

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

**Lecture – 59**

**Hydrogen atom energy spectrum and degeneracy using Runge – Lenz vector**



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**SO(4) = SU(2) x SU(2)**

- We can rewrite so(4) generators such that the algebra resembles product of two su(2) algebras

$$\hat{I} = \frac{1}{2}(\hat{L} + \hat{M}'); \quad \hat{K} = \frac{1}{2}(\hat{L} - \hat{M}')$$

- That is.,
  - $[I_i, I_j] = i\hbar\epsilon_{ijk}I_k$
  - $[K_i, K_j] = i\hbar\epsilon_{ijk}K_k$
  - $[\hat{I}, \hat{K}] = 0$
- Clearly,  $[\hat{I}, H] = 0; [\hat{K}, H] = 0$ .
- Hence we can write states which are simultaneous eigenstates of H,  $I_z$ ,  $K_z$

So, get back to the slide here. So, if you see the slide the SO 4 generators you can try to rewrite a linear combination with the rescale Runge-Lenz vector with L such that you see the I is exactly like an SU 2 algebra. There is another SU 2 algebra with the K and these two do not talk to each other. What do I mean by do not talk to each other? Any of the components of I with any of the components of K the commutator is 0.

What such a thing we call it in discrete groups? We call it as like a direct product group. If we have g 1 and g 2, elements of g 1 and g 2 commute orderly it does not matter, you call it is a

direct product group. Similarly, the  $SO(4)$  algebra involves two sub algebras which are  $SU(2)$  and  $SU(2)$  the corresponding group  $SO(4)$  will be a direct product of two  $SU(2)$  groups, ok. I think one of the assignment problems had to do with this. If you have done the assignments then you will appreciate what I am saying, ok.

Now, tell me if I given this information that Hamiltonian commutes with  $I$ , Hamiltonian commutes with  $K$ . Well  $I$  has  $i_x, i_y, i_z$ ,  $K$  has  $k_x, k_y, k_z$ . Now, what do I write for a state? State should be a simultaneous eigenstate of Hamiltonian  $I_z$  and  $k_z$ . If course, you can also say because  $SU(2)$  you know that it should also be a eigenstate of  $i^2$  and  $k^2$ , right or you can write this states of  $SU(2)$  has highest weight comma the weight vectors, right.



This is what we do, ok. So, hence we can write the states which are simultaneous eigenstates of Hamiltonian because it commutes with  $I$  and  $K$ , the Hamiltonian, you can write it as a simultaneous eigenstate of Hamiltonian  $I_z$  and  $K_z$ . Is everything clear to you?.

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$SO(4) = SU(2) \times SU(2)$

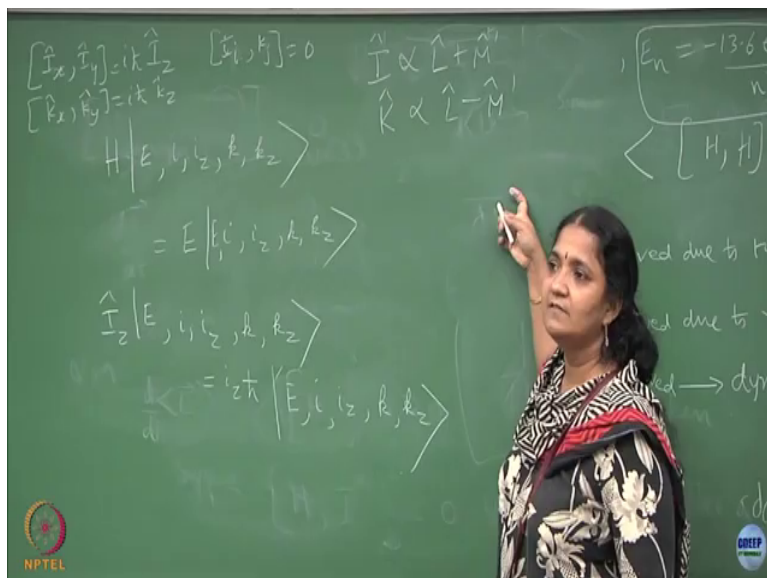
- The simultaneous eigenstate is denoted as  $|E, i, i_z, k, k_z\rangle$
- We can construct two Casimir operators which commutes with all  $so(4)$  generators and H:
$$C_1 = \hat{L} \cdot \hat{L} + \hat{K} \cdot \hat{K} \quad C_2 = \hat{L} \cdot \hat{L} - \hat{K} \cdot \hat{K}$$
- Using the form of  $\mathbf{M}$  and  $\mathbf{L}$ , you can check that  $C_2$  is a null operator
- This implies that  $i$  and  $k$  are constrained to be same
- Hence  $C_1 |E, i, i, k, k_z\rangle = 2i(i+1)\hbar^2 |E, i, i_z, k, k_z\rangle$

