#### Introduction to Quantum Mechanics

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# Part I Theory

# 1 The Wave Function

# 1.1 The Schrodinger Equation

Looking for Particle's wave function

$$\Psi(x,t)$$

by solving the Schrodinger equation

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

$$\hbar = rac{h}{2\pi} = 1.054573 imes 10^{-34} 
m Js$$

# 1.2 The Statistical Interpretation

Born's statistical interpretation

$$\int_a^b |\Psi(x,t)|^2 dx = \{ ext{probability of finding the particle between a and b}\}$$

• All quantum mechanics has to offer is statistical information about the possible results.

# 1.3 Probability

#### 1.3.1 Discrete Variables

The average value of some *function* of *j* is given by

$$\langle f(j)
angle = \sum_{j=0}^{\infty} f(j) P(j)$$

The variance of the distribution

$$\sigma^2 \equiv \langle (\Delta j)^2 
angle$$

The standard deviation

$$\sigma = \sqrt{\langle j^2 
angle - \langle j 
angle^2}$$

#### 1.3.2 Continuous Variables

ho(x): probability density

$$P_{ab} = \int_a^b \rho(x) \, \mathrm{d}x$$

Rules:

$$\int_{-\infty}^{\infty} 
ho(x) \, \mathrm{d}x = 1$$
  $\langle x 
angle = \int_{-\infty}^{\infty} x 
ho(x) \, \mathrm{d}x$   $\langle f(x) 
angle = \int_{-\infty}^{\infty} f(x) 
ho(x) \, \mathrm{d}x$ 

$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

## 1.4 Normalization

**Normalizing** the wave function (square-integrable)

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, \mathrm{d}x = 1$$

Proof the Schrodinger equation automatically preserves the normalization of the wave function:

$$egin{aligned} rac{\partial \Psi}{\partial t} &= rac{i\hbar}{2m} rac{\partial^2 \Psi}{\partial x^2} - rac{i}{\hbar} V \Psi, & rac{\partial \Psi^*}{\partial t} &= -rac{i\hbar}{2m} rac{\partial^2 \Psi^*}{\partial x^2} + rac{i}{\hbar} V \Psi^* \ & \downarrow & \ rac{\partial}{\partial t} |\Psi|^2 &= rac{\partial}{\partial t} (\Psi^* \Psi) &= \Psi^* rac{\partial \Psi}{\partial t} + rac{\partial \Psi^*}{\partial t} \Psi \ & \downarrow & \ rac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x)|^2 \, \mathrm{d}x &= \int_{-\infty}^{\infty} rac{\partial}{\partial t} |\Psi(x)|^2 \, \mathrm{d}x &= 0 & \mathrm{QED} \end{aligned}$$

## 1.5 Momentum

For a particle in state  $\Psi$ , the expectation value of x is

$$\langle x 
angle = \int_{-\infty}^{\infty} x |\Psi(x)|^2 \, \mathrm{d}x = \int \Psi^* \left[ x 
ight] \Psi \, \mathrm{d}x$$

the expectation value of momentum is

$$\langle p 
angle = m rac{d \langle x 
angle}{dt} = -i \hbar \int \left( \Psi^* rac{\partial \Psi}{\partial x} 
ight) dx = \int \Psi^* \left[ -i \hbar (\partial/\partial x) 
ight] \Psi \, \mathrm{d}x$$

ullet operator:  $x o ext{position}; -i\hbar(\partial/\partial x) o ext{momentum}$ 

the expectation of any  ${\cal Q}(x,p)$  is

$$\langle Q(x,p)
angle = \int \Psi^*[Q(x,-i\hbar\partial/\partial x)]\Psi\,\mathrm{d}x$$

· Ehrenfest's theorem

$$rac{d\langle p
angle}{dt}=\left\langlerac{\partial V}{\partial x}
ight
angle$$

proof: 
$$rac{d\langle p
angle}{dt}=-i\hbar\intrac{\partial}{\partial t}\left(\Psi^*rac{\partial\Psi}{\partial x}
ight)=-i\hbar\left(rac{i}{\hbar}
ight)\int-|\Psi|^2rac{\partial V}{\partial x}dx$$

# 1.6 The Uncertainty Principle

• de Broglie formula

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

· Heisenberg's uncertainty principle

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

# 2 Time-Independent Schrodinger Equation

# 2.1 Stationary States

Separation of variables  $\Psi(x,t)=\psi(x)\varphi((t)$ 

$$rac{darphi}{dt} = -rac{iE}{\hbar}arphi \qquad o \qquad arphi(t) = e^{iEt/\hbar} \ -rac{\hbar^2}{2m}rac{d^2\psi}{dx^2} + V\psi = E\psi \qquad ext{time-independent Schrodinger equation}$$

