Application to Rotational Motion

Schrödinger equations for three basic types of motion: translation, vibration, **rotation** → "quantization"

3. **Rotational motion**
   (1) Rotation in 2-D
   (2) Rotation in 3-D
   (3) Spin

(1) Rotation in 2-D (a particle on a ring)

Mass m, radius r (in xy plane)

Total energy = kinetic energy (V=0)

$E = p^2/2m$

Angular momentum L_z (or J_z, z-direction)
(perpendicular to xy plane)

$L_z = J_z = \pm pr$

$\Rightarrow$ $E = J_z^2/2mr^2 = J_z^2/2I$ ($I = mr^2$, moment of inertia)

Q.M. angular momentum, rotational energy $\Rightarrow$ "quantized"

$|r|$: fixed $\Rightarrow$ "rigid rotor"

Diatomic: reduced mass, $\mu = m_1 m_2/(m_1+m_2)$

Schrödinger equation

$$-(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2)\Psi(x,y) + V(x,y)\Psi(x,y) = E\Psi(x,y)$$

$x, y \to r, \phi$ change of variables

$\partial f/\partial x = (\partial r/\partial x)\partial f/\partial r + (\partial \phi/\partial x)\partial f/\partial \phi$

$f(x,y) \to f(r,\phi)$

✓ $\partial/\partial x = (\partial r/\partial x)\partial/\partial r + (\partial \phi/\partial x)\partial/\partial \phi$

$r = \sqrt{(x^2 + y^2)}$, $\phi = \tan^{-1}(y/x)$, $x = r\cos\phi$, $y = r\sin\phi$

$\partial r/\partial x = \frac{1}{2}(x^2 + y^2)^{-1/2} \cdot 2x = 2x/2\sqrt{(x^2 + y^2)} = x/r = \cos\phi$

$\partial \phi/\partial x = (-y/x^2)/[1 + (y/x)^2] = -y/(x^2 + y^2) = -r\sin\phi/r^2 = -\sin\phi/r$

✓ $\partial/\partial y = (\partial r/\partial y)\partial/\partial r + (\partial \phi/\partial y)\partial/\partial \phi$

$\partial r/\partial y = 2y/2\sqrt{(x^2 + y^2)} = r\sin\phi/r = \sin\phi$

$\partial \phi/\partial y = (1/x)/[1 + (y/x)^2] = x/(x^2 + y^2) = r\cos\phi/r^2 = \cos\phi/r$

✓ $\partial^2/\partial x^2 = (\partial/\partial x)(\partial/\partial x) = [\cos\phi(\partial/\partial r) - (-\sin\phi/r)(\partial/\partial\phi)]^2$, r is fixed $\rightarrow \partial/\partial r = 0$

$= (1/r^2)\sin\phi\,[(\partial/\partial\phi)\sin\phi(\partial/\partial\phi)] = (\sin\phi/r^2)[\cos\phi(\partial/\partial\phi) + \sin\phi(\partial^2/\partial\phi^2)]$

✓ $\partial^2/\partial y^2 = [(\cos\phi/r)(\partial/\partial\phi)]^2 = (\cos\phi/r^2)(\partial/\partial\phi)[\cos\phi(\partial/\partial\phi)]$

$= (\cos\phi/r^2)[-\sin\phi(\partial/\partial\phi) + \cos\phi(\partial^2/\partial\phi^2)]$

$\therefore (\partial^2/\partial x^2 + \partial^2/\partial y^2) = (1/r^2)(\partial^2/\partial\phi^2)$, $V(x,y) = 0$ (no external force)

$\Rightarrow$ $-(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2)\Psi(x,y) + V(x,y)\Psi(x,y) = E\Psi(x,y)$

