

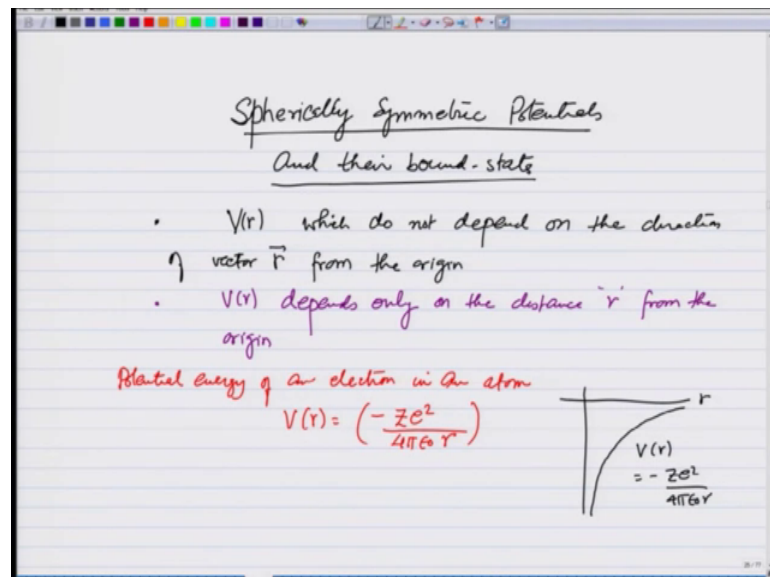
Introduction to Quantum Mechanics
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Lecture - 03

Schrödinger equation for particles in spherically symmetric potentials, angular momentum operator

From this lecture onward for 3 or 4 lectures we are now going to concentrate on this Spherically Symmetric Potentials and their bound-states.

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So, let me explain what spherically symmetric potentials are these are potentials $V(r)$ which do not depend on the direction of vector r from the origin. So, this is what they do not do what they do is they depend $V(r)$ depends only on the distance r from the origin and these will include potential energy of an electron in an atom where the potential energy $V(r)$ is given as minus Ze^2 over $4\pi\epsilon_0 r$ it depends only on r and the way it behaves from the origin is like this.

So, if this is r then it behaves like this depends only on the distance this is $V(r)$ equals minus Ze^2 over $4\pi\epsilon_0 r$ or electron or any other particle in a potential say one-half $k r^2$ which is also known as 3-dimensional harmonic oscillator or any other potential that depends on distance r only let me take one more example potential box in 3-dimensions. So, that would be something like this it is minus say some constant

$V = 0$ up to a distance a and then it becomes ∞ .

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• Electron in a potential $\frac{1}{2}kr^2$ (3 dimensional harmonic oscillator)

• Potential box in 3d

$V(r)$

$-V$

a

r

$V(r) = \text{depends only on } r$

Angular momentum in Q. Mech.
Corresponding operators
and their properties

This is r , $V(r)$ and this is a distance a this is another example of a 3-dimensional potentials all these potentials or potential energies have V the potential energy that depends only on r . And we want to explore that in the process we are also going to introduce the idea of angular momentum in quantum mechanics the corresponding, the corresponding operators and their properties. So, this is a program that will run over the next 3 4 lectures. So, let us begin as to why angular momentum becomes important in this case.

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$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$$

Since $V(r)$, it is good to work in spherical polar coordinates

Classically: Angular momentum of a particle moving in spherically symmetric potential is conserved

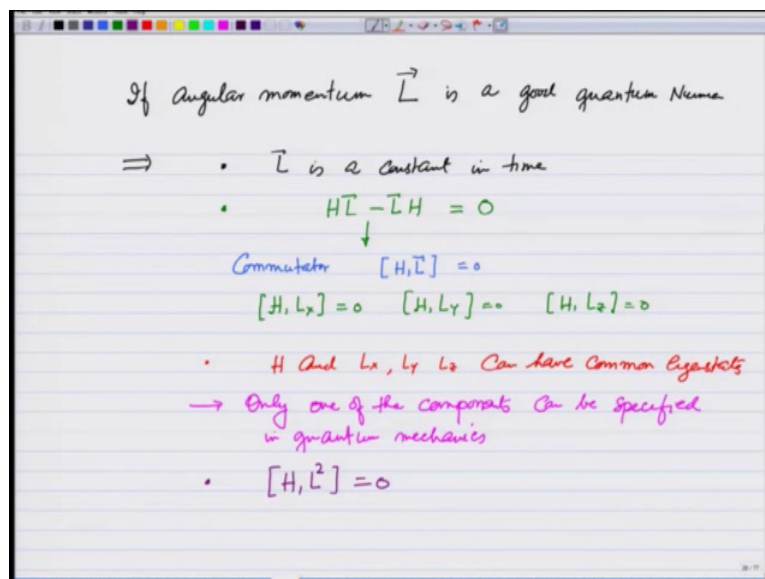
In quantum mechanics Angular momentum could be a good quantum number