Three Answers:

stationary states

$$\Psi(x,t)=\psi(x)e^{iEt/\hbar}$$

- states of definite total energy
  - $\circ$  Hamiltonian :  $H(x,p)=rac{p^2}{2m}+V(x)$
  - Hamiltonian operator:

$$\hat{H} = -rac{\hbar^2}{2m}rac{\partial^2}{\partial x^2} + V(x)$$

• Rewrite time-independent S\_e :

$$\hat{H}\psi=E\psi$$

- $\circ~$  expectation value of the total energy :  $\langle H 
  angle = E$  &  $\langle H^2 
  angle = E^2$
- $\circ$  variance:  $\sigma_H=0$
- linear combination of separable solutions

$$\Psi(x,t) = \sum_{n=1}^\infty c_n \psi(x) e^{-iE_n t/\hbar} = \sum_{n=1}^\infty c_n \Psi_n(x,t)$$

- $\circ~$  stationary states  $\Psi_n(x,t)=\psi_n(x)e^{iEt/\hbar}$
- $\circ \ |c_n|^2$  : probability that a measurement of the energy would return the value  $E_n$

$$\sum_{n=1}^{\infty}|c_n|^2=1 \ \langle H
angle =\sum_{n=1}^{\infty}|c_n|^2E_n$$

#### Four therom

- ullet For normalizable solutions, the separation constant E must be real
- $\psi(x)$  can always be taken to real
- If V(-x) = V(x) then  $\psi(x)$  can always be taken to be either even or odd
- ullet E must  $>V_{min}$

# 2.2 The Infinite Square Well

$$V(x) = egin{cases} 0 & 0 \leq x \leq a \ \infty & otherwise \end{cases}$$

Outside the well,  $\psi(x)=0$ 

Inside the well (simple harmonic oscillator equation)

$$rac{d^2\psi}{dx^2} = -k^2\psi, \qquad ext{where} \, k \equiv rac{\sqrt{2mE}}{\hbar}$$

- $E \geq 0$
- general solution:  $\psi(x) = A\sin(kx) + B\cos(kx)$
- boundary conditions:  $\psi(0) = \psi(a) = 0$
- · distinct solutions & normalize

$$\psi_n(x)\sqrt{rac{2}{a}}\sin\left(rac{n\pi}{a}x
ight), \qquad ext{with } E_n=rac{n^2\pi^2\hbar^2}{2ma^2} \quad (n=1,2,3,...)$$

- ground state:  $\psi_1$
- ullet propeties for  $\psi_n$ 
  - alternately even or odd
  - o each successive state has one more node(zero-crossing)

matually orthogonal

$$\int \psi_m(x)^* \psi_n(x) \, \mathrm{d}x = \delta_{mn}$$

complete

$$f(x) = \sum_{n=1}^\infty c_n \psi_n(x) \qquad c_n = \int \psi_n(x)^* f(x) \,\mathrm{d} x$$

• \*

$$egin{aligned} \Psi(x,t) &= \sum_{n=1}^{\infty} c_n \sqrt{rac{2}{a}} \sin\left(rac{n\pi}{a}x
ight) e^{-i(n^2\pi^2\hbar/2ma^2)t} \ c_n &= \sqrt{rac{2}{a}} \int_0^a \sin\left(rac{n\pi}{a}x
ight) \Psi(x,0) \,\mathrm{d}x \ \hat{H}\psi_n &= E_n\psi_n \quad o \quad \langle H
angle &= \sum |c_n|^2 E_n \end{aligned}$$

## 2.3 The Harmonic Oscillator

$$V(x)=rac{1}{2}m\omega^2x^2 \ \hat{H}=rac{1}{2m}\left[\hat{p}+(m\omega x)^2
ight]$$

# 2.3.1 Algebratic Method

$$egin{aligned} \left[\hat{A},\hat{B}
ight] &\equiv \hat{A}\hat{B} - \hat{B}\hat{A} 
ightarrow \left[x,\hat{p}
ight] = i\hbar \ \hat{a}_{\pm} &\equiv rac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x) 
ightarrow egin{aligned} x &= \sqrt{rac{\hbar}{2m\omega}}(\hat{a}_{+} + \hat{a}_{-}) \ \hat{p} &= i\sqrt{rac{\hbar m\omega}{2}}(\hat{a}_{+} - \hat{a}_{-}) \end{aligned} \ &\downarrow \ \hat{a}_{+}\hat{a}_{-} &= rac{1}{\hbar\omega}\hat{H} - rac{1}{2} \ \hat{a}_{-}\hat{a}_{+} &= rac{1}{\hbar\omega}\hat{H} + rac{1}{2} \end{aligned} 
ightarrow egin{aligned} \star &\hbar\omega\left(\hat{a}_{\pm}\hat{a}_{\mp} \pm rac{1}{2}
ight)\psi = E\psi \ \hat{H}(\hat{a}_{+}\psi) &= (E + \hbar\omega)(\hat{a}_{+}\psi) \ \hat{H}(\hat{a}_{-}\psi) &= (E - \hbar\omega)(\hat{a}_{-}\psi) \end{aligned}$$

