1 Intuition of Quantum Mechanics

1.1 Wave & Wave Function

Wave

$$\lambda k = 2\pi \quad \omega T = 2\pi \tag{1}$$

De Broglie Relation:

$$p = \frac{h}{\lambda} \quad \hbar = \frac{h}{2\pi} \implies p = \hbar k \quad \hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{2}$$

Schrodinger Equation: (Ψ is the wave function)

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \tag{3}$$

1.2 Complex Number

Euler's Formula:

$$e^{a+ib} = e^a(\cos b + i\sin b), \quad a \in \mathbb{R}, b \in \mathbb{R} \tag{4}$$

Complex Conjugate:

$$z = a + ib \quad z^* = a - ib \quad |z|^2 = zz^* = a^2 + b^2, \quad a, b \in \mathbb{R} \tag{5}$$

$$c = e^{\ln(c)} \implies (c^{a+ib})^* = (c^*)^{a-ib}, \quad C \in \mathbb{C}, a, b \in \mathbb{R} \tag{6}$$

Trig $\leftrightarrow$ Hyperbolic: ($a \in \mathbb{C}$)

$$\sin(ia) = i\sinh(a) \implies \sinh(a) = -i\sin(ia) \tag{7}$$

$$\cos(ia) = \cosh(a) \implies \cosh(a) = \cos(ia) \tag{8}$$

1.3 Probability

Gaussian Integral: ($a > 0$)

$$\int_{-\infty}^{\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}}, \quad \int_{-\infty}^{\infty} x^2 e^{-ax^2}\,dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}, \quad \int_{-\infty}^{\infty} x^{2n+1} e^{-ax^2}\,dx = 0 \tag{9}$$

Axiom of Probability:

$$\rho(x,t) = |\Psi(x,t)|^2 \quad \int_{-\infty}^{\infty} \rho(x,t)dx = \langle\Psi|\Psi\rangle = 1 \tag{10}$$

$$\langle\Psi|\Psi\rangle = C \neq \infty \text{ or } 0 \text{ (normalizable)} \implies \Psi(x,t) \to \frac{1}{\sqrt{C}}\Psi(x,t) \tag{11}$$

Expectation Value:

$$\langle O\rangle = \langle\Psi|O\Psi\rangle, \quad \sigma_O = \sqrt{\langle O^2\rangle - \langle O\rangle^2}, \quad O \in \text{observable} \tag{12}$$

Commutator:

$$\mathbf{comm}(A,B) = [A,B] = AB - BA \text{ Use test function} \tag{13}$$

Uncertainty Principle:

$$\sigma_A \sigma_B \geq \frac{1}{2}|\langle \mathbf{comm}(A,B)\rangle| \implies \sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{14}$$

1.4 Probability Current

Probability Density:

$$\frac{d}{dt}\int_a^b \rho(x,t)dx = J(a,t) - J(b,t) \implies J(x,t) = \frac{\hbar}{2mi}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right) \tag{15}$$

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0 \text{ (Conservation of Probability)} \tag{16}$$

Plane Wave

$$\psi(x) = \mathcal{A}e^{ikx} \implies J = \frac{\hbar k}{m}|\mathcal{A}|^2 > 0 \quad \text{(Incident from left)} \tag{17}$$

$$\psi(x) = \mathcal{B}e^{-ikx} \implies J = -\frac{\hbar k}{m}|\mathcal{B}|^2 < 0 \quad \text{(Incident from right)} \tag{18}$$

Transmission & Reflection Coefficients:

$$T = \frac{|J_{transmitted}|}{|J_{incident}|}, \quad R = \frac{|J_{reflected}|}{|J_{incident}|} \tag{19}$$

2 Solving Schrodinger Equation

2.1 TISE

Separation of Variables:

$$\Psi(x,t) = \psi(x)\phi(t) \implies \frac{i\hbar}{\phi(t)}\frac{d\phi(t)}{dt} = \frac{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)}{\psi(x)} = E \tag{20}$$

Time-Dependent Part:

$$\phi(t) = e^{-\frac{i}{\hbar}Et} \implies \Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}} \tag{21}$$

Time-Independent Schrodinger Equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x), \quad \hat{H}\psi(x) = E\psi(x) \tag{22}$$

Existance of Minium Energy:

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = (V(x) - E)\psi, \quad E < V_{min} \implies \text{sign}(\frac{d^2\psi}{dx^2}) = \text{sign}(\psi) \implies \psi \text{ blows up!} \tag{23}$$

If $E < V_{min}$ the solution is exponentially divergent and not physically acceptable. Therefore allowed energies must be bounded below.

Scattering State:

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = (V(x) - E)\psi, \quad E > V_{max} \implies \text{sign}(\frac{d^2\psi}{dx^2}) \neq \text{sign}(\psi) \implies \psi \text{ oscillates!} \tag{24}$$

$E > V_{max}$ will cause ψ to oscillate, so it is called scattering state. Without linear combination with 2 linear independent states, it is not normalizable.