$\Rightarrow$ $-(\hbar^2/2m)(1/r^2)(d^2/d\phi^2)\Psi(\phi) = E\Psi(\phi)$

$mr^2 = I$ (moment of inertia), $\Psi''(\phi) + (2IE/\hbar^2)\Psi(\phi) = 0$

let $2IE/\hbar^2 = m_l^2$

$\Psi(\phi) = A\exp(im_l\phi)$, $m_l = \pm\sqrt{(2IE)}/\hbar$

Normalization,

$\therefore \Psi(\phi) = \exp(im_l\phi)/\sqrt{(2\pi)}$

Cyclic boundary condition: Ψ should be single-valued

$\Psi(\phi + 2\pi) = \Psi(\phi)$

$\Psi(\phi + 2\pi) = \exp[im_l(\phi + 2\pi)]/\sqrt{(2\pi)}$

$= [\exp(im_l\phi)\exp(im_l 2\pi)]/\sqrt{(2\pi)}$

$= \exp(im_l\phi)/\sqrt{(2\pi)} = \Psi(\phi)$

$\therefore \exp(im_l 2\pi) = 1 \Rightarrow m_l = 0, \pm1, \pm2, \pm3, \ldots.$

$(\cos(m_l 2\pi) + i\sin(m_l 2\pi) = 1)$

$2IE/\hbar^2 = m_l^2 \Rightarrow$ $\mathbf{E_{m\mathit{l}} = (m_\mathit{l}\hbar)^2/2I}$, $m_l = 0, \pm1, \pm2, \pm3, \ldots.$

cf. Classical Mechanics

$E = p^2/2m = (L/r)^2/2m = L^2/2I$, $L = rp$

$J_z = \mathbf{L = m_\mathit{l}\hbar}$, $m_l = 0, \pm1, \pm2, \pm3, \ldots.$

- de Broglie relation

$$\lambda = h/p = h/(J_z/r) = h/(m_l\hbar/r) = h/(m_l h/2\pi r) = 2\pi r/m_l$$

$$m_l\lambda = 2\pi r$$

- angular momentum (J_z) is quantized: $m_l\hbar$

- Energy is quantized, $E_{m_l} = (m_l\hbar)^2/2I$, $m_l = 0, \pm1, \pm2, \pm3, \ldots.$

$|m_l|$: doubly degenerate except $m_l = 0$

- Wavefunction,

$$\Psi_{m_l}(\phi) = \exp(im_l\phi)/\sqrt{(2\pi)}$$
$$= 1/\sqrt{(2\pi)}[\cos(m_l\phi) + i\sin(m_l\phi)]$$

real part of Ψ

-Probability, $\Psi_{m_l}^* \Psi_{m_l} = 1/(2\pi)$

Equal probability of finding the particle anywhere on the ring

$\Rightarrow$Uncertainty principle: angle & angular momentum $\rightarrow$ inability to specify them

cf. orbital angular momentum

(2) Rotation in 3-D (a particle on a sphere)

Electrons in atoms, rotating molecules: free to move anywhere on the surface of a sphere of radius r

e.g., diatomic molecule

Schrödinger equation

$$H\Psi = E\Psi$$

$$H = -(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + V(x,y,z)$$
$$= -(\hbar^2/2m)\nabla^2 + V$$

In polar coordinates (r: fixed)

$\nabla^2 = \partial^2/\partial r^2 + (2/r)\partial/\partial r + (1/r^2)\Lambda^2$ Λ^2 : legendrian

$\Lambda^2 = (1/\sin^2\theta)(\partial^2/\partial\phi^2) + (1/\sin\theta)(\partial/\partial\theta)\sin\theta(\partial/\partial\theta)$

R is const $\Rightarrow \partial/\partial r = 0,\ \partial^2/\partial r^2 = 0$

Free to move $\Rightarrow V = 0$

$\nabla^2 = (1/r^2)[(\partial^2/\partial\theta^2) + (\cos\theta/\sin\theta)(\partial/\partial\theta) + (1/\sin^2\theta)(\partial^2/\partial\phi^2)]$

$-(\hbar^2/2m)\nabla^2\Psi = E\Psi$

$-(\hbar^2/2m\, r^2)[(\partial^2/\partial\theta^2) + (\cos\theta/\sin\theta)(\partial/\partial\theta) + (1/\sin^2\theta)(\partial^2/\partial\phi^2)]\Psi(\theta, \phi) = E\Psi(\theta, \phi)$

$\Psi(\theta, \phi) = \Theta(\theta)\,\Phi(\phi)$: separation of variables

$\Phi(\partial^2/\partial\theta^2)\Theta + (\cos\theta/\sin\theta)\Phi(\partial/\partial\theta)\Theta + (\Theta/\sin^2\theta)(\partial^2/\partial\phi^2)\Phi = -(2IE/\hbar^2)\Theta\Phi$

$(1/\Theta)(\partial^2/\partial\theta^2)\Theta + (1/\Theta)(\cos\theta/\sin\theta)(\partial/\partial\theta)\Theta + (1/\Phi)(1/\sin^2\theta)(\partial^2/\partial\phi^2)\Phi = -(2IE/\hbar^2)$

