Quantum Physics 1
Class 19

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3D Problems

Review:

Quantum Postulates:

- $\hat{A}\varphi_a = a\varphi_a$
- properties of $\hat{A}$, Hermitian operators
- $[\hat{x}, \hat{p}] = i\hbar$
- $[\hat{A}, \hat{B}] = 0$, possess same eigenfunct. (w/ different eigenvalues)
- $\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle$

Matrix representation of Hermitian operators

consider $A_{nn'} = \int \varphi_n^* \hat{A} \varphi_{n'}\, dx$; with φ_n basis

$$\Rightarrow (A) = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & \ddots & \\ \vdots & & & \ddots \end{pmatrix}$$

& Hermitian adjoint ; $(A^\dagger) = \begin{pmatrix} A_{11}^* & A_{12}^* & \cdots \\ A_{21}^* & \ddots & \\ \vdots & & \ddots \end{pmatrix}$

w/t $A^{\dagger}_{nn'} \equiv \int \varphi_n^* A^{\dagger} \varphi_{n'} \, dx$

$$= \int (\hat{A} \varphi_n)^* \varphi_{n'} \, dx$$

$$= \left[\int \varphi_{n'}^* \hat{A} \varphi_n \right]^*$$

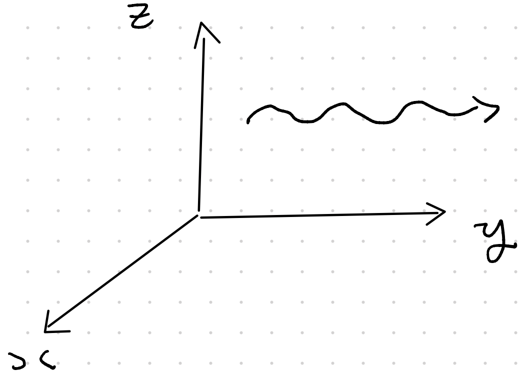
with Hermitian operator:

$$A^{\dagger}_{nn'} = A^*_{n'n} = A_{nn'}$$

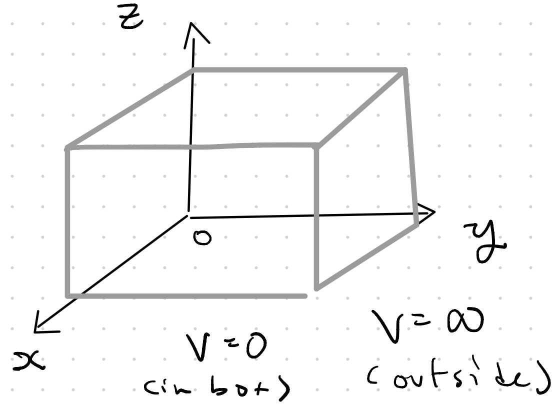
eg) $A_{12} = A^*_{21}$

Bound States & Free Particle

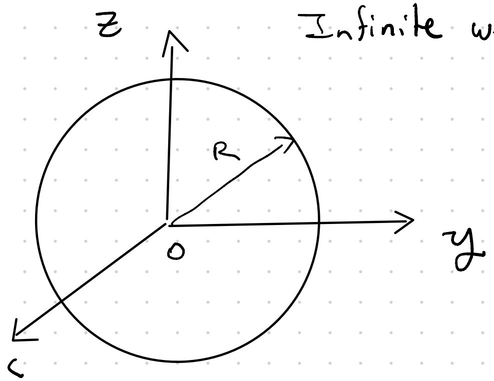
Free particle, $V=0$

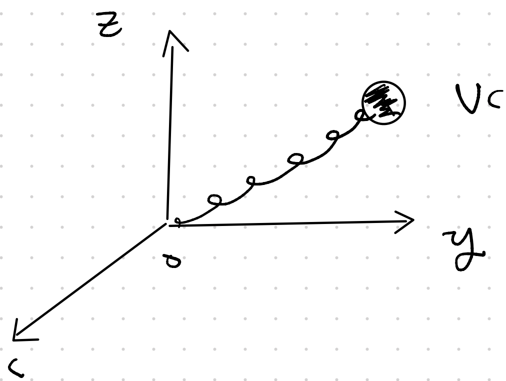


Infinite well



Infinite well (particle in a "box")

