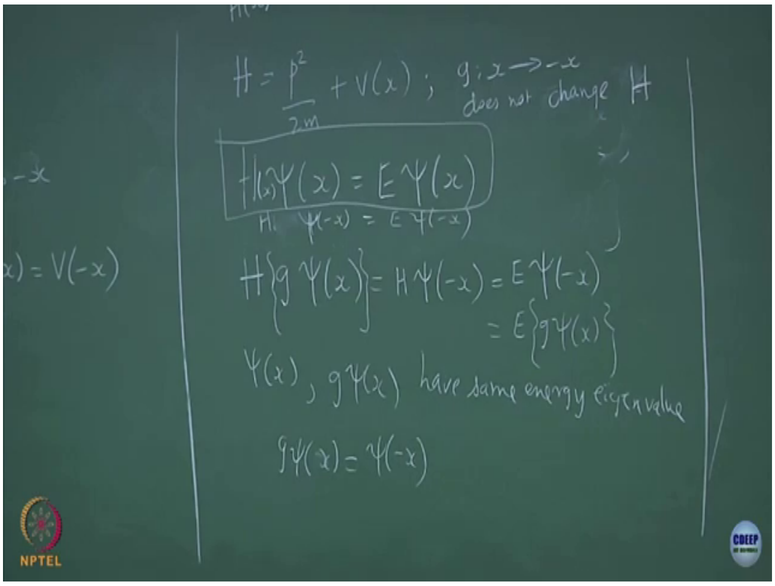

So, tell me I have a Hamiltonian for the harmonic oscillator, what is the Hamiltonian it is the total energy which I can write it as V of x and when you write the Schrodinger equation you write high psi of x equal to e psi of x right.

But we also know that the Hamiltonian this Hamiltonian does not change right under the groups symmetric this group symmetric let me call it as ordered to symmetry it is calling it as C 2, but you can call it also as a inversion right x going to y, what is the meaning of it? So, typically when I see the Hamiltonian I have to list out what are the groups symmetries.

So, what are the groups symmetries here the non-trivial element of that group is only g which takes x 2 minus x does not change; does not change Hamiltonian you all agree, because of this symmetric portage if you had some asymmetry potential that condition will not be true, clear.

So, if I do H g on psi of x what is g on psi of x is going to do psi of minus x ok. So, in this eigenvalue equation if I replace x 2 minus x so, this is actually dependent on x right if suppose this is this coordinate is dummy coordinate you could write H of minus x psi of minus x equals to psi of minus x at H of minus x is same as H of x right H of x is same as H of minus x you all agree.

So, which means the second replace it again as Hamiltonian on psi of minus x is E on psi of x are you all with me. So, then what happens H on psi of minus x is again E of psi of minus x clear. So, what I have shown, what I have shown this is an eigenvalue equation, I also see that there is a group summary the group is the group with this character table with the non trivial element g that groups symmetry that non trivial element of that groups symmetry does not alter my Hamiltonian.

So, that is why I am calling that to be the symmetry of this Hamiltonian. Once I put this in what am I getting I am showing that psi of x and g psi of x have same energy do you all with me? Both are same energy, what is this definition what is this called.

Student: (Refer Time: 26:26).

It will be degenerate if psi of x cannot be written as constant multiple of g of psi of x otherwise it will be non degenerate right and g of sign psi of x I am going write it a psi of minus x allowed.

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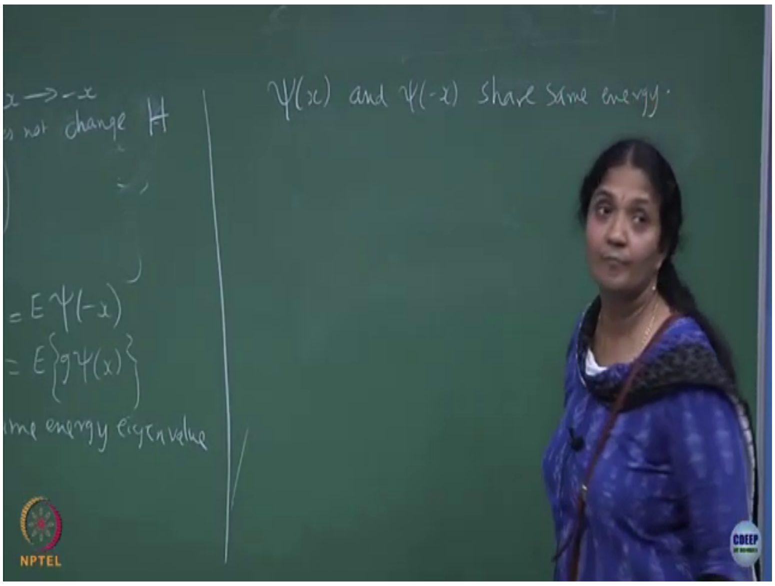

So, psi of x and psi of minus x, psi of x and psi of minus x share same energy ok, what is that next step you know from harmonic oscillator solving, have you seen degenerate energy eigenvalues in the 1 d harmonic oscillator?.