Put $(1/\Phi)(\partial^2/\partial\phi^2)\Phi = -m_l^2$, m_l: separation constant

$\Rightarrow$ (i) $d^2/d\phi^2)\Phi + m_l^2\Phi = 0$

(ii) $(d^2/d\theta^2)\Theta + (\cos\theta/\sin\theta)(d/d\theta)\Theta + [(2IE/\hbar^2) - (m_l^2/\sin^2\theta)]\Theta = 0$

$\Rightarrow$ (i) $\Phi = \exp(im_l\phi)/\sqrt{(2\pi)}$, $m_l = 0, \pm1, \pm2, \pm3, \ldots.$

(ii) $s = \cos\theta$, $\beta = 2IE/\hbar^2$

$G(s) = \Theta(\cos\theta)$, $d\Theta/d\theta = -\sin\theta(dG/ds)$,

$d^2\Theta/d\theta^2 = \sin^2\theta(d^2G/ds^2) - \cos\theta(dG/ds)$,

$\therefore (1-s^2)(d^2G/ds^2) - 2s(dG/ds) + [\beta - (m_l^2/1-s^2)] = 0$

$\beta = 2IE/\hbar^2$

$\beta = l(l + 1)$, $l = 0,1,2,3\ldots$ (quantum number)

$-l \leq m_l \leq l$, $m_l = -l, -l+1, \ldots 0,1,2, \ldots l$

$\Psi(\theta, \phi) = \Theta(\theta)\, \Phi(\phi) =$

Normalized wavefunction, $Y_{l,ml}(\theta, \phi) = \Theta_{l,ml}(\theta)\, \Phi_{l,ml}(\phi)$ (spherical harmonics) e.g., Table 9.3 (구판 12.3)

- wavefunction

$Y_{l,m_l}(\theta, \phi)$

- Probability, $Y_{l,ml}{}^2(\theta, \phi)$

- $E = l(l + 1)(\hbar^2/2I)$, $l = 0,1,2,3\ldots$

  energy is quantized, independent of m_l

  same energy ⇒ $(2l + 1)$ different wavefunctions

  ⇒ quantum number l is $(2l + 1)$-fold degenerate

- angular momentum (L, L_z)

  classical mechanics: angular momentum L, $E = L^2/2I$ ($L = J$ in the textbook)

  ⇒ magnitude of angular momentum (L) $= [l(l + 1)]^{1/2}\hbar$, $l = 0,1,2,3\ldots$

  z-component of angular momentum (L_z) $= m_l\hbar$, $m_l = -l, -l+1,\ldots 0,1,2,\ldots l$

  c.f.)

- space quantization

$L = [l(l + 1)]^{1/2}\hbar$, $l = 0,1,2,3\ldots$
$L_z = m_l\hbar$, $m_l = -l, -l+1,\ldots 0,1,2,\ldots l$

Q. M.: a rotating body may not take up
an arbitrary orientation

1921. Stern & Gerlach

⇒ Angular momentum is quantized

- Uncertainty principle

if L_z is known, impossible to know the other two components (L_x, L_y)

(3) Spin

- Stern-Gelach observed 2 bands of Ag atoms:
  angular momentum $l \rightarrow 2l + 1$ orientations
  $\Rightarrow$ to get 2 orientations $\rightarrow l = ½$??, l must be integer

$\Rightarrow$suggestion: not due to orbital angular momentum (motion of electron around atomic nucleus), but motion of electron about its own axis **"spin"**

Ag: [Kr]$4d^{10}\underline{5s^1}$

Magnitude of spin angular momentum = $[s(s + 1)]^{1/2}\hbar$, s = 0,1,2,3…

z-axis: $m_s\hbar$, m_s = s, s-1,….,-s

Electron: only one value of s is allowed, s = ½

angular momentum $1/2\sqrt{3}\hbar = 1/2\sqrt{3}\hbar$

$\Rightarrow$ Intrinsic property of the electron

$2s + 1$ = different orientations

$m_s = +1/2$, $\alpha \uparrow$
$m_s = -1/2$, $\beta \downarrow$

- proton, neutron ($s = ½$) $\Rightarrow$ angular momentum, $(3/4)^{1/2}\hbar$: ½ spin "fermions" (constitute matter)
- mesons, photon, $s = 1 \Rightarrow$ angular momentum, $(2)^{1/2}\hbar$: integer spin (including 0) "boson" (responsible for the forces that bind fermions together)

c.f. l(angular momentum quantum number), m_l(orbital magnetic q. #), s(spin angular q. #), m_s(spin magnetic q. #)