H , and Ang. Mom operator have common eigenfunctions

So, the Hamiltonian in such cases where the potential is spherically symmetric is minus H cross square over $2m$, Laplacian plus V r notice that we are talking about a 3-dimensional case because the potential depends on r distance from the origin and therefore, the kinetic energy is necessarily as del^2 not a simple d^2 by $d x^2$ square d^2 by $d y^2$ square derivative and since V depends only on r it is good to work in spherical polar coordinates. So, it will be a good idea for all of you who are going through these lectures to review your spherical polar coordinates.

Now classically, classically what we expect in such potentials is that angular momentum of a particle moving in spherically symmetric potentials is conserved this is what we know for example, you know Kepler's laws and all those things follow from there what do we expect in quantum mechanics. So, in quantum mechanics correspondingly recall from your previous lecture angular momentum could we not yet proved could be a good quantum number and what do we mean by that? That means, that the H and angular momentum operator have common eigen functions. Let me explore that a bit more.

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So, if angular momentum and rather than writing it again and again let me call this vector [laughter], angular momentum L is a good quantum number this means number one L is a constant and time it does not vary, number 2 $H L$ minus $L H$ if I change the order of these operators and subtract this should be 0 this is what we have learnt last time.

Let me give this a name because we will keep coming again and again we call this a

commutator and denote it as this $H L$. So, commutator of H and L is going to be 0 what that means, in terms of components of angular movement of $H L$ x the x component of L will be 0 $H L y$ commutator would be 0 and H is that commutator would be 0. And if they are 0 this also implies that H and $L x$ or $L y$ or $L z$ not necessarily each one of these, but H with $L x$ H with $L y$ or H with $L z$ can have common eigen states then only the wave function that is a solution of the Schrodinger equation would have the each component being conserved, because the wave function does not change with time and therefore, that eigen value remains the same. What we will see in here I just put a avert that only and we will see why one of the components can be specified in quantum mechanics. Let me give that statement to you and I will show it later.

What other thing we can do is that the total angular momentum L square commutator also vanishes. So, all these mean that angular momentum is conserved. So, what I am going to do next is devote some time to find out what this angular momentum operator is what its components are represented as and what are these other properties and what is the Schrodinger equation therefore, for particle moving in a spherically symmetric potential.

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Angular Momentum operator

Classically $\vec{L} = \vec{r} \times \vec{p}$

Quantum Mechanics $\vec{L}_{op} = \vec{r} \times \vec{p}_{op}$

$\vec{L} = \frac{\hbar}{i} \vec{r} \times \vec{\nabla}$ ($\vec{p}_{op} = \frac{\hbar}{i} \vec{\nabla}$)

$\vec{L} = \frac{\hbar}{i} (x\hat{x} + y\hat{y} + z\hat{z}) \times (\hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z})$

$L_x = \frac{\hbar}{i} (y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$

$L_y = \frac{\hbar}{i} (z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$

$L_z = \frac{\hbar}{i} (x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$

So, let us now focus on the angular momentum operator. Now classically you have angular momentum which is r cross p . So, the corresponding operator in quantum mechanics will be L operator I will write operator now and then drop it later L operator

and L operator would be given as \mathbf{r} cross \mathbf{p} operator. So, [laughter], I will drop now operator form it is given as \mathbf{H} cross over \mathbf{i} \mathbf{r} cross the gradient operator because \mathbf{p} operator is \mathbf{H} cross over \mathbf{i} times the variant.