There occurs a "lowest rung" :  $\hat{a}_-\psi_0=0$  ightarrow

$$\psi_0 = \left(rac{m\omega}{\pi\hbar}
ight)^{1/4} e^{-rac{m\omega}{2\hbar}x^2}, \qquad ext{with} \qquad E_0 = rac{1}{2}\hbar\omega$$

Exited states, increasing the energy by  $\hbar\omega$  with each step:

$$\psi_n = A_n (\hat{a}_+)^n \psi_0(x), \qquad ext{with} \qquad E_n = \left(n + rac{1}{2}
ight) \hbar \omega$$

Normalization algebraically

$$\begin{array}{ll} \bullet \ \ \hat{a}_+\psi_n=c_n\psi_{n+1}, & \hat{a}_-\psi_n=d_n\psi_{n-1} \\ & \int_{-\infty}^{\infty} f^*(\hat{a}_\pm g)\,\mathrm{d}x = \int_{-\infty}^{\infty} (\hat{a}_\mp f)^*g\,\mathrm{d}x \\ & \downarrow \\ \left\{ \begin{matrix} c_n=\sqrt{n+1} \\ d_n=\sqrt{n} \end{matrix} \right. & \leftarrow \left\{ \begin{matrix} \int_{-\infty}^{\infty} (\hat{a}_\pm\psi_n)^*(\hat{a}_\pm\psi_n)\,\mathrm{d}x = \int_{-\infty}^{\infty} (\hat{a}_\mp\hat{a}_\pm\psi_n)^*\psi_n\,\mathrm{d}x \\ \hat{a}_+\hat{a}_-\psi_n=n\psi_n, & \hat{a}_-\hat{a}_+\psi_n=(n+1)\psi_n \end{matrix} \right. \\ & \bigstar \quad \psi_n=\frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0(x) \end{array}$$

### 2.3.2 Analytic Method

$$rac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi \qquad \xi\equiv\sqrt{rac{m\omega}{\hbar}}x \quad K\equivrac{2E}{\hbar\omega}$$

To begin with at very large  $\xi$ 

$$egin{align} rac{d^2\psi}{d\xi^2} pprox \xi^2\psi & |x| o \infty & \psi(\xi) = h(\xi)e^{-\xi^2/2} \ & rac{d\psi}{d\xi}, rac{d^2\psi}{d\xi^2} & rac{d^2h}{d\xi^2} - 2\xirac{dh}{d\xi} + (K-1)h = 0 \ \end{pmatrix}$$

In the form of *power serires* in  $\xi$ 

$$h(\xi)=\sum_{j=0}^\infty a_j \xi^j \quad rac{dh}{d\xi}\,,rac{d^2h}{d\xi^2} \ 
ightarrow \ \sum_{j=0}^\infty [(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j] \xi^j=0$$

$$a_{j+2} = rac{(2j+1-K)}{(jh+1)(j+2)} a_j \quad o \quad h(\xi) = h_{\mathrm{even}}(\xi) + h_{\mathrm{odd}}(\xi)$$

For physically acceptable solutions:

$$K=2n+1\Rightarrow E=(n+1/2)\hbar\omega$$
 , for  $n=0,1,2,\ldots$   $\downarrow$   $a_{j+2}=rac{-2(n-j)}{(jh+1)(j+2)}a_{j}$ 

Nomalized stationary state

$$igsplace \psi_n(x) = \left(rac{m\omega}{\pi\hbar}
ight)^{1/4} rac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

• The first few of  $H_n(\xi)$ 

$$\cdot H_0 = 1$$

$$\cdot H_1 = 2\xi$$

$$H_2 = 4\xi^2 - 2$$

$$H_3 = 8\xi^3 - 12\xi$$

# 2.4 The Free Particle

$$V(x)=0 \ rac{d^2\psi}{dx^2}=-k^2\psi, \quad ext{where} \quad k\equivrac{\sqrt{2mE}}{\hbar} \ \Psi(x,t)=Ae^{ik\left(x-rac{\hbar k}{2m}t
ight)}+Be^{-ik\left(x-rac{\hbar k}{2m}t
ight)}$$