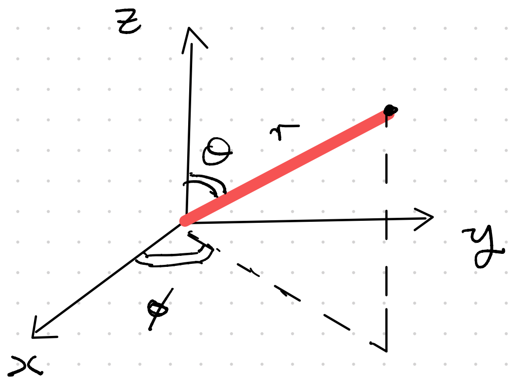




$V(x,y,z) = \frac{1}{2} m\omega^2 r^2$

$= \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2)$

NB: Can use separation of variables in cartesian coord. and/or spherical coordinate systems. Choice depends on the symmetry of the problem.



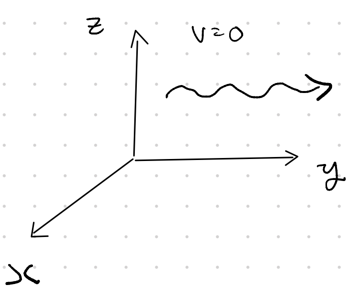
Spherical Coordinate System

For $V(r) \propto -\frac{1}{r} \propto \frac{1}{\sqrt{x^2+y^2+z^2}}$

using separation of variables not possible in cartesian coordinates.

But works in spherical coordinates.

Example of s ation of variables:



$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right]=E\psi(x,y,z)$$

$$\psi(x,y,z)=\phi_x(x)\,\phi_y(y)\,\phi_z(z)$$

In-class 19.1

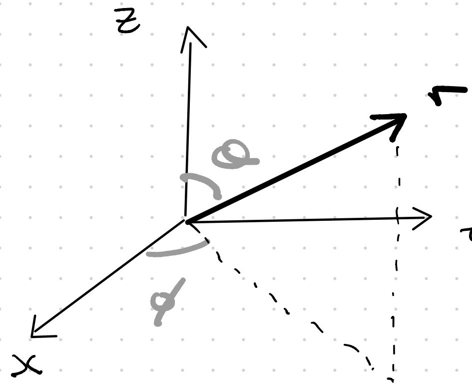
Consider 3D S.E.

Recall:
$$-\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)}\psi=(E-V(r))\psi$$

$\nabla^2 \equiv$ laplacian operator

Spherical Coordinates:

$$\left.\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}\right\}$$



∇^2 in spherical coord.:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi)$$
$$=(E-V(r))\psi(r,\theta,\phi)$$

$$\Rightarrow \left(\frac{\hat{p}_r^2}{2m}+\frac{\hat{L}^2}{2mr^2}\right)\psi=(E-V)\psi$$

where $\hat{p}_r^2 \equiv -\hbar^2\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]$

$$\hat{L}^2 \equiv -\hbar^2 \left[\frac{1}{\sin\theta} \cdot \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

$$\text{\&} \quad \psi(r, \theta, \phi) = \underbrace{R(r)}_{\text{radical}} \underbrace{Y(\theta, \phi)}_{\text{angular}}$$

Separation of Variables (spherical coordinates)

