Quantum Mechanics

Graduate course

Dr. Gassem Alzoubi

Textbook: Quantum mechanics concepts and applications (2nd edition)

by Nouredine Zettili (N. Zettili)

topics: Most materials from chps 6 – 11 will be covered

Instructor: Dr. Gassem Alzoubi

The Hashemite university dept of phys

Chapter 6: Three-dimensional motion

sections 6.1 and 6.2 are self study [3D problems in Cartesian coordinates]

section 6.3: 3D problems in spherical coordinates:

consider a particle moving in 3d under the potential $V(x,y,z)$, then the schrodinger equation takes the form

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad ; \text{where } H = \frac{P^2}{2m} + V(\vec{r}) \;;$$

now in 3d $\vec{p}$ is given by $\vec{p} = \frac{\hbar}{i}\vec{\nabla}$; $P_x = \frac{\hbar}{i}\frac{d}{dx}$

$P_y = \frac{\hbar}{i}\frac{d}{dy}$

$\Rightarrow$ the schrodinger eq^n becomes

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi \quad \text{--- (1)}$$

$P_z = \frac{\hbar}{i}\frac{d}{dz}$

where ∇^2 is the laplacian

now if the potential V is independent of time, then the general solution of equation (1) is given by

$$\Psi_n(\vec{r},t) = \psi_n(\vec{r})\, e^{-i\frac{E_n}{\hbar}t} \quad ----- \quad (2)$$

by substituting (2) in (1), we end up with the time-independent schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi \quad ----- \quad (3)$$

in this course we will be discussing mostly spherically symmetric potentials (central fields) where $V(\vec{r}) = V(r)$

four types of potentials will be studied

1) The free particle $V(r) = 0$

2) The spherical square potential well $V(r) = \begin{cases} -V_0, & r<a \\ 0, & r>a \end{cases}$

3) The Isotropic Harmonic oscillator $V(r) = \frac{1}{2}m\omega^2 r^2$
$\hookrightarrow (\omega_x = \omega_y = \omega_z = \omega)$

4) The coulomb potential (H atom) $V(r) = \frac{-e^2}{r}$

now since the Hamiltonian is spherically symmetric, we are going to use the spherical coordinates (r, θ, ϕ), where

$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$

in spherical coordinates, ∇^2 is given by

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

$$= \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \underbrace{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}}_{= -L^2/\hbar^2 \text{ angular part}}\right]$$ see appendix B.3

$$\Rightarrow \nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{r^2\hbar^2}$$; substitute this into eq^n(3)

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\psi(r) + \frac{L^2}{2mr^2}\psi(r) + V(r)\psi(r) = E\psi(r) \quad \text{--(4)}$$

since the Hamiltonian is a sum of radial part and angular part, ~~then~~ we can look for solutions that are products of radial and angular part, that is

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\,Y_{lm}(\theta,\phi) \quad \text{---- (5)}$$

Substituting this solution into the scrodinger equation (4) we have

$$-\frac{\hbar^2}{2m}Y_{lm}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{nl}}{dr}\right) + \left[V(r) + \frac{L^2}{2mr^2}\right]R_{nl}Y_{lm} = E R_{nl}Y_{lm}$$

Now using $L^2 Y_{lm} = \hbar^2 l(l+1)\,Y_{lm}$, we have

$$-\frac{\hbar^2}{2m}Y_{lm}\frac{1}{r^2}\left(r^2\frac{dR_{nl}}{dr}\right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]R_{nl}Y_{lm} = E R_{nl}Y_{lm}$$

divide by Y_{lm} and rearrange

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{nl}}{dr}\right) + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}\right]R_{nl} = 0$$

multiply by r,

$$\underbrace{\frac{1}{r}\frac{d}{dr}\left(r^2\frac{dR_{nl}}{dr}\right)}_{\Downarrow \text{ can be written as}} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}\right]rR_{nl} = 0$$

$$\frac{d^2}{dr^2}(rR_{nl}) + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}\right](rR_{nl}) = 0$$

$$\Rightarrow \frac{d^2}{dr^2}(rR_{nl}) + \frac{2m}{\hbar^2}\left[E - V_{eff}(r)\right] rR_{nl} = 0 \qquad \cdots (6)$$

where $V_{eff}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$ → effective potential

$V(r)$ → Central Potential

$\frac{\hbar^2 l(l+1)}{2mr^2}$ → repulsive or centrifugal Potential (tend to repel the particle away from the center)

equation (6) is called the radial equation

let $U_{nl}(r) = rR_{nl}(r)$ ⇒ the radial eq^n becomes

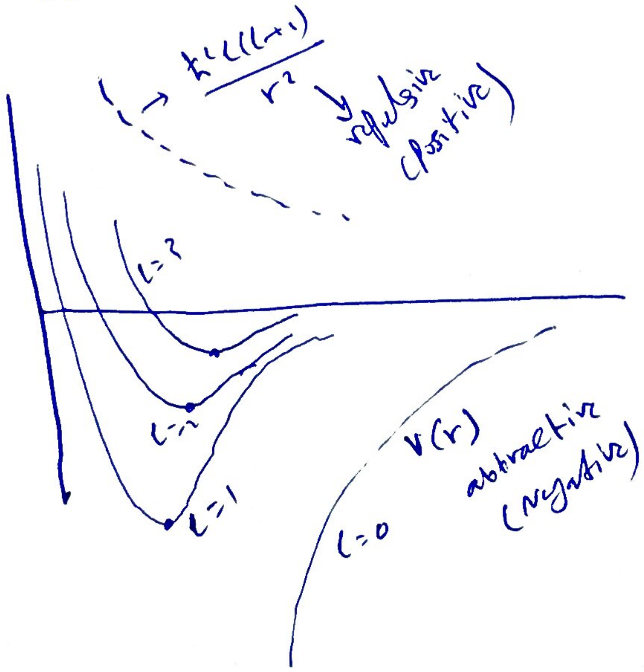
$$\frac{d^2 U_{nl}(r)}{dr^2} + k_l^2(r)\, U_{nl}(r) = 0 \quad (7) \quad ; \text{ where } k_l^2(r) = \frac{2m}{\hbar^2}(E - V_{eff})$$

→ 1d motion with $0 < r < \infty$

notice that the wavefunction $\psi_{nlm}(r)$ must be finite for all values of r $(0 < r < \infty)$, so if $R_{nl}(r)$ is finite ⇒

$U_{nl}(r) = rR_{nl}(r)$ must vanish at $r = 0$

- for equation (7) to describe bound states, the Potential $V(r)$ must be attractive (i.e negative) because $\frac{\hbar^2 l(l+1)}{r^2}$ is repulsive.



We see that as l increases, the depth of V_{eff} decreases and minimum moves to the right away from the center. the farther the particle from the center, the less bound it will be

Remark: when a particle has orbital and spin degrees of freedom, its total wave function is

$$\Psi_{n,l,m_l,m_s}(\vec{r}) = \psi_{nlm_l}(\vec{r})\,|s,m_s\rangle = R_{nl}(r)\,Y_{lm_l}(\theta,\phi)\,\underbrace{|s,m_s\rangle}_{\text{sometimes called } \chi},$$

here, the spin operator $\hat{\vec{S}}$ acts only on the spin part $|s,m_s\rangle$

the orbital operator $\hat{\vec{L}}$ acts only on the spatial part Y_{lm}