where  $C_1 = \frac{1}{2}(\hat{L}^2 + \hat{M}^2) = -\frac{\hbar^2}{2} - \frac{\mu \kappa^2}{4H}$ .



So, that is what I have done here. I have written the corresponding highest weight  $i_z$ , highest weight  $k_z$  and it should be a simultaneous eigenstate of Hamiltonian also. So, I have put the energy on the states. What is the meaning of this? I am sure somebody can help me out. Hamiltonian on  $|E, i, i_z, k, k_z\rangle$  will give you  $E |E, i, i_z, k, k_z\rangle$  and if you take  $i_z$  operator on  $|E, i, i_z, k, k_z\rangle$  then it will be  $i_z \hbar |E, i, i_z, k, k_z\rangle$ . I am putting  $\hbar$  cross because I am using them even in the definition on the Runge-Lenz vector  $k_z$ , ok.

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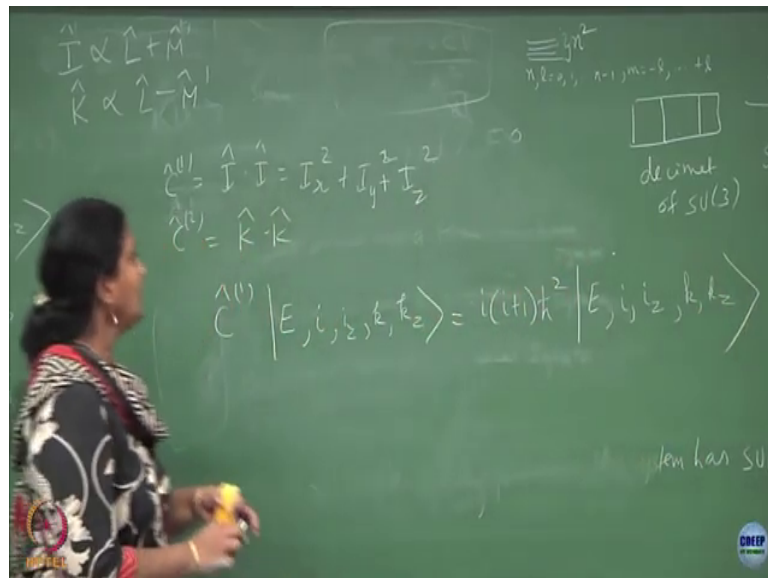
Similarly, for  $k_z$ . So,  $I$  satisfy this algebra, right I wrote you also already  $I_x, I_y$  is  $i\hbar$  cross  $I_z$ ,  $K_x, K_y$  is  $i\hbar$  cross  $K_z$ . And you also have  $I_x$  with  $k_y$  or any of the components, in fact, I will call it as  $i$  and  $K_j$  this is going to be 0 that is why this is  $SU(2)$  sub algebra,  $SU(2)$  sub algebra then the total algebra of  $SO(4)$ . How did we write  $I$  and  $K$ ?

We wrote  $I$  and  $K$  as think up to some constant it is  $L$  plus  $M$  prime  $M$  prime is the rescaled Runge-Lenz vector up to constants and  $K$  is  $M$  prime, ok. So, these are the  $SO(4)$  generators and you took a linear combination of the  $SO(4)$  generators so that you get the familiar  $SU(2)$  algebra which I know how to work out. And when I play around only with the familiar  $SU(2)$  algebras, clear.