Now, $\left(\frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} \right) \psi(r,\theta,\phi) = (E - V(r))\, \psi(r, \theta, \phi)$

assume: $\psi = R(r)\, Y(\theta,\phi)$; $\hat{P}_r \equiv -\hbar^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)\right]$

$$\Rightarrow \left(\frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} \right) R(r)\, Y(\theta,\phi) = (E - V)\, R(r)\, Y(\theta,\phi) \quad \ldots (1)$$

$$\boxed{\text{In-class 19.2}}$$

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(1) $\times\ 2mr^2/\hbar^2$

$$\Rightarrow \left(\frac{2mr^2}{\hbar^2}\right) \frac{\hat{P}_r}{2m} \cdot R(r) Y(\theta,\phi) + \frac{\hat{L}^2}{\hbar^2} R(r) Y(\theta,\phi) = \frac{2mr^2}{\hbar^2}(E - V(r)) \cdot R(r) Y(\theta,\phi)$$

- Divide by $R(r)\, Y(\theta,\phi)$:

$$\Rightarrow \frac{2mr^2}{\hbar^2 R(r)} \frac{\hat{p}_r^2}{2m} (R(r)) + \underbrace{\frac{1}{\hbar^2} \frac{1}{Y(\theta,\phi)} \hat{L}^2 Y(\theta,\phi)}_{\text{constant, } \lambda} = \frac{2mr^2}{\hbar^2} [E - V(r)]$$

Separation of variables gives two equations:

$$\boxed{\hat{L}^2 Y(\theta, \phi) = \lambda \hbar^2 Y(\theta, \phi)} \quad \ldots \text{ 2}$$

$$\boxed{\frac{2mr^2}{\hbar^2} \frac{\hat{p}_r^2}{2m} R(r) + \lambda R(r) = \frac{2mr^2}{\hbar^2} (E - V(r)) R(r)} \quad \ldots \text{ 3}$$

NB $Y(\theta, \phi)$: spherical harmonics

In-class 19.3

Consider θ dependence:

$$\boxed{\left(-\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{m^2}{\sin^2\theta}\right) \Theta = \lambda \Theta}$$

where $\Theta \equiv$ Legendre polynomial

Textbook [Apendix B] :

Boundary conditions lead to : $\lambda = l(l+1)$

$l = 0, 1, 2, \ldots$

& For each l ; $m = -l, -l+1, \ldots, l-1, l$

$Y(\theta, \phi) = \Theta(\cos\theta)\,\Phi(\phi)$ apply for all $V(r)$, including $V(r) = 0$.

Now example of Legendre Polynomial :

$\Theta_0 = 1$

$\Theta_1 = \cos\theta$

$\Theta_2 = \frac{1}{3}(3\cos^3\theta - 1), \ldots$

$\boxed{\text{In-class 19.4}}$

$$\frac{\partial^2 \Phi}{\partial \phi^2} + m^2 \Phi = 0$$

$$\Rightarrow \Phi(\phi) = e^{im\phi}$$

$$e^{im\phi} = e^{im(\phi + 2\pi)}$$

$$\therefore \; e^{i2\pi m} = 1$$

$$\Rightarrow \; 2\pi m = 0\pi, \pm 2\pi, \pm 4\pi$$

$$\text{or } m = 0, \pm 1, \pm 2, \ldots$$

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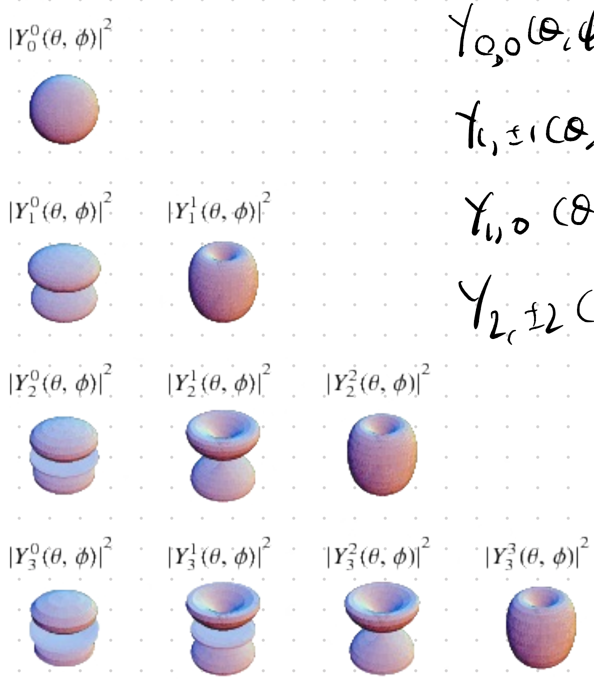
examples of spherical harmonics



