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.

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

1.3. The Uncertainty Principle.

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

2. Time-Independent Schrödinger Equation

2.1. Stationary States.

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi &= E\psi\\ \Psi(x,t) &= \sum_{n=1}^{\infty}c_n\psi_n(x)e^{-i\frac{E_n t}{\hbar}}\end{aligned}$$

2.2. The Infinite Square Well.

$$\begin{aligned}V(x) &= \begin{cases}0 & 0\leq x\leq L\\ \infty & \text{otherwise}\end{cases}\\ E_n &= \frac{n^2\pi^2\hbar^2}{2mL^2}\\ \psi_n(x) &= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\\ \langle\psi_i|\psi_j\rangle &= \delta_{ij}\\ c_n &= \langle\psi_n|\Psi(x,t=0)\rangle\end{aligned}$$

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

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

2.3. The Harmonic Oscillator.

2.3.1. *Base State.*

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

2.3.2. *Ladder Operators.*

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

2.3.3. *Solving.*

$$\begin{aligned}\hat{a_+}\psi_n &= \sqrt{n+1}\psi_{n+1}\\ \hat{a_-}\psi_n &= \sqrt{n}\psi_{n-1}\\ \psi_n &= \frac{1}{\sqrt{n!}}(\hat{a_+})^n\psi_0\\ E_n &= \left(n+\frac{1}{2}\right)\hbar\omega\end{aligned}$$

2.3.4. *Operators.*

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

2.4. The Free Particle.

$$\begin{aligned}k^2 &= \frac{2mE}{\hbar^2}\\ k &\in \mathbb{R}\\ E &= \frac{\hbar^2k^2}{2m}\\ p &= \hbar k\\ \Psi(x,t) &= \underbrace{Ae^{ikx-i\frac{E}{\hbar}t}}_{\text{right mover}} + \underbrace{Be^{-ikx-i\frac{E}{\hbar}t}}_{\text{left mover}}\\ \Phi(k) &= \frac{1}{\sqrt{a\pi}}\frac{\sin(ka)}{k}\end{aligned}$$

2.5. Step Potential.

$$\begin{aligned}V(x) &= \begin{cases}0 & x<0\\ V_0 & x\geq 0\end{cases}\\ J_x &= -\frac{\hbar i}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]\\ T &\equiv \left|\frac{J_{trans}}{J_{inc}}\right| \quad 0\leq T\leq 1\\ R &\equiv \left|\frac{J_{refl}}{J_{inc}}\right| \quad 0\leq R\leq 1\end{aligned}$$

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

$$\begin{aligned}k_1^2 &= \frac{2mE}{\hbar^2}\\ \Psi_{\text{I}} &= \underbrace{Ae^{ik_1x}}_{\text{Incident}} + \underbrace{Be^{-ik_1x}}_{\text{Reflected}}\\ k_2^2 &= \frac{2m(E-V_0)}{\hbar^2}\\ \Psi_{\text{II}} &= \underbrace{Ce^{ik_2x}}_{\text{Transmited}} + \underbrace{De^{-ik_2x}}_{\text{DNE}}\\ T &= \frac{4}{\left[1+\frac{k_2}{k_1}\right]^2}\frac{k_2}{k_1}\\ R &= \frac{\left[1-\frac{k_2}{k_1}\right]^2}{\left[1+\frac{k_2}{k_1}\right]^2}\end{aligned}$$

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

$$\begin{aligned}k_1^2 &= \frac{2mE}{\hbar^2}\\ \Psi_{\text{I}} &= \underbrace{Ae^{ik_1x}}_{\text{Incident}} + \underbrace{Be^{-ik_1x}}_{\text{Reflected}}\\ k_2^2 &= \frac{2m(E-V_0)}{\hbar^2}\\ \Psi_{\text{II}} &= \underbrace{Ce^{-k_2x}}_{\text{Transmited}} + \underbrace{De^{k_2x}}_{\text{DNE}}\\ T &= 0\\ R &= 1\end{aligned}$$

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.

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

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.

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

The identity operator is

$$\hat{I} = \sum|\alpha\rangle\langle\alpha|$$

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

$$\hat{O}\,|n\rangle = o_n\,|n\rangle$$

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.*

$$\begin{aligned}\hat{a_+}\,|n\rangle &= \sqrt{n+1}\,|n+1\rangle\\ \hat{a_-}\,|n\rangle &= \sqrt{n}\,|n-1\rangle\end{aligned}$$

3.3.3. *Wave Function.*

$$\begin{aligned}|\Psi\rangle &= \sum_n A_n\,|n\rangle\\ A_n &= \langle n|\Psi\rangle\\ |\Psi\rangle &= \sum_n\langle n|\Psi\rangle\,|n\rangle\end{aligned}$$

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4. Quantum Mechanics in Three Dimensions

4.1. Schrödinger Equation in Spherical Coordinates.

4.1.1. *Legendre.*

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

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

4.1.2. *Spherical Harmonics.*

$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta)$$
$$\epsilon = \begin{cases}(-1)^m & m \geq 0\\ 1 & m \leq 0\end{cases}$$
$$\left\langle Y_l^m \middle| Y_{l'}^{m'}\right\rangle = \delta_{ll'}\delta_{mm'}$$

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$
$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$
$$Y_1^{\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$$
$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$$
$$Y_2^{\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$$
$$Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm 2i\phi}$$

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.*

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

4.2.2. *Radial.*

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

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$
$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$
$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

4.2.3. *Wave Function.*

$$n \in \mathbb{N}$$
$$0 \leq l < n$$
$$-l \leq m \leq l$$

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3\frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}} \cdot e^{-r/na}\left(\frac{2r}{na}\right)^l\left[L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)\right]Y_l^m(\theta,\phi)$$

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

4.3. Angular Momentum.

$$L_x = yp_z - zp_y$$
$$L_y = zp_x - xp_z$$
$$L_z = xp_y - yp_x$$
$$[L_x, L_y] = i\hbar L_z,\ [L_y, L_z] = i\hbar L_x,\ [L_z, L_x] = i\hbar L_y$$
$$L^2 \equiv L_x^2 + L_y^2 + L_z^2$$
$$\left[L^2, L_x\right] = 0,\ \left[L^2, L_y\right] = 0,\ \left[L^2, L_z\right] = 0$$
$$L_\pm \equiv L_x \pm iL_y$$
$$[L_z, L_\pm] = \pm\hbar L_\pm$$
$$\left[L^2, L_\pm\right] = 0$$

4.4. Spin.

$$S_i = \frac{\hbar}{2}\sigma_i$$
$$\sigma_x \equiv \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$
$$\sigma_y \equiv \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$
$$\sigma_z \equiv \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$