So, now, it is quite easy to find out what these are. So, L operator is \mathbf{H} cross over \mathbf{i} x , in x direction plus y in y direction plus z in z direction cross x partial with respect to x plus y partial with respect to y plus z partial with respect to z that is the operator for angular momentum and if you work it out that I will leave it is a very simple exercise for you is that it gives you L_x to be equal to \mathbf{H} cross over \mathbf{i} y partial with respect to z minus z partial with respect to y .

L_y comes out to be \mathbf{H} cross over \mathbf{i} , z partial with respect to x minus x partial with respect to y and L_z comes out to be \mathbf{H} cross over \mathbf{i} x partial with respect to y minus y partial with respect to x . So, these are the components or the operators of angular momentum components in Cartesian coordinates.

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Angular momentum in Spherical polar coordinates

$$\vec{L} = \frac{\hbar}{2} \vec{r} \times \vec{p}$$

$$= \frac{\hbar}{2} r \hat{r} \times \left(\hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \frac{\hat{\phi}}{r \sin \theta} \frac{\partial}{\partial \phi} \right)$$

$$\vec{L} = \frac{\hbar}{2} \left[\hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right]$$

$$\hat{\theta} = \cos \theta \cos \phi \hat{x} + \cos \theta \sin \phi \hat{y} - \sin \theta \hat{z}$$

$$\hat{\phi} = -\sin \phi \hat{x} + \cos \phi \hat{y}$$

$$L_x = \frac{\hbar}{2} \left(-\sin \phi \frac{\partial}{\partial \theta} - \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right)$$

$$L_y = \frac{\hbar}{2} \left(\cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right)$$

$$L_z = \frac{\hbar}{2} \frac{\partial}{\partial \phi}$$

But as I said earlier we are going to work in terms of spherical polar coordinates because angular momentum really comes into play when we are dealing with such systems. So, its angular momentum comes into play when we are dealing with systems with its spherical symmetry where it is conserved. So, let us also write angular momentum in spherical polar coordinates.

So, again L this is understood as an operator is $\mathbf{H} \times \mathbf{r}$ and I am going to write this \mathbf{p} the gradient operator in terms of this spherical polar coordinates. So, this is going to be $\mathbf{H} \times \mathbf{r}$ distance then \mathbf{r} unit vector cross \mathbf{r} unit vector partial with respect to r plus θ unit vector $\frac{1}{r}$ partial with respect to θ plus ϕ unit vector over $r \sin \theta$ partial with respect to ϕ . This is going to be the operator and when you write this further it is $\mathbf{H} \times \mathbf{r}$ cross \mathbf{r} unit vector is 0. So, that goes away and then you get $\mathbf{r} \times \theta$ $\mathbf{r} \times \theta$ is in ϕ direction. So, I get the ϕ component r cancels d by $d\theta$ and then I have $r \times \phi$ $r \times \phi$ is in minus θ direction. So, this becomes minus $\theta \frac{1}{\sin \theta}$ partial with respect to ϕ .

So, this is the angular momentum operator in spherical polar coordinates. Let us now write the components of L_x , L_y and L_z using spherical polar coordinates. For that I am going to use θ is equal to cosine of θ , cosine of ϕ in x direction plus cosine of $\theta \sin$ of ϕ in y direction minus \sin of θ in z direction and the ϕ unit vector is equal to minus sign of ϕ in x direction plus cosine of ϕ in y direction and I substitute these n and collect different terms.

So, what I am going to get then is that L_x will come out to be $\mathbf{H} \times \mathbf{r}$ in the brackets I am going to get minus $\sin \phi \frac{d}{d\theta}$ and minus co-tangent θ cosine of $\phi \frac{d}{d\phi}$. L_y is going to come out as $\mathbf{H} \times \mathbf{r}$ cosine of $\phi \frac{d}{d\theta}$ and then I have minus cotangent of $\theta \sin$ of $\phi \frac{d}{d\phi}$. And finally, L_z is the simplest and this comes out to be $\mathbf{H} \times \mathbf{r}$ $\frac{d}{d\phi}$ this is here as a component. So, the components of angular momentum in x , y and z direction are given in terms of spherical polar coordinates like this.

Let us rewrite them on the next page and discuss some of the properties.

