

Introduction to Quantum Mechanics
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Lecture - 05

Equation for the radial component of wavefunction for spherically symmetric potentials and general properties of its solution

We been looking at the Schrodinger equation for spherically symmetric systems.

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$[H, L^2] = 0$

$\Rightarrow L^2$ is a good quantum number

$H = -\frac{\hbar^2}{2m} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{L^2}{2mr^2} + V(r)$

Schrodinger equation

$-\frac{\hbar^2}{2m} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \psi + \frac{L^2}{2mr^2} \psi + V(r) \psi = E \psi$

$\psi(\vec{r}) = R(r) Y_{lm}(\theta, \phi)$

Do separation of variables

$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{l(l+1)\hbar^2}{2mr^2} R + V(r)R = ER$

And we have shown that H and L square is equal to 0 which implies that L square is a good quantum number. And the Hamiltonian is shown is minus h cross square over 2 m d by dr r square d by dr plus L square operator over 2 m r square plus V r. And therefore, the Schrodinger equation is minus h cross square over 2 m d by dr r square d by dr times psi plus L square operating on psi 2 m r square plus v r psi equals E psi.

I could tell you that psi r vector can be written as R which depends only on r and some other function which I have given as Y lm theta and phi and then write this and do separation of variables. And what you would find is that equation becomes minus h cross square over 2 m there is r square here: 1 over r square d by dr r square d R by dr plus l, l plus 1 h cross square over 2 m r square R plus V r R equals E R and that is because Y lm's give you this l l plus 1 term. Let me do this explicitly and show it to you.

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$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{L^2}{2mr^2} \psi + V(r)\psi = E\psi$$

$$\psi = R(r) Y(\theta, \varphi)$$

$$\frac{\hbar^2}{r^2} \left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) Y + \frac{R}{2mr^2} L^2 Y + V(r) R Y = E R Y \right]$$

$$= -\frac{\hbar^2}{2m} \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{1}{2mY} L^2 Y + V(r) = E$$

$$-\frac{\hbar^2}{2m} \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + V(r) - E = -\frac{1}{2mY} L^2 Y = \lambda$$

Depends only on r
depends only on (θ, φ)

So, when I have minus h cross square over 2 m, 1 over r square d by dr of r square d psi over dr plus L square over 2 m r square psi plus v r psi equals e psi. And write psi equals some function R of r other function which I am writing y theta and phi; then what I get is minus h cross square over 2 m 1 over r square the full derivative of r square d R by dr times Y plus L acts only on those functions which is a functions of theta and phi because involves no derivative respect to R. So, I get R over 2 m r square L square on Y plus V r R Y equals E R Y.

And then you divide this whole thing by 1 over R Y and multiply by r square to get minus h cross square over 2 m, 1 over R d over dr r square d R over dr plus 1 over 2 m Y L square Y plus V r equals E. And then I change sides of certain terms and write this as minus h cross square over 2 m, 1 over R d by dr of r square d R over dr plus V r minus E is equal to minus 1 over 2 m Y, L square Y.

And it is so happens that this term the term on the left hand side depends only on r; term on the right hand side here depends only on theta and phi. And for them to be equal therefore this must be equal to sum constant lambda.

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$$-\frac{1}{2m} L^2 Y = \lambda Y$$

$$\lambda = -\frac{l(l+1)\hbar^2}{2m}$$

$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{l(l+1)\hbar^2}{2mr^2} R + V(r)R = ER$$

E depends on the angular momentum l
 E depends on $R(r)$ through $V(r)$

(*) Angular part of ψ for sph sym systems is the same for all $V(r)$; These are eigenfunctions of L^2 .

And therefore, what you find is that minus 1 over 2 m, L square Y is equal to lambda Y. Immediately you know that this is the Eigen function Y is the Eigen function for L square, and therefore lambda should be equal to nothing but minus l, l plus 1 h cross square over 2 m in this case because there is an extra 2 m sitting her. And you bring it back to the r equation and the equation you end up getting is minus h cross square over 2 m, d by dr of r square d R by dr and there will be 1 over r square in front plus l l plus 1 h cross square over 2 m r square R plus v r R equals E R.