So, if I want to determine  $I$  there are ways of defining  $i$ ,  $i$  is such that any of those  $I$  plus  $I$  minus which you generate with  $I_x$  plus  $I_y$ , if  $I_z$  is  $i$  then it will be 0  $I$  plus will be 0.

Similarly, if it is  $k_z$  is  $k$ ,  $I$  plus on that state will be 0 that is one way of determining what is  $K$  and what is  $I$  in the lie algebra language, but you could also define a Casimir. What is the Casimir? I defined that also the Casimir operator is one which commutes with all the generators, quadratic Casimir.

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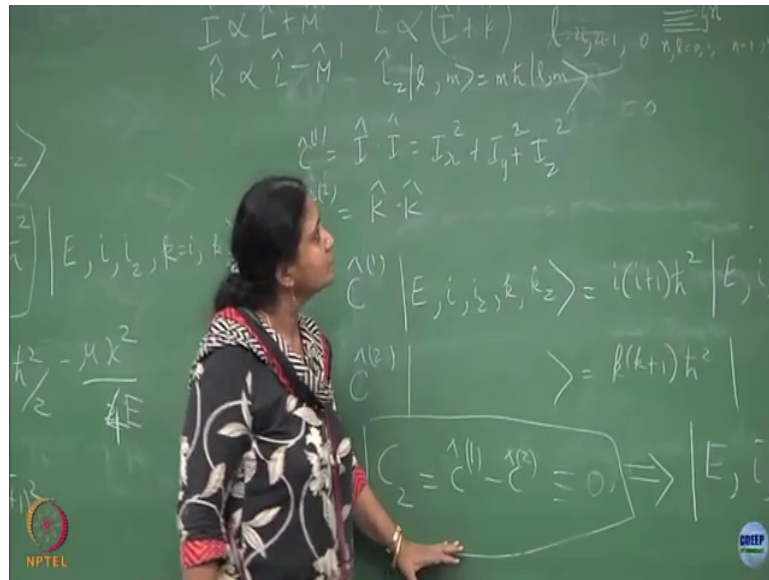


So, it can define a Casimir which is  $I \cdot I$  what is that  $I_x$  square,  $I_y$  square,  $I_z$  square, right, you can define one Casimir like this. You can define another Casimir which is  $K \cdot K$ . And, if you take this Casimirs operated on the same states what will you get? Someone? What will you get?  $I$  into  $i$  plus  $1$   $\hbar$  cross square it is an eigenstate.

Casimir means it commutes with it is a linear combination of the quadratic bilinear in the generators, it commutes with all the generators. In fact this commutes with each of the components of  $I_x$ ,  $I_y$ ,  $I_z$ , it also commutes with the Hamiltonian because of that, it also

commutes with  $k_x$ ,  $k_y$ ,  $k_z$  because this commutator is 0. So, that is why it is also you can write an eigenvalue equation involving this. If it did it with  $C_2$  what will happen?  $C_2$  will give you  $k$  into  $k$  plus  $1$   $h$  cross  $1$ , clear, ok.

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So, these information we are going to exploit to do work further evaluation and determining what is this energy, fine, clear, ok.

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### SO(4) = SU(2) x SU(2)

- The simultaneous eigenstate is denoted as  $|E, i, i_z, k, k_z\rangle$
- We can construct two Casimir operators which commutes with all so(4) generators and H:
 
$$C_1 = \hat{L} \cdot \hat{L} + \hat{K} \cdot \hat{K} \quad C_2 = \hat{L} \cdot \hat{L} - \hat{K} \cdot \hat{K}$$
- Using the form of **M** and **L**, you can check that  $C_2$  is a null operator
- This implies that  $i$  and  $k$  are constrained to be same
- Hence  $C_1 |E, i, i_z, k, k_z\rangle = 2i(i+1)\hbar^2 |E, i, i_z, k, k_z\rangle$

where 
$$C_1 = \frac{1}{2}(\hat{L}^2 + \hat{M}^2) = -\frac{\hbar^2}{2} - \frac{\mu \kappa^2}{4H}$$

