#### QUANTUM MECHANICS FALL 2018

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1. The Wave Function

### 1.1. The Schrödinger Equation.

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi$$

#### 1.2. Operators.

$$\begin{split} \langle \hat{x} \rangle &= \langle \Psi | \hat{x} | \Psi \rangle \\ \langle \hat{p} \rangle &= m \frac{d \left\langle \hat{x} \right\rangle}{dt} = \langle \Psi | -i \hbar \frac{\partial}{\partial x} | \Psi \rangle \\ \left\langle \hat{H} \right\rangle &= \langle \Psi | -\frac{\hbar^2}{2m} \frac{\partial}{\partial x} + V(x) | \Psi \rangle \\ \left[ \hat{A}, \hat{B} \right] &= \hat{A} \hat{B} - \hat{B} \hat{A} \end{split}$$

#### 1.3. The Uncertainty Principle.

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

# 2. TIME-INDEPENDENT SCHRÖDINGER $\qquad \qquad \text{Equation}$

#### 2.1. Stationary States.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-i\frac{E_n t}{\hbar}}$$

#### 2.2. The Infinite Square Well.

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & \text{otherwise} \end{cases}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$\langle \psi_i | \psi_j \rangle = \delta_{ij}$$

$$c_n = \langle \psi_n | \Psi(x, t = 0) \rangle$$

The probability of being in state n is equal to  $|c_n|^2$ .

$$\left\langle \hat{H} \right\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

#### 2.3. The Harmonic Oscillator.

### 2.3.1. Base State.

$$\begin{split} \Psi_0 &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \\ E_0 &= \frac{\hbar\omega}{2} \end{split}$$

#### 2.3.2. Ladder Operators.

$$\hat{a_+} = \frac{1}{\sqrt{2m\omega\hbar}} \left[ -i\hat{p} + m\omega x \right]$$

$$\hat{a_-} = \frac{1}{\sqrt{2m\omega\hbar}} \left[ i\hat{p} + m\omega x \right]$$

$$\left[ \hat{a_-}, \hat{a_+} \right] = 1$$

2.3.3. Solving.

$$\hat{a_+}\psi_n = \sqrt{n+1}\psi_{n+1}$$

$$\hat{a_-}\psi_n = \sqrt{n}\psi_{n-1}$$

$$\psi_n = \frac{1}{\sqrt{n!}}(\hat{a_+})^n\psi_0$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

2.3.4. Operators.

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left( \hat{a_+} + \hat{a_-} \right)$$

$$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} \left( \hat{a_+} - \hat{a_-} \right)$$

#### 2.4. The Free Particle.

$$k^{2} = \frac{2mE}{\hbar^{2}}$$

$$k \in \mathbb{R}$$

$$E = \frac{\hbar^{2}k^{2}}{2m}$$

$$p = \hbar k$$

$$\Psi(x,t) = \underbrace{Ae^{ikx-i\frac{E}{\hbar}t}}_{\text{right mover}} + \underbrace{Be^{-ikx-i\frac{E}{\hbar}t}}_{\text{left mover}}$$

$$\Phi(k) = \frac{1}{\sqrt{a\pi}} \frac{\sin(ka)}{k}$$

#### 2.5. Step Potential.

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \ge 0 \end{cases}$$

$$J_x = -\frac{\hbar i}{2m} \left[ \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right]$$

$$T \equiv \left| \frac{J_{trans}}{J_{inc}} \right| \quad 0 \le T \le 1$$

$$R \equiv \left| \frac{J_{refl}}{J_{inc}} \right| \quad 0 \le R \le 1$$

### 2.5.1. Case 1. $E > V_0$

$$k_1^2 = \frac{2mE}{\hbar^2}$$

$$\Psi_{\rm I} = \underbrace{Ae^{ik_1x}}_{\rm Incident} + \underbrace{Be^{-ik_1x}}_{\rm Reflected}$$

$$k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

$$\Psi_{\rm II} = \underbrace{Ce^{ik_2x}}_{\rm Transmited} + \underbrace{De^{-ik_2x}}_{\rm DNE}$$

$$T = \frac{4}{\left[1 + \frac{k_2}{k_1}\right]^2} \frac{k_2}{k_1}$$

$$R = \frac{\left[1 - \frac{k_2}{k_1}\right]^2}{\left[1 + \frac{k_2}{k_1}\right]^2}$$

2.5.2. Case 2. 
$$E < V_0$$

$$k_1^2 = \frac{2mE}{\hbar^2}$$

$$\Psi_{\rm I} = \underbrace{Ae^{ik_1x}}_{\rm Incident} + \underbrace{Be^{-ik_1x}}_{\rm Reflected}$$

$$k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

$$\Psi_{\rm II} = \underbrace{Ce^{-k_2x}}_{\rm Transmited} + \underbrace{De^{k_2x}}_{\rm DNE}$$

$$T = 0$$

$$R = 1$$

#### 3. Formalism

3.1. **Observables.** Observances are represented by hermitian operators, and  $\langle O \rangle = \mathbb{R}$ .

$$\hat{O} | \psi \rangle = o | \psi \rangle$$

### 3.2. The Uncertainty Principle.

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B}\right] \right\rangle \right)^2$$

Observables whose operators do not commute car called incompatible observables, meaning that measuring one changes the other.