So, the energy E depends on L and radial function r only. So, energy E depends on the angular momentum as is expected higher than low, but more the kinetic energy and E depends on R r through potential v r. So, you notice that the angular part of the wave function for a spherically symmetric potentials is the same. So, angular part of psi for spherically symmetric systems is the same for all v r. And what is it these are eigen functions of L square operator. It is only with r component that the person that depends on v r.

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$$\psi = R^{(r)} Y_{lm}(\theta, \phi)$$

ψ is an eigenfunction of L^2 and L_z

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\ell(\ell+1)}{2mr^2} R + V(r)R = ER$$

$$= \left[-\frac{\hbar^2}{2m} \frac{d^2R}{dr^2} - \frac{\hbar^2}{mr} \frac{dR}{dr} + \frac{\ell(\ell+1)}{2mr^2} R + V(r)R \right] = ER$$

- R should be finite everywhere ← & Continuous
- For bound states $R \rightarrow 0$ as $r \rightarrow \infty$ ↘ Continuous
- $\left(\frac{dR}{dr} \right)$ should also be finite everywhere ↙ And Continuous

So, my psi is nothing but R Y and I can write this Y lm theta and phi. So, psi is also now psi is and Eigen function of L square and L z as is expected, because these are conserved quantities and in addition I get this r. And equation for r is minus h cross square over 2 m 1 over r square d by dr r square d R by dr plus L l plus 1 over 2 m r square R plus v r R equals E R. And this can be written further as minus h cross square over 2 m d 2 R over dr square minus h cross square over m r d R over dr plus L l plus 1 over 2 m r square R plus v r R equals E R when we expand this

Now, this equation involves both the second derivative and first derivative r; we would like to simplify it but before that let us say that R should be finite everywhere. Because psi should be finite, if I whatever solution I find r should be finite everywhere including r equals 0 and r going far away. For bound state R should go to 0 as R goes to infinity because for bound states part we cannot escape to infinity.

So, now we got we are going to do is simplify this equation by writing r in a certain term or before that I should also mention that d R over dr should also be finite everywhere and the finite. And with this also there is one more condition this should be continuous. So, finite and continuous; should also a finite and continuous everywhere.

Let us now simplify this equation.

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$$-\frac{\hbar^2}{2m} \frac{d^2 R}{dr^2} - \frac{\hbar^2}{m r} \frac{dR}{dr} + \frac{l(l+1)\hbar^2}{2mr^2} R + VR = ER$$

$R(r) = \frac{u}{r}$

Since R is finite everywhere, $u \rightarrow 0$ as $r \rightarrow 0$ faster than r or as r

$$\frac{dR}{dr} = \frac{1}{r} \frac{du}{dr} - \frac{1}{r^2} u$$

$$\frac{d^2 R}{dr^2} = \frac{1}{r} \frac{d^2 u}{dr^2} - \frac{2}{r^2} \frac{du}{dr} + \frac{2}{r^3} u$$

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r} \frac{d^2 u}{dr^2} - \frac{2}{r^2} \frac{du}{dr} + \frac{2}{r^3} u \right] - \frac{\hbar^2}{m r} \left[\frac{1}{r} \frac{du}{dr} - \frac{1}{r^2} u \right] + \frac{l(l+1)\hbar^2}{2mr^3} u + V(r) \frac{u}{r} = E \frac{u}{r}$$

So, the equation I have is minus \hbar cross square over $2m$ $d^2 R$ over dr square minus \hbar cross square over $m r$ dR over dr plus $l(l+1)\hbar$ cross square over $2m r$ square R plus $V R$ equals $E R$. Let us write $R = u/r$. And since R is finite everywhere u should go to 0 as r tends to 0 faster than r or as r then only r would remain finite as r goes to 0. But what does this condition do; so in addition to this condition that I have on u which I am going to apply what does the substitution do is simplifies things for me. Because now dR/dr is going to be $du/dr \cdot 1/r$ plus minus $1/r^2 u$ and $d^2 R/dr^2$ is going to be equal to $1/r d^2 u/dr^2$ minus $2/r^2 du/dr$ plus $2/r^3 u$.