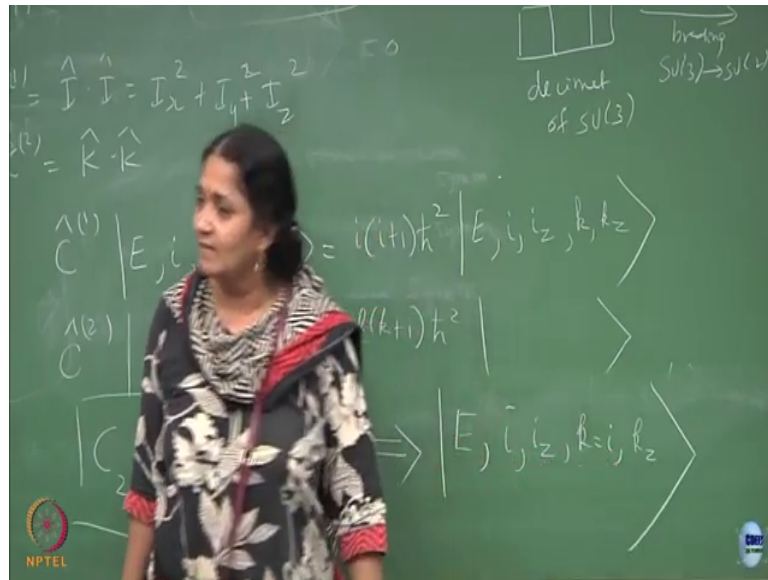
So, coming back to the slide I am going to take an interesting combination of  $\hat{L} \cdot \hat{L}$  which was one of the quadratic Casimir,  $\hat{K} \cdot \hat{K}$  is one of the quadratic Casimir. I am going to take a linear combination with a plus sign and what we call it is  $C_1$  that is also going to be an eigenstate of this operator and another one  $C_2$  which is difference of the two quadratic Casimir, ok.

I leave it to you to check that  $C_2$  will turn out to be 0. If you substitute explicitly the values of  $\hat{L}$  in terms of  $\hat{L}$  plus  $\hat{M}$  prime and  $\hat{K}$  as  $\hat{L}$  minus  $\hat{M}$  prime  $C_2$  will turn out to be a 0 operator. What is that mean? If  $C_2$  is the 0 operator null operator  $C_1$  eigen value is this,  $C_2$  eigen value is this. I want to define a  $C_2$  which is  $C_1$  minus  $C_2$ , ok.

If this is equal to 0 the physics of the system shows that this is 0, ok, the hydrogen atom spectrum or hydrogen atom operators Runge-Lenz rescale explicitly if you substitute the  $C_1$

and C 2 you find that the difference is 0 this is a constraint from the hydrogen atom system. Just looking at SU 2 cross SU 2 you will not have this constraint. If you fall back on the Runge-Lenz vector you see that this is an additional information I get, ok.

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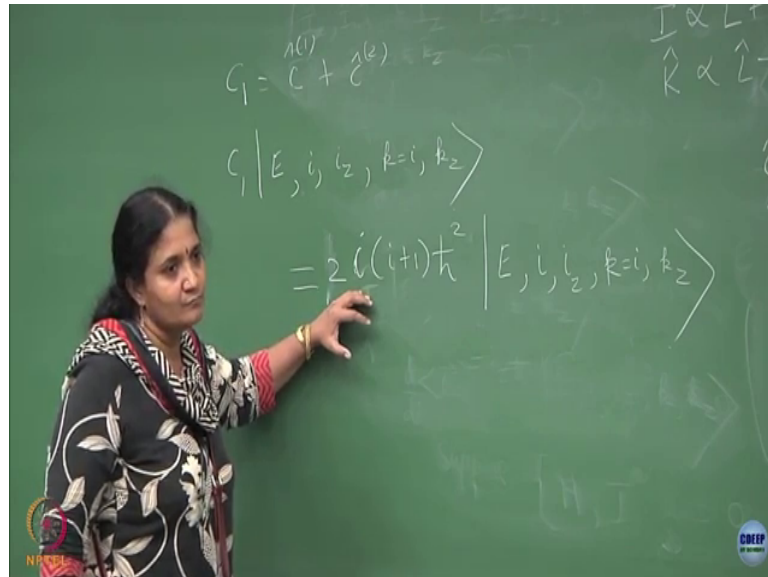
This information forces, this is the information pertinent to the hydrogen atom problem which forces that my states have to be E, i, i z, k equal to i k z. This is a subspace. The system gets into a subspace where this eigen value should be same as this eigenvalue which forces that the highest weight has to be i, ok.