3.3. **Dirac Notation.** We can express functions as a basis vector in Hilbert space.

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha \end{pmatrix} \quad \langle \alpha| = (\alpha_1^* \alpha_2^* \cdots \alpha_n^*)$$

The identity operator is

$$\hat{I} = \sum |\alpha\rangle \left<\alpha\right|$$

For some operator  $\hat{O}$  and eigenvalues  $o_n$ 

$$\hat{O}\left|n\right\rangle = o_n\left|n\right\rangle$$

3.3.1. Matrix Operators.

$$O_{nm} \equiv \langle n|\hat{O}|m\rangle$$

Hermitian if

$$O_{nm} = O_{mn}^*$$

 $3.3.2.\ Harmonic\ Oscillator.$ 

$$\begin{array}{l} \hat{a_{+}} \left| n \right\rangle = \sqrt{n+1} \left| n+1 \right\rangle \\ \\ \hat{a_{-}} \left| n \right\rangle = \sqrt{n} \left| n-1 \right\rangle \end{array}$$

 $3.3.3.\ Wave\ Function.$ 

$$\begin{split} |\Psi\rangle &= \sum_{n} A_{n} |n\rangle \\ A_{n} &= \langle n|\Psi\rangle \\ |\Psi\rangle &= \sum_{n} \langle n|\Psi\rangle |n\rangle \end{split}$$

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4. Quantum Mechanics in Three

#### 4.1. Schrödinger Equation in Spherical Coordinates.

4.1.1. Legendre.

$$P_l(x) \equiv \frac{1}{2^l l!} \left(\frac{d}{dx}\right)^l (x^2 - l)^l$$

$$P_l^m(x) \equiv (1 - x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_l(x)$$

$$\begin{split} P_0 &= 1 & P_0^0 &= 1 \\ P_1 &= x & P_1^1 &= \sin \theta \\ P_2 &= \frac{1}{2}(3x^2 - 1) & P_1^0 &= \cos \theta \\ P_3 &= \frac{1}{2}(5x^3 - 3x) & P_2^1 &= 3\sin \theta \cos \theta \\ P_4 &= \frac{1}{8}(35x^4 - 30x^2 - 3)P_2^0 &= \frac{1}{2}(3\cos^2 \theta - 1) \end{split}$$

# 4.2. The Hydrogen Atom.

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

$$E_n = -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] \frac{1}{n^2} \ n \in \mathbb{N}$$

$$a \equiv \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.529 \times 10^{-10} m$$

$$E_1 = -13.6eV$$

4.2.1. Laguerre.

Lagrantic. 
$$L_q(x) \equiv e^x \left(\frac{d}{dx}\right)^q (e^{-x}x^q)$$

$$L_{q-p}^p(x) \equiv (-q)^p \left(\frac{d}{dx}\right)^p L_q(x)$$

$$L_0 = 1$$

$$L_1 = -x + 1$$

$$L_2 = x^2 - 4x + 2$$

$$L_3 = -x^2 + 9x^2 - 18x + 6$$

4.2.3. Wave Function.

$$n \in \mathbb{N}$$

$$0 \le l < n$$

$$-l \le m \le l$$

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}}$$

$$\cdot e^{-r/na} \left(\frac{2r}{na}\right)^l \left[L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right)\right] Y_l^m(\theta,\phi)$$

$$\begin{split} \psi_{100}(r,\theta,\phi) &= \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}} \\ \langle \psi_{nlm} | \psi_{n'l'm'} \rangle &= \delta_{nn'} \delta_{ll'} \delta_{mm'} \end{split}$$

$$4.1.2.\ Spherical\ Harmonics.$$

$$Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos\theta)$$

$$\epsilon = \begin{cases} (-1)^m & m \ge 0\\ 1 & m \le 0 \end{cases}$$

$$\left\langle Y_l^m \middle| Y_{l'}^{m'} \right\rangle = \delta_{ll'} \delta_{mm'}$$

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$$

$$Y_1^{\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2 \theta - 1)$$

$$Y_2^{\pm 1} = \mp \left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{\pm i\phi}$$

$$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$$

$$R_{nl}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}}$$

$$\cdot e^{-r/na} \left(\frac{2r}{na}\right)^l \left[L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right)\right]$$

$$R_{10} = 2a^{-3/2} \exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2} \left(1 - \frac{1}{2}\frac{r}{a}\right) \exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a} \exp(-r/2a)$$

# 4.3. Angular Momentum.

## 4.4. **Spin.**

$$S_i = \frac{\hbar}{2}\sigma_i$$

$$\sigma_x \equiv \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}$$

$$\sigma_y \equiv \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix}$$

$$\sigma_z \equiv \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$$