Let us now substitute this in the Schrodinger equation here and get minus \hbar cross square over $2m$ substitute for this $1/r d^2 u/dr^2$ minus $2/r^2 du/dr$ plus $2/r^3 u$ minus \hbar cross square over $m r$ in the bracket I get $1/r du/dr$ minus $1/r^2 u$. Then I get plus $l(l+1)\hbar$ cross square over $2m r$ cubed u plus $V r u$ is equal to $E u$ over r .

Now let us cancel certain terms. The term with du/dr cancels with du/dr here. The term with u/r^3 cancels with this term here.

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$$-\frac{\hbar^2}{2m} \frac{u''}{r} + \frac{l(l+1)\hbar^2 u}{2mr^3} + V(r) \frac{u}{r} = E \frac{u}{r}$$

$$u'' = \frac{d^2 u}{dr^2}$$

$$\boxed{-\frac{\hbar^2}{2m} u'' + \frac{l(l+1)\hbar^2}{2mr^2} u + V(r) u = E u}$$

$$V_{\text{eff}} = V(r) + \frac{l^2}{2mr^2}$$

$$-\frac{\hbar^2}{2m} u'' + V_{\text{eff}}(r) u = E u$$

$$V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2}$$

So, all I am left with is minus \hbar^2 over $2m$ u'' plus $l(l+1)\hbar^2$ over $2mr^3$ plus $V(r) \frac{u}{r}$ equals $E \frac{u}{r}$. Where u'' is nothing but $d^2 u / dr^2$. Multiplied by r throughout in the equation becomes minus \hbar^2 over $2m$ u'' plus $l(l+1)\hbar^2$ over $2mr^2$ plus $V(r) u$ equals $E u$ where u'' is nothing but $d^2 u / dr^2$ multiplied by r throughout, and the equation becomes minus \hbar^2 over $2m$ u'' plus $l(l+1)\hbar^2$ over $2mr^2$ plus $V(r) u$ equals $E u$.

This is like the Schrodinger equation for one dimensional motion except that this $V(r)$ also has an additional term here or this is a u . Here recall from classical mechanics that in motion in central forces there is $V_{\text{effective}}$ which was $V(R) + L^2 / 2mr^2$. So, this term here is very similar to that you get a $V_{\text{effective}}$ which is $L^2 / 2mr^2$ except in quantum mechanics I get $l(l+1)$. So, the equation is nothing but minus \hbar^2 over $2m$ u'' plus $V_{\text{effective}}(r) u$ equals $E u$ exactly like the Schrödinger equation where $V_{\text{effective}}(r) = V(r) + l(l+1)\hbar^2 / 2mr^2$.

Now for potentials that are regular near $r = 0$ some general properties about r can be inferred from this equation.

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$$-\frac{\hbar^2}{2m} u'' + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)u = E u$$

$$V(r) \rightarrow -\frac{1}{r} \text{ or better}$$

$$\text{Equation becomes } -\frac{\hbar^2}{2m} u'' + \frac{l(l+1)\hbar^2}{2mr^2} u = 0 \quad \text{as } r \rightarrow 0$$