2.2 Infinite Potential Well

Condition:

$$V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & \text{otherwise} \end{cases} \implies \psi(x)\text{is a } C^0 \text{ function.} \tag{25}$$

Equation:

$$\lim_{x\to 0^+} \psi(x) = \lim_{x\to 0^-} \psi(x) = \lim_{x\to a^+} \psi(x) = \lim_{x\to a^-} \psi(x) = 0 \tag{26}$$

Solution:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} \tag{27}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n \in \mathbb{N} \tag{28}$$

Expectation Values:

$$\langle x\rangle = \frac{a}{2}, \quad \langle x^2\rangle = a^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right), \quad \langle p\rangle = 0, \quad \langle p^2\rangle = \frac{n^2\pi^2\hbar^2}{a^2} \tag{29}$$

2.3 SHM

Condition:

$$V(x) = \frac{1}{2}m\omega^2x^2, \quad \omega \in \mathbb{R}^+ \text{ (parameter)} \implies \psi(x)\text{is a } C^\infty \text{ function.} \tag{30}$$

Ladder Operators:

$$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega x\right) \implies \hat{H} = \hbar\omega\left(a_+a_- + \frac{1}{2}\right), \mathbf{comm}(a_-, a_+) = 1 \tag{31}$$

Induction: (We assume $\psi_n(x)$ is an solution - base case. Similar for a_-)

$$\hat{H}a_+\psi_n(x) = a_+\left(\hat{H}\psi_n(x) + \hbar\omega\psi_n(x)\right) = (E_n + \hbar\omega)a_+\psi_n(x) \tag{32}$$

Ground State:

$$a_-\psi_0(x) = 0 \implies \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} \tag{33}$$

$$a_+\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x) \quad a_-\psi_n(x) = \sqrt{n}\psi_{n-1}(x) \tag{34}$$

General Solution:

$$\psi_n(x) = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0(x) \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{35}$$

Position & Momentum:

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a_+ + a_-), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\,(a_+ - a_-) \tag{36}$$

Expectation Values:

$$\langle x\rangle = 0, \quad \langle x^2\rangle = \frac{\hbar}{2m\omega}(2n+1), \quad \langle p\rangle = 0, \quad \langle p^2\rangle = \frac{\hbar m\omega}{2}(2n+1) \tag{37}$$

2.4 Free Particle

Condition:

$$V(x) = 0 \implies \frac{d^2}{dx^2}\psi(x) + k^2\psi(x) = 0, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \in \mathbb{R} \tag{38}$$

General Solution:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \implies \psi(x) = C\sin(kx) + D\cos(kx) \tag{39}$$

3 Continuous and Fourier Transform

3.1 Fourier Transform

Definition:

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx \iff f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{f}(k)e^{ikx}dk \tag{40}$$

3.2 Finite Potential Well

Condition:

$$V(x) = \begin{cases} 0, & 0 < x < a \\ V_0, & \text{otherwise} \end{cases} \implies \psi(x)\text{is a } C^1 \text{ function.} \tag{41}$$

Equation: (4 boundary conditions)

$$\forall c, c \in \mathbb{R}, \quad \lim_{x\to c^+}\psi(x) = \lim_{x\to c^-}\psi(x), \quad \lim_{x\to c^+}\frac{d\psi}{dx}(x) = \lim_{x\to c^-}\frac{d\psi}{dx}(x) \tag{42}$$

General Solution: (Scattering, $E > V_0$, wave from left, $B_3 = 0$)

$$\psi(x) = \begin{cases} A_1e^{ik_1x} + B_1e^{-ik_1x}, & x < 0 \\ A_2e^{ik_2x} + B_2e^{-ik_2x}, & 0 < x < a \\ A_3e^{ik_1x}, & x > a \end{cases} \quad k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, \quad k_2 = \sqrt{\frac{2mE}{\hbar^2}} \tag{43}$$

Solutions: (Let $\Delta = 2\cos(k_2a) - i\left(\frac{k_1}{k_2} + \frac{k_2}{k_1}\right)\sin(k_2a)$)

$$A_3 = \frac{2e^{-ik_1a}}{\Delta}A_1, \quad B_1 = \frac{-i\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)\sin(k_2a)}{\Delta}A_1 \tag{44}$$

$$A_2 = \frac{(1+\frac{k_1}{k_2})\,e^{-ik_2a}}{\Delta}A_1, \quad B_2 = \frac{(1-\frac{k_1}{k_2})\,e^{ik_2a}}{\Delta}A_1 \tag{45}$$

$$T = \frac{4}{|\Delta|^2} = \left[1 + \frac{V_0^2\sin^2(k_2a)}{4E(E-V_0)}\right]^{-1}, \quad R = 1 - T \tag{46}$$