This two are SU 2 algebras, but the eigen value of the second SU 2 algebra highest weight, should be same as the highest weight of the first SU 2 algebra because this constraint comes from my system under investigation hydrogen atom where the Runge-Lenz vector scale



satisfies this condition. So, looking at this you can say that this  $i$  has to be equal to  $k$ , ok. So, that is a subspace. Is this clear?

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So, once I put this condition then I can write the  $C_1$ ,  $C_1$  is. What will this be? It will add up now,  $C_1$  will give you  $i$  into  $i + 1$   $\hbar$  plus square  $C_2$  will also give you, into, plus  $1$   $\hbar$  cross square, but  $k$  is  $i$ . So, you will get this to be twice  $i$  into  $i + 1$   $\hbar$  cross square on; you all with me? Because  $C_1$  will give you  $i$  into  $i + 1$   $\hbar$  cross square  $C_2$  will give you  $k$  into  $k + 1$   $\hbar$  cross square, but  $k$  into  $k + 1$   $\hbar$  cross square because of this condition which came out from this input will force you and so, you have twice  $i$  into  $i + 1$   $\hbar$  cross square, clear, ok.

So, this  $C_1$  getting back to the slide, the  $C_1$  which I have written  $C$  subscript one that turns out to be write out in terms of we wrote it as  $\mathbf{L} \cdot \mathbf{L}$  plus  $\mathbf{K} \cdot \mathbf{K}$ , but rewrite it in terms of angular momentum, orbital angular momentum and Runge-Lenz vector re-scaled.



Please do that exercise, it turns out that it is going to be  $L^2$  plus  $M^2$  and you can write the quantum mechanical form of  $M^2$  to see the expression in terms of the Hamiltonian or energy eigen. This step I am not doing it here, but please check it out, ok. So, it is going to be the  $C_1$  eigenvalue which I wrote has to capture the energy of this state. So, this expression tells you that there is a relation which captures the energy of the state, ok. So, let me get to that state on the screen.

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### SO(4) = SU(2) x SU(2)

- From the two equations:
 
$$C_1 |E, i, i_z, k, k_z\rangle = 2i(i+1)\hbar^2 |E, i, i_z, k, k_z\rangle$$

$$C_1 = \frac{1}{2}(\hat{L}^2 + \hat{M}^2) = -\frac{\hbar^2}{2} - \frac{\mu\kappa^2}{4E}$$
- E is determined by equating
 
$$\hbar^2 2i(i+1) = -\frac{\hbar^2}{2} - \frac{\mu\kappa^2}{4E}$$
- The exact expression is
 
$$E_i = \frac{-\mu\kappa^2}{2\hbar^2(2i+1)^2}$$

So,  $C_1$  on  $i, i_z, k, k_z$  is equal to  $i(i+1)\hbar^2$ . This I have already explained. From here what do you have to do? You have to equate  $\hbar^2 2i(i+1)$  has to be equated to

