

Quantum Mechanics

- Momentum and position operators

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad [x, p] = i\hbar, \quad \mathbf{p} = -\frac{\hbar}{i} \nabla, \quad [x_i, p_j] = i\hbar \delta_{ij}, \quad [p_i, f(\mathbf{x})] = \frac{\hbar}{i} \frac{\partial f}{\partial x_i}$$

- Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t}(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}, t) \right) \Psi(\mathbf{x}, t),$$

- Stationary state:

$$\Psi(x, t) = \psi(x) e^{-iEt/\hbar}, \quad -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x)$$

- Expectation values

$$\langle Q \rangle(t) = \int dx \Psi^*(x, t) (Q \Psi(x, t))$$

- Time evolution of expectation value. For Q Hermitian (Ehrenfest thm)

$$i\hbar \frac{d}{dt} \langle Q \rangle = \langle [Q, H] \rangle$$

- Commutator identity

$$[A, BC] = [A, B]C + B[A, C]$$

- Uncertainty ΔQ of a Hermitian operator Q

$$(\Delta Q)^2 = \langle Q^2 \rangle - \langle Q \rangle^2 = \langle (Q - \langle Q \rangle)^2 \rangle$$

- Infinite square well

$$V(x) = \begin{cases} 0, & \text{for } 0 < x < a, \\ \infty & \text{otherwise} \end{cases}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}, \quad n = 1, 2, \dots$$

- Harmonic Oscillator

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m \omega^2 \hat{x}^2 = \hbar \omega \left(\hat{N} + \frac{1}{2} \right), \quad \hat{N} = \hat{a}^\dagger \hat{a}$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right),$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\omega\hbar}{2}} (\hat{a}^\dagger - \hat{a}),$$

$$[\hat{x}, \hat{p}] = i\hbar, \quad [\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{N}, \hat{a}] = -\hat{a}, \quad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger.$$

$$\hat{a} \phi_0 = 0, \quad \phi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp \left(-\frac{m\omega}{2\hbar} x^2 \right).$$

$$\phi_1(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x \exp \left(-\frac{m\omega}{2\hbar} x^2 \right)$$

$$\phi_2(x) = -\frac{1}{\sqrt{2}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \left(1 - 2 \frac{m\omega}{\hbar} x^2 \right) \exp \left(-\frac{m\omega}{2\hbar} x^2 \right)$$

$$\phi_n = \frac{1}{\sqrt{n!}} (a^\dagger)^n \phi_0$$

$$\hat{H} \phi_n = E_n \phi_n = \hbar \omega \left(n + \frac{1}{2} \right) \phi_n, \quad \hat{N} \phi_n = n \phi_n, \quad (\phi_m, \phi_n) = \delta_{mn}$$

$$\hat{a}^\dagger \phi_n = \sqrt{n+1} \phi_{n+1}, \quad \hat{a} \phi_n = \sqrt{n} \phi_{n-1}.$$

- Central potentials: $V(\mathbf{r}) = V(r)$

$$\psi(r, \theta, \phi) = \frac{u(r)}{r} Y_{\ell m}(\theta, \phi)$$

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

$$u(r) \sim r^{\ell+1}, \quad \text{as } r \rightarrow 0.$$

$Y_{lm}(\theta, \varphi)$	$Y_{lm}(x, y, z)$
$Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$	$Y_{00}(x, y, z) = \frac{1}{\sqrt{4\pi}}$
$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos \theta$	$Y_{10}(x, y, z) = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$
$Y_{1,\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin \theta$	$Y_{1,\pm 1}(x, y, z) = \mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$
$Y_{20}(\theta, \varphi) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$	$Y_{20}(x, y, z) = \sqrt{\frac{5}{16\pi}} \frac{3z^2 - r^2}{r^2}$
$Y_{2,\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{15}{8\pi}} e^{\pm i\varphi} \sin \theta \cos \theta$	$Y_{2,\pm 1}(x, y, z) = \mp \sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$
$Y_{2,\pm 2}(\theta, \varphi) = \sqrt{\frac{15}{32\pi}} e^{\pm 2i\varphi} \sin^2 \theta$	$Y_{2,\pm 2}(x, y, z) = \mp \sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2ixy}{r^2}$

- Hydrogen atom:

$$H = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{r}$$

$$E_n = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2}, \quad a_0 = \frac{\hbar^2}{me^2} \simeq 0.529 \times 10^{-10} \text{m}, \quad \frac{e^2}{2a_0} \simeq 13.6 \text{eV}$$

$$\psi_{n,\ell,m}(\vec{x}) = A \left(\frac{r}{a_0} \right)^\ell \left(\text{Polynomial in } \frac{r}{a_0} \text{ of degree } n - (\ell + 1) \right) e^{-\frac{Zr}{na_0}} Y_{\ell,m}(\theta, \phi)$$

$$n = 1, 2, \dots, \quad \ell = 0, 1, \dots, n-1, \quad m = -\ell, \dots, \ell$$

$$\psi_{n,\ell,m}(\vec{x}) = \frac{u_{n\ell}(r)}{r} Y_{\ell,m}(\theta, \phi)$$

$$u_{1,0}(r) = \frac{2r}{a_0^{3/2}} \exp(-r/a_0)$$

$$u_{2,0}(r) = \frac{2r}{(2a_0)^{3/2}} \left(1 - \frac{r}{2a_0} \right) \exp(-r/2a_0)$$

$$u_{2,1}(r) = \frac{1}{\sqrt{3}} \frac{1}{(2a_0)^{3/2}} \frac{r^2}{a_0} \exp(-r/2a_0)$$

$$\hat{L}_x = \hat{y} \hat{p}_z - \hat{z} \hat{p}_y, \quad \hat{L}_y = \hat{z} \hat{p}_x - \hat{x} \hat{p}_z, \quad \hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x.$$

$$\hat{L}^2 \equiv \hat{L}_x \hat{L}_x + \hat{L}_y \hat{L}_y + \hat{L}_z \hat{L}_z, \quad L_{\pm} = L_x \pm i L_y$$

Angular momentum: $[L_x, L_y] = i\hbar L_z$ et cycl.

Ladder operators:

$$L_+ |\ell, m\rangle = \hbar \sqrt{(\ell+m+1)(\ell-m)} |\ell, m+1\rangle$$

$$L_- |\ell, m\rangle = \hbar \sqrt{(\ell+m)(\ell-m+1)} |\ell, m-1\rangle$$

Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$