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$$L_x = -\frac{\hbar}{i} \left(\sin \theta \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right)$$

$$L_y = \frac{\hbar}{i} \left(\cos \theta \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right)$$

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

- \hat{L} operator involves derivatives with respect to angular coordinates θ and ϕ only.

$$[\hat{L}, f(r)] = \hat{L} f(r) - f(r) \hat{L} = 0$$

$$\hat{L} f(r) \psi - f(r) \hat{L} \psi = f(r) \hat{L} \psi - f(r) \hat{L} \psi = 0$$

Hamiltonian for spherically symmetric systems

So, what we have found is that L_x is equal to $i\hbar$ will take the minus sign out minus \hbar cross over i , $\sin \theta$ d by $d \theta$ plus $\cot \theta$ $\cos \phi$ d by $d \phi$ L_y comes out to be \hbar cross over i , $\cos \theta$ d by $d \theta$ minus $\cot \theta$ $\sin \phi$ d by $d \phi$ and L_z comes out to be \hbar cross over i d by $d \phi$.

So, you notice that number one, L operator involves derivative with respect to angular coordinates θ and ϕ only there is no derivative with respect to r . So, if you take the commutator of L with any function of r which means L operating on f minus f L this will necessarily come out to be 0 how do we show that. Let us take this $L f r$ operating on say some ψ minus $f r L$ operating on some ψ now L has derivatives with respect to θ and ϕ only. So, it when it operates on f it gives you 0. So, this comes out to be again $f r L$ operating only on ψ minus $f r L$ operating on ψ because L operating on $f r$ gives you 0 and this is 0. So, L would commute or its commutator with any function of r alone not r vector r alone the radial distance is going to be 0.

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The image shows a whiteboard with handwritten mathematical notes. At the top, the Hamiltonian is given as $\mathcal{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$. Below this, two commutators are shown: $[\mathcal{L}, -\frac{\hbar^2}{2m} \nabla^2] = 0$ and $[\mathcal{L}, V(r)] = 0$. These lead to the conclusion $[\mathcal{H}, \mathcal{L}] = 0$. A red arrow points to the text " \mathcal{L} is a conserved quantity". Below that, it says " \mathcal{L} and \mathcal{H} ~~do~~ have common eigenfunctions". In green, it states " \mathcal{L}^2, L_z and \mathcal{H} will have common eigenfunctions for spherically symmetric potentials." At the bottom, three commutators are listed in blue: $[L_x, L_y] = \hbar L_z$, $[L_y, L_z] = \hbar L_x$, and $[L_z, L_x] = \hbar L_y$.

In particular now if I take the Hamiltonian for this spherically symmetric systems and calculate its commutator with L will turn out to be 0, so what I am doing is I am taking the Hamiltonian for the spherically symmetric systems minus \hbar^2 cross square over $2m$, L square plus $V(r)$, now ∇^2 involves only derivatives with respect to r and θ and the order does not matter. So, L with minus \hbar^2 cross squared over $2m$ ∇^2 is anyway 0. And we have just seen that L commutator with function V with that depends only on r it is also 0.

So, we conclude that $\mathcal{H} \mathcal{L}$ is 0 which implies that L is a conserved quantity or L and \mathcal{H} can have common eigen functions I am not making a very definitive statements that they do they can because we see in the next lecture that all functions cannot be made simultaneously eigen functions of L_x , L_y and L_z . So, what we are going to have instead is I will just cut this and say that L^2 , L_z and \mathcal{H} will have common eigen functions for spherically symmetric potentials. We will show that for the dawn.

Now, once we have got an L_x , L_y and L_z it is easy to show that L_x , L_y commutator is going to come out to be $\hbar L_z$, L_y , L_z commutator will come out to be $\hbar L_x$ and L_z , L_x commutator will come out to be $\hbar L_y$.

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Commutators of \vec{L} components

$$L_x = \frac{\hbar}{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \quad L_y = \frac{\hbar}{i} \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$L_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

$$\left. \begin{aligned} L_x L_y - L_y L_x &= i\hbar L_z \\ L_y L_z - L_z L_y &= i\hbar L_x \\ L_z L_x - L_x L_z &= i\hbar L_y \end{aligned} \right\} \vec{L} \times \vec{L} = i\hbar \vec{L}$$

Commutator of (L_i, L_j) $i \neq j$ is NOT ZERO
 These components cannot have simultaneous / common eigenfunctions.