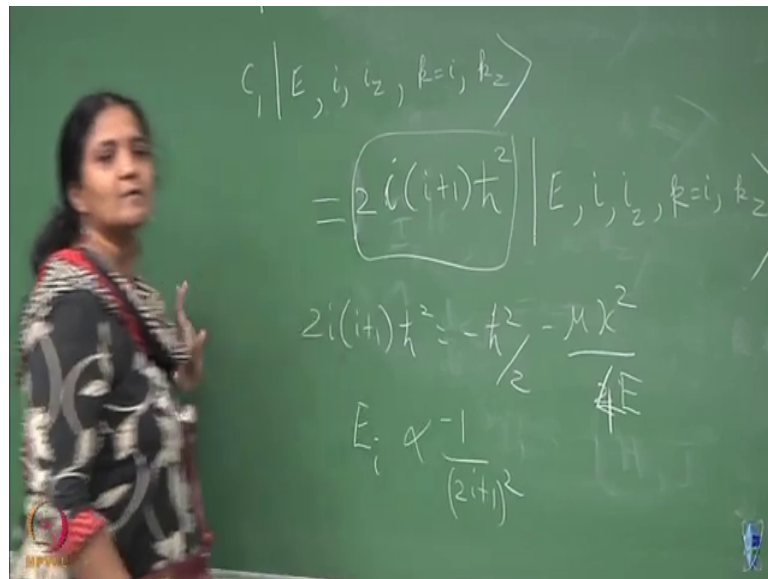
the right hand side of this operator which operates on the states. So, the corresponding Hamiltonian will give me energy  $E$ . So, the eigen value which you find here should be related to this expression, you all agree, is that clear?  $C_1$  operator the operator form in terms of the Hamiltonian is this.

So, you have another eigenvalue for it and that eigenvalue must be same as this expression. From here you can determine for a state with  $l$  highest weight here you can determine the energy eigenvalue. Please simplify this. Please simplify and see what you get it will turn out to be your expected answer provided you call this  $2l + 1$  as principle quantum number  $M$ , ok.

So, this simplify, please simplify this and see that you will end up getting this. I did not do anything other than exploiting Runge-Lenz vector is a conserved quantity and try to recast, so that it looks like an  $SO(4)$  algebra and  $SO(4)$  can be seen as two  $SU(2)$ . And then I had this additional information using the Runge-Lenz vector and orbital angular momentum it satisfies this condition and that force me that  $l$  and  $k$  are not independent,  $k$  has to be equal to  $l$ .

Once I have that condition I end up getting this eigenvalue, but this eigenvalue should be same as  $-\frac{\hbar^2}{2m} \mu^2$  by  $4E$ , ok.

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I am going to put from here you can determine what is E, and I am putting a subscript to remember that the state on which it was operating had this i and this turns out to be proportional to minus 1 over 2 i plus 1 plus 1 square, ok. So, far so good, ok.

So, we are going to use the fact that C subscript 1 is also in terms of the orbital angular momentum and the scaled Runge-Lenz vector is related to the Hamiltonian in the corresponding eigenvalue will be the energy E as I said on the board, so that is going to give us I am just summarizing the on the slide, so the C 1 eigenvalue will be it will have eigenvalue i into i plus 1 for i square and k square is again i call to k.

So, you have this. And substituting and equating both of these eigenvalues which is what I have done here. You end up getting an expression for the energy eigenvalue which is what I

explained now. So, clearly you see that  $i$  can be half odd integers in general because they are SU 2 quantum numbers  $2i + 1$  will always be integers.

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### SO(4) = SU(2) x SU(2)



- Replace  $(2i+1) = n$  in the energy eigenvalues

$$E_i = \frac{-\mu\kappa^2}{2\hbar^2(2i+1)^2},$$

- The eigenvalues are the familiar hydrogen atom energy levels:

$$E_n = -\frac{\mu e^4}{2\hbar^2 n^2}$$

- We know that the energy levels are  $n^2$  fold degenerate ignoring spin quantum number
- We can see this from the  $su(2) \times su(2)$  algebra

So, replace  $2i + 1$  to be  $n$  which is nothing it is similar to your principle angular momentum principle quantum number which you see in your hydrogen atom. So, essentially the energy eigenvalue replacing  $2i + 1$  as  $n$  you get energy eigenvalue to be your familiar energy level stationary states of your hydrogen atom which is proportional to  $1/L^2$ . Remember this  $n$  is  $2i + 1$  and  $n$  be in the hydrogen atom context we call it principle quantum number and it is integer and  $i$  could be half integers, but  $2i + 1$  will always be an integer.