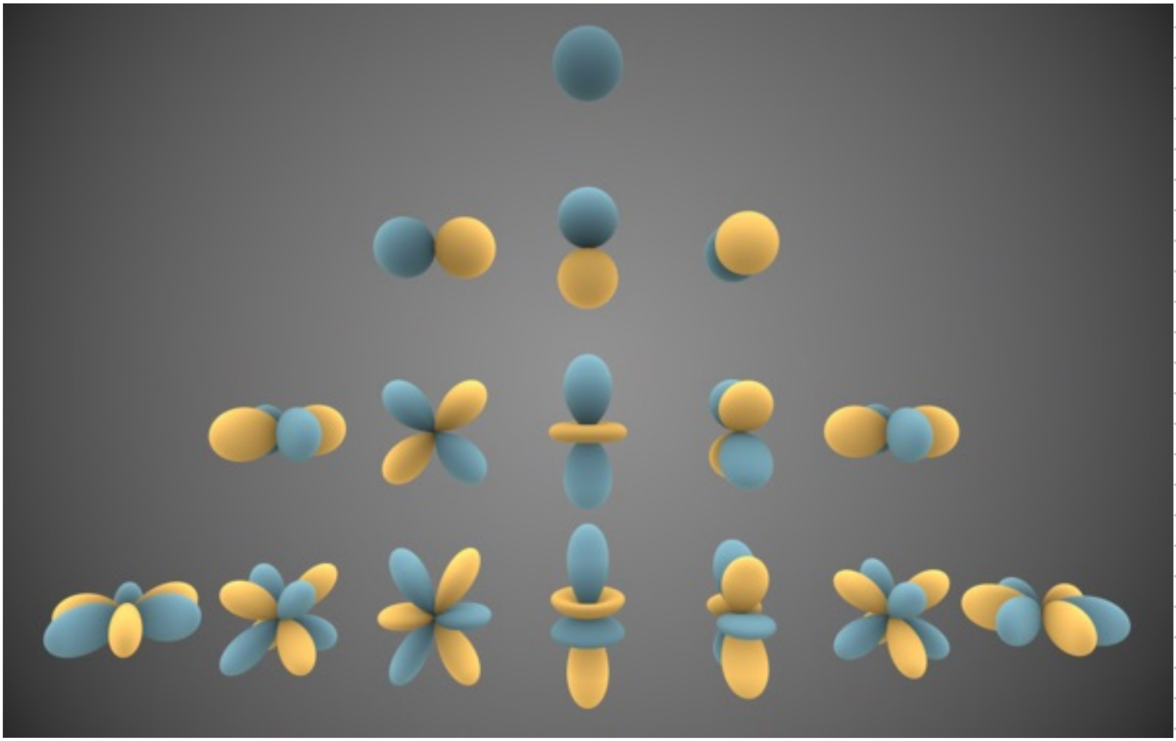
$$Y_{0,0}(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$$

$$Y_{1,\pm 1}(\theta,\phi) = \mp \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\phi}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{2,\pm 2}(\theta,\phi) = \sqrt{\frac{15}{3\pi}} \sin^2\theta \, e^{\pm 2i\phi}$$

$\mathrm{Re}(Y_{\ell m}(\theta,\phi))$



Wikipedia