Let us write these commutators of L components. So, what you will see is that L_x which is \hbar cross over i y d by d z minus z d by d y , L_y which is \hbar cross over i z d by d x minus x d by d z and L_z which is equal to \hbar cross over i x d by d y minus y d by d x . If you calculate the commutator; that means, $L_x L_y$ minus $L_y L_x$ if you calculate this just plug in the things and get it this comes out to be $i\hbar$ cross L_z and the cyclic combination. So, $L_y L_z$ minus $L_z L_y$ will come out to with $i\hbar$ cross L_x and the next cycle combination is going to be $L_z L_x$ minus $L_x L_z$ is going to be $i\hbar$ cross L_y . All this can be combined to write together as L cross L keeping the order of operators correctly is going to be $i\hbar$ cross L again.

So, what we notice is that the commutator of $L_i L_j$, i not equals to j is not zero and then the commutator is not zero. Again recall that these components cannot have simultaneous or common eigen functions; more on that in the next lecture.

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Operator for L^2

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$= -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right)$$

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\phi^2}$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left(\frac{L^2}{-\hbar^2} \right)$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} L^2$$

$$-\frac{\hbar^2}{2m} \nabla^2 = -\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2mr^2} \left\{ \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} \right\}$$

Now, what I want to do is from this I want to calculate the operator for operator for L square the magnitude of the angular momentum. So, L square is going to be L x square plus L y square plus L z square and I can substitute all that I calculated earlier and you will see that this will come out to be h cross square 1 over sin theta d by d theta sin theta d by d theta plus 1 over sin square theta double derivative with respect to phi this is what L square x let us relate it to the Laplacian.

So, I know that the Laplacian is 1 over r square d by d r r square d by d r plus 1 over sin theta d by d theta sin theta d by d theta plus there is a r square also plus 1 over r square sin square theta d 2 by d phi square. So, you see that this is equal to nothing, but 1 over r square partial with respect to r, r square d by d r plus 1 over r square and the operator for L square over minus h cross square.

So, I can write this del square as 1 over r square d by d r, r square d by d r minus 1 over h cross square r square L operator square and consequently minus h cross square over 2 m del square is going to be minus h cross square over 2m r square d by d r r square d by d r plus L operator square over 2m r square. This is kind of reminiscent of classical theory where we write the energy kinetic energy as p r square over 2m plus L square over 2 m r square. So, L square over 2 m r square is the kinetic energy of a particle going around in an orbit the non radial component of the kinetic energy and that rightly is expressed in the quantum mechanical language as L square operator divided by 2m r square.

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The image shows a whiteboard with handwritten mathematical expressions. At the top, the Hamiltonian operator H is given as
$$H = -\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2mr^2} + V(r)$$
 This is enclosed in a rectangular box. Below this, it is noted that L is a conserved quantity. The commutator $[H, L^2] = 0$ is shown, with a note that eigenfunctions of H and L^2 are common. Further down, the commutation relations $[L_x, L] = iL$ and $[L^2, L_i] = 0$ are written. Finally, for a spherically symmetric system, it is stated that $[H, L] = 0$ and $[L^2, H] = 0$.

And therefore, the Hamiltonian now for a spherically symmetric problems can be written as minus \hbar cross square over $2 m r$ square partial with respect to r plus L operator square divided by $2 m r$ square plus $V(r)$ this is the Hamiltonian for spherically symmetric system. I can write this because L now is a conserved quantity and you can see from this that $[H, L^2] = 0$ this means eigen functions of H and L^2 are common.

So, just to conclude this lecture what we have is we have shown derive the L , L operator that we have shown that $[L_x, L] = iL$ and that means, that I cannot find simultaneous eigen functions for all components of L . It is also easy to show after I calculate L^2 that $[L^2, L_i] = 0$ for any component would be 0. So, I can find common eigen functions of L^2 and any component, but only one component because all other components I cannot find it because of the first $[L_x, L] = iL$ the common eigen functions for all components.

And we also seen that for this spherically symmetric systems $[H, L] = 0$. That means, I can find common eigen functions of H and L at the angular momentum, but because of the commutation relation between different components of L I will be able to find common eigen functions of H and only one component of angular momentum which we usually choose to be L_z and $[L^2, H] = 0$.

We will use these to find the solutions of Schrodinger equation for these spherically

symmetric problems.