The next thing which we you have to which I already promise you that I will do is how to find the  $n^2$  degenerate, how can you show that each level is  $n^2$  degenerate and for

that you need to see the physical orbital angular momentum, ok. The orbital angular momentum as I was explaining here on the board if  $\hat{I}$  and  $\hat{K}$  is  $L$  plus  $M$  prime and  $L$  minus  $M$  prime, the physical orbital angular momentum is actually a linear combination of  $\hat{I}$  and  $\hat{K}$ , ok.



So, this is going to be like an angular momentum addition of two angular momentum. So, you will end up having the eigenvalues. So, these  $L_z$  will be on the eigenstates are  $l m$  with eigenvalue  $m \hbar$ , where  $m$  will take values from minus  $l$  to plus  $l$  and what are the all values allowed for  $L$  is given by the angular momentum addition, ok. So, it will be from  $l$  minus  $K$  to  $l$  plus  $K$ . So, you will have because  $l$  is equal to  $K$  is the constraint which comes from this condition the  $L$  values take value from  $2l$ ,  $2l - 1$  up to  $0$ , ok.

So, you do see that if you replaced  $2l + 1$  as  $n$ , then  $l$  goes from  $0, 1$  to  $n - 1$  which is what you physically see the azimuthal quantum number given a principle quantum number  $n$  you will have a azimuthal quantum number taking  $0, 1$  up till  $n - 1$  which comes naturally from the angular momentum addition which allows the range of  $l$  to be  $2l$ ,  $2l - 1$  up to  $0$ , ok. And from there you can determine the degeneracy to  $n^2$ .

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### Physical orbital angular momentum $L$

- Note that the orbital angular momentum  $L$  is given by addition of the two  $su(2)$  generators :
 
$$\hat{L} = \hat{I} + \hat{K}$$
- The eigenstates of  $L_z$   $|\ell m\rangle$
- Where the range of  $\ell$  will be from
 
$$i+k, i+k-1, \dots, |i-k|$$
- With the condition  $i=k$ ,  $\ell = 2i, 2i-1, \dots, 0$
- in terms of  $n=2i+1$ , we get  $\ell = 0, 1, 2, \dots, n-1$  giving degeneracy
 
$$= \sum_{\ell=0}^{n-1} (2\ell+1) = n^2.$$

I am explaining this again on the slide that the orbital angular momentum  $L$  is given by addition of two  $SU(2)$  generators  $I$  and  $K$ . The eigenstates of a  $L$  is  $z$  we denote it by  $l$  and  $l_z$  and the range of  $l$  will be from  $i+k$  to  $2i$  minus  $k$ , with the condition which we have imposed that  $i$  and  $k$  are not independent, but  $i$  is equal to  $k$  that forces the  $L$  which is the orbital angular momentum quantum number to run from  $2i$  or  $2i-1$  up to  $0$ .

Replacing it in terms of  $n$  which is  $2i+1$  we get  $l$  to be  $0, 1$  up till  $n-1$ , directly giving us the degeneracy to be similar to  $l$  going from  $0$  to  $n-1$  each of those magnetic quantum numbers will be  $2l+1$  dimension. So, if you sum up you will end up getting  $n^2$  which is the degeneracy of an energy level which is whose energy is  $1/n^2$ , proportional to  $1/n^2$ , ok.

So, I hope I have given you a feel of how group theory is actually useful to get the energy spectrum in a neat way, exploiting the conserve quantities has generators and trying to write a algebra and find out the constraints and determine the energy eigenvalues.

This is what has happened in the hydrogen atom spectrum; with the tool which have taught can be used for any abstract system or any complex system where you may find a set of conserve quantities, you can try to find the algebra for those generators and see whether they resemble some known lie algebras and you can exploit these powers and get certain quantities in an elegant fashion, ok.

I hope you enjoyed the course. And there are certain things like wave function in the hydrogen atom cannot be explicitly determined, but definitely the energy eigenvalues you do not need to go through those complex equations to solve, but use the symmetries including the dynamical symmetry due to Runge-Lenz vector, where we have written it as SO 4 and getting the energies of the stationary states to be proportional to minus 1 over n square in a neat fashion including the degeneries which is n square, ok.

Thank you.