No, you know why, because of the same groups symmetry which you mechanically use right, equalently look at this character table the character table tells you that your wave functions which you write must be either an irreducible representation of A or B or this representation symmetric or anti symmetric this is this statement. So, let me try and say this little more clearly.

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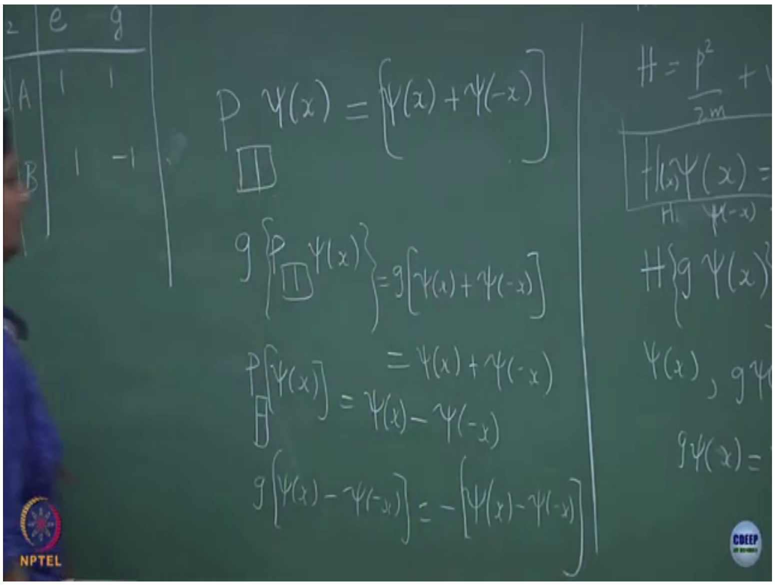

So, psi of x there exists a projector a symmetrizer associated with one of the irreps, what is the symmetrizer mean I told you already. Symmetrizer means that all the group elements should not change the configuration like what will happen is that it has to become ok. The projector will project my wave function any arbitrary wave function into a symmetric combination by this what I mean is if I do a group operation on that projected state g on psi of x right projected state is psi of x plus psi of minus x.

So, g on psi of x plus psi of minus x will turn out to be same you will remain in the same space irrespective of the group operation. So, there should be a projector a predictor this is (Refer Time: 29:57) given now, but I will systematized it at some point right now you take it.

And then the group operation does not take you from this space to this space ok, similarly if you do P on psi of x what will this P? Psi of x minus psi of minus x right and whenever you do a group operation on psi of x minus psi of minus x it will be minus of psi of ok. So, look at this relation that g, g gives you a plus 1 eigen value here and g gives you a minus 1 eigen value here and let us go and look at this character table.

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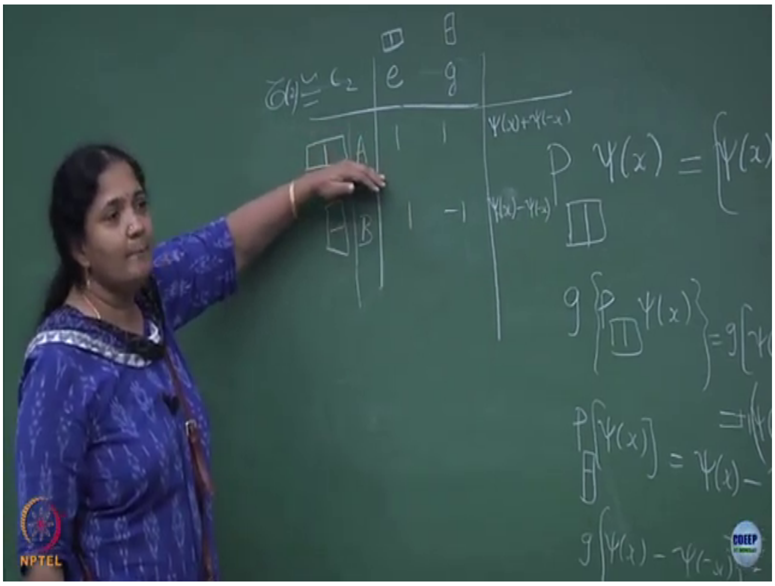

The g gives me a plus 1 eigenvalue means this is a good candidate because g operating on this is plus 1 times, if you look at minus 1 if you want to get it is psi of x minus psi of minus x. So, all your harmonic oscillator wave functions should either belong to this irrep or this irrep it can be dangling, because the groups symmetry of the harmonic oscillator is respected by this order to group ok. It has to be necessarily what is this wave function property, it is even function, it is odd function, this is what you see in your harmonic oscillator.