$$u'' - \frac{l(l+1)u}{r^2} = 0$$

$$u \sim r^\alpha \quad \alpha(\alpha-1) - l(l+1) = 0$$

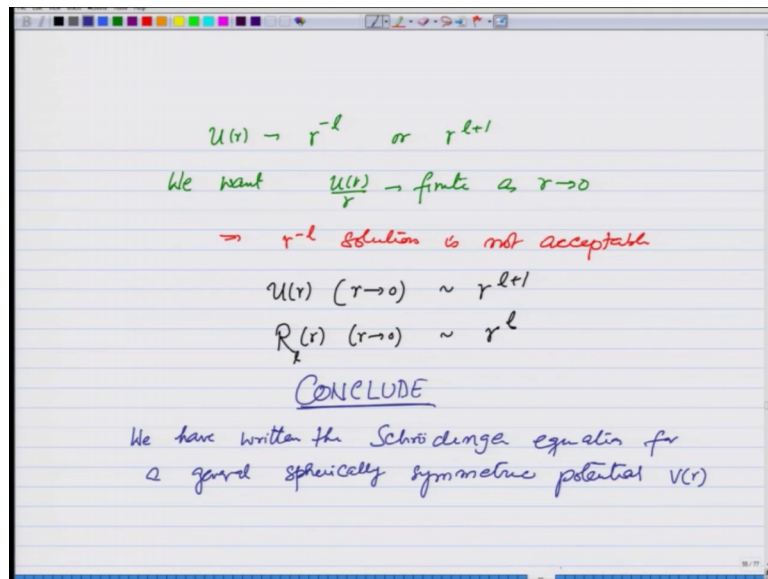
$$\alpha = -l, \quad \alpha = l+1$$

$$u(r) \text{ as } r \rightarrow 0 \quad r^{-l} (r^{l+1})$$

So, the equation that I have is minus \hbar^2 over $2m$ u'' plus $l(l+1)\hbar^2$ over $2mr^2$ plus $V(r)u$ equals $E u$. So, $V(r)$ that goes as maybe minus $1/r$ or better; better I mean it does not blow up faster than $1/r$. The equation becomes minus \hbar^2 over $2m$ u'' plus $l(l+1)\hbar^2$ over $2mr^2$ u is equal to 0 as r tends to 0 , because I can neglect $E u$ I can neglect $V(r)$ and therefore this is equation that becomes. And if you solve this u basically if you rearrange terms you get $u'' - l(l+1)u/r^2 = 0$.

If I take u to be of the order of r raised to α you get $\alpha(\alpha-1) - l(l+1) = 0$. So, α could be either equal to minus l or α could be equal to $l+1$. So, the solution $u(r)$ as r tends to 0 goes as either r^{-l} or r^{l+1} .

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So, what we found is that $u(r)$ causes either r raised to minus L or r raised to L plus 1. We want $u(r)/r$ to be finite as r tends to 0 because r should remain finite, and therefore r raised to minus L solution is not acceptable. So, $u(r)$ as r tends to 0 goes as r raised to L plus 1. The solution of the Schrodinger equation as r tends to 0 goes as r raised to l .

So, you see that r depends on L . Now through this we find out. So, that is one property we can see for u from here. Now other properties as you go far away r tend into infinity and all that those will depend on what $V(r)$ is like. But this is general thing that you can find out from a u equation. And what will be solving now is the u equation because that is easier to solve

So, let me just now conclude this lecture by saying that we have return the Schrodinger equation for a general spherically symmetric potential $V(r)$.

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$R(r) \quad (\psi = R(r) Y_{lm}(\theta, \phi))$

$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{l(l+1)\hbar^2}{2mr^2} R + VR = ER$$

- $R(r) = \frac{u(r)}{r}$

$$-\frac{\hbar^2}{2m} u'' + \frac{l(l+1)\hbar^2}{2mr^2} u + V(r)u = Eu$$

$$\equiv -\frac{\hbar^2}{2m} u'' + V_{\text{eff}}(r)u = Eu$$
- Irrespective of $V(r)$ $R(r) \sim r^l$ as $r \rightarrow 0$

And then by writing the radial component where psi is given as the radial component times Y_{lm} theta and phi we found that, equation for $r \geq 2m$ $\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{l(l+1)\hbar^2}{2mr^2} R + VR = ER$. Then by writing $R(r)$ as $\frac{u(r)}{r}$ we found the equation for u which is like the one dimensional equation $u'' + \frac{l(l+1)}{2mr^2} u + V(r)u = Eu$; which is equivalent to $-\frac{\hbar^2}{2m} u'' + V_{\text{eff}}(r)u = Eu$. And, we finally found for irrespective of $V(r)$; as long as regular does not blow faster than $1/r$ as r goes to 0 $R(r)$ goes as r^l as r tends to 0.

In the next lecture we are going to focus on a particular system and that will be the hydrogen atom.