3.3 Finite Potential Barrier

Condition:

$$V(x) = \begin{cases} V_0, & 0 < x < a \\ 0, & \text{otherwise} \end{cases} \implies \psi(x)\text{is a } C^1 \text{ function.} \tag{47}$$

General Solution: (Scattering, $E < V_0$ tunneling, wave from left, $B_3 = 0$)

$$\psi(x) = \begin{cases} A_1 e^{ikx} + B_1 e^{-ikx}, & x < 0 \\ A_2 e^{\kappa x} + B_2 e^{-\kappa x}, & 0 < x < a \\ A_3 e^{ikx}, & x > a \end{cases} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{48}$$

Solutions ($E < V_0$, let $\Delta = 2\cosh(\kappa a) - i\left(\frac{k}{\kappa} - \frac{\kappa}{k}\right)\sinh(\kappa a)$):

$$A_3 = \frac{2e^{-ika}}{\Delta} A_1, \quad B_1 = \frac{-i\left(\frac{k}{\kappa} + \frac{\kappa}{k}\right)\sinh(\kappa a)}{\Delta} A_1 \tag{49}$$

$$A_2 = \frac{(1 + \frac{ik}{\kappa})\, e^{-\kappa a}}{\Delta} A_1, \quad B_2 = \frac{(1 - \frac{ik}{\kappa})\, e^{\kappa a}}{\Delta} A_1 \tag{50}$$

$$T = \frac{4}{|\Delta|^2} = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)}\right]^{-1}, \quad R = 1 - T \tag{51}$$

Solutions ($E > V_0$, replace $\kappa \to -ik'$, i.e. $\sinh \to i\sin$, $\cosh \to \cos$):

$$T = \left[1 + \frac{V_0^2 \sin^2(k'a)}{4E(E - V_0)}\right]^{-1}, \quad R = 1 - T, \quad k' = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \tag{52}$$

3.4 Delta Potential Well

Condition:

$$V(x) = -\alpha\delta(x) \implies \psi(x) \text{is a } C^0 \text{ function.} \tag{53}$$

Equation:

$$\lim_{x \to 0^+} \psi(x) = \lim_{x \to 0^-} \psi(x) \tag{54}$$

$$\text{Take } \int_{0^-}^{0^+} dx \text{ for TISE} \implies \lim_{x \to 0^+} \frac{d\psi}{dx}(x) - \lim_{x \to 0^-} \frac{d\psi}{dx}(x) = -\frac{2m\alpha}{\hbar^2}\psi(0) \tag{55}$$

Bound State: ($E < 0$, one bound state)

$$\psi(x) = \begin{cases} A_1 e^{\kappa x}, & x < 0 \\ B_1 e^{-\kappa x}, & x > 0 \end{cases} \quad \kappa = \frac{m\alpha}{\hbar^2}, \quad E = -\frac{m\alpha^2}{2\hbar^2}, \quad A_1 = B_1 = \sqrt{\kappa} \tag{56}$$

Expectation Values:

$$\langle x \rangle = 0, \quad \langle x^2 \rangle = \frac{1}{2\kappa^2}, \quad \langle p \rangle = 0, \quad \langle p^2 \rangle = \hbar^2\kappa^2 = -2mE \tag{57}$$

Scattering: ($E > 0$, wave from left)

$$\psi(x) = \begin{cases} A_1 e^{ikx} + B_1 e^{-ikx}, & x < 0 \\ A_2 e^{ikx}, & x > 0 \end{cases} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \beta = \frac{m\alpha}{\hbar^2 k} \tag{58}$$

$$B_1 = \frac{i\beta}{1 - i\beta} A_1, \quad A_2 = \frac{1}{1 - i\beta} A_1, \quad T = \frac{1}{1 + \beta^2}, \quad R = \frac{\beta^2}{1 + \beta^2} \tag{59}$$

3.5 Delta Potential Barrier

Condition:

$$V(x) = +\alpha\delta(x) \implies \psi(x) \text{ is a } C^0 \text{ function.} \tag{60}$$

Equation:

$$\lim_{x\to 0^+}\psi(x)=\lim_{x\to 0^-}\psi(x),\quad \lim_{x\to 0^+}\frac{d\psi}{dx}(x)-\lim_{x\to 0^-}\frac{d\psi}{dx}(x)=+\frac{2m\alpha}{\hbar^2}\psi(0) \tag{61}$$

Scattering: ($E>0$, wave from left, no bound states)

$$\psi(x)=\begin{cases}A_1e^{ikx}+B_1e^{-ikx}, & x<0\\ A_2e^{ikx}, & x>0\end{cases}\quad k=\sqrt{\frac{2mE}{\hbar^2}},\quad \beta=\frac{m\alpha}{\hbar^2k} \tag{62}$$

$$B_1=\frac{-i\beta}{1+i\beta}A_1,\quad A_2=\frac{1}{1+i\beta}A_1,\quad T=\frac{1}{1+\beta^2},\quad R=\frac{\beta^2}{1+\beta^2} \tag{63}$$