Harmonic oscillator without doing a calculation just purely from groups symmetry I can say that the wave functions have to be either symmetric wave function or anti symmetric wave function it cannot be both it cannot be a function without any symmetry it is purely from this group symmetry ok. How do we get these projectors I will explain, but as of now once you get into this thing you can see clearly that g if you write a function and this has to be psi of minus x it has to be proportional to it I should say ok.

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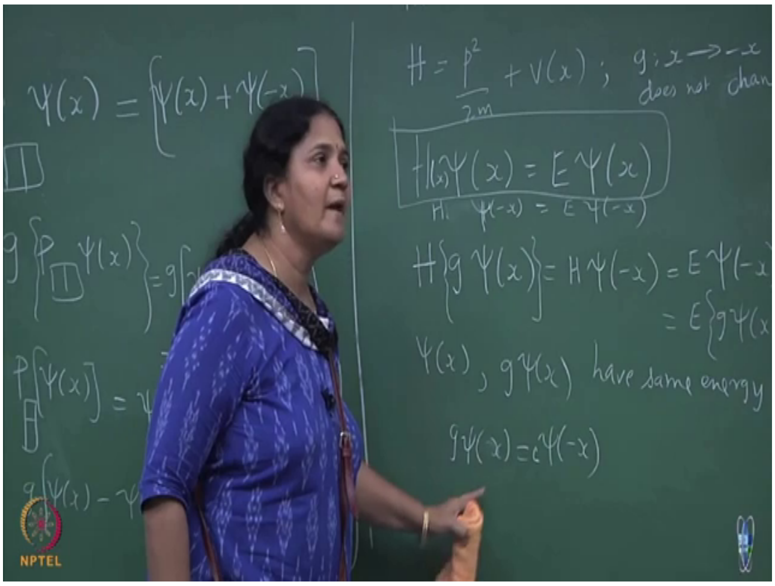

So, it should be sums I should put here it is not exactly equal to I should say sum C eigen value C ok. This breaks it into either the wave function should be symmetric anti symmetric and it will be only a non degenerate wave function.

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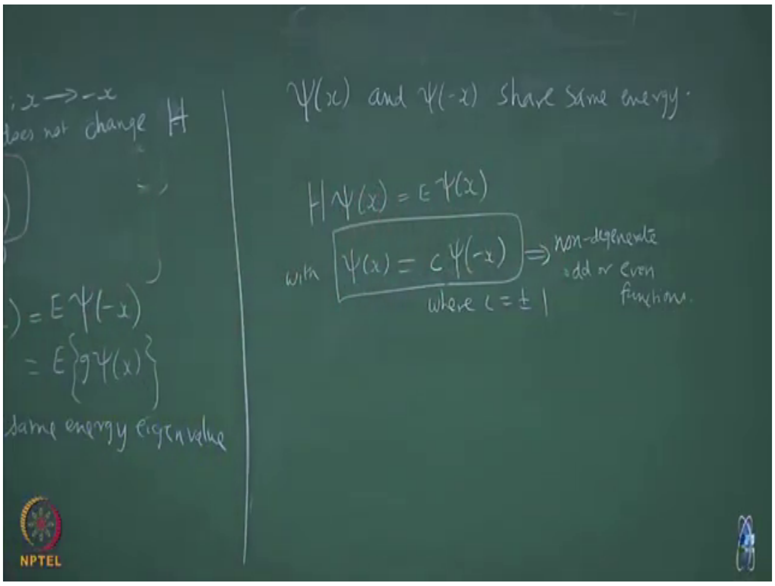

Once I put this in you can show that with psi of x equal to sum C psi of minus x where C is plus or minus 1, this condition that it is proportional these 2 are not independent if it does not equal to it then you would have said it is degenerate wave function right. In this case since it is proportional to this proportionality constant C you can fix because the group is of order 2.

So, you if you take square it is C square have to be plus 1 the only option is C has to be plus or minus. So, the this implies non degenerate odd or even functions ok. So, this is what you get without solving the problem and you can determine the actual wave function with the symmetry properties required by your irreps.