Represents a wave traveling to right and another going to left, as well write

$$\Psi_k(x,t) = Ae^{i\left(kx-rac{\hbar k^2}{2m}t
ight)} \ k \equiv \pm rac{\sqrt{2mE}}{\hbar}, ext{with} egin{cases} k>0 \Rightarrow ext{traveling to the right} \ k<0 \Rightarrow ext{traveling to the left} \end{cases}$$

This wave function is not normalizable

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \mathrm{d}x = |A|^2 \int_{-\infty}^{+\infty} \mathrm{d}x = |A|^2(\infty)$$

· Plancherel's therem

$$f(x) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} \mathrm{d}k \leftrightarrow F(k) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} \mathrm{d}x$$

Now this can be normalized

$$\Psi(x,t) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - rac{\hbar k^2}{2m}t
ight)} \mathrm{d}k \ \left\{ \Psi(x,0) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} \mathrm{d}k 
ight. \ \left. \phi(k) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} \mathrm{d}x 
ight.$$

 $ullet v_{
m classical} = v_{
m group} = 2 v_{
m phase}$ 

### 2.5 The Delta-Function Potential

#### 2.5.1 Bound States and Scattering States

$$\begin{cases} E < V(\infty) \Rightarrow \text{ bound state} \\ E > V(\infty) \Rightarrow \text{ scattering state} \end{cases}$$

#### 2.5.2 The Delta-Fuction Well

$$V(x) = -\alpha \delta(x)$$

(1) bound state E < 0

$$egin{align} rac{d^2\psi}{dx^2} = \kappa^2\psi, & ext{where} \quad \kappa \equiv rac{\sqrt{-2mE}}{\hbar} \ & \psi \ & \psi(x) = egin{cases} Be^{\kappa x}, & (x < 0) \ Fe^{-\kappa x}, & (x > 0) \end{cases} \end{split}$$

- boundary conditions at x=0:
  - $\circ \; \psi$  is always continuous;  $\Rightarrow F = B$
  - $\circ d\psi/dx$  is continuous except at points where the potential is infinite.

$$\psi(0)=B\Rightarrow \kappa=rac{mlpha}{\hbar^2}$$

Proof: ( $\epsilon o 0$ )

$$-rac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}rac{d^2\psi}{d^2x}dx+\int_{-\epsilon}^{+\epsilon}V(x)\psi(z)dx=E\int_{-\epsilon}^{+\epsilon}\psi(x)dx=0$$

$$egin{aligned} \Rightarrow \Delta \left(rac{d\psi}{dx}
ight) &= rac{2m}{\hbar^2} \lim_{\epsilon o 0} \int_{-\epsilon}^{+\epsilon} -lpha \delta(x) \psi(z) dx = -rac{2mlpha}{\hbar^2} \psi(0) \ \left\{ egin{aligned} d\psi/dx|_+ &= -B\kappa \ d\psi/dx|_- &= +B\kappa \end{aligned} 
ight. &\Rightarrow \Delta \left(rac{d\psi}{dx}
ight) = -2B\kappa \end{aligned}$$

Norminized  $ightarrow B = \sqrt{\kappa}$ 

$$\psi(x)=rac{\sqrt{mlpha}}{\hbar}e^{-mlpha|x|/\hbar^2}; \qquad E=-rac{mlpha^2}{2\hbar^2}$$

(2) scattering state E>0

$$egin{aligned} rac{d^2\psi}{dx^2} &= -k^2\psi, \quad ext{where} \quad k \equiv rac{\sqrt{2mE}}{\hbar} \ \psi \ \psi(x) &= egin{cases} Ae^{ikx} + Be^{-ikx}, & (x < 0) \ Fe^{ikx} + Ge^{-ikx}, & (x > 0) \end{cases} \end{aligned}$$

· Boundary conditions

$$F+G=A+B \ \left\{ egin{aligned} &\Delta(d\psi/dx)=ik(F-G-A+B) \ &\psi(0)=(A+B) \end{aligned} 
ight. \Rightarrow \ ik(F-G-A+B)=-rac{2mlpha}{\hbar^2}(A+B) \ F-G=A(1+2ieta)-B(1-2ieta), \qquad ext{where }eta\equivrac{mlpha}{\hbar^2k} \end{aligned}$$

When wave come from left:

A: amplitude of the incident wave

B: amplitude of the reflected wave

F: amplitude of the transmitted wave

$$B=rac{ieta}{1-ieta}A, \qquad F=rac{1}{1-ieta}A, \qquad G=0$$

The *relative* probability of reflection and transmission:

$$R\equivrac{|B|^2}{|A|^2}=rac{eta^2}{1+eta}=rac{1}{1+(2\hbar^2E/mlpha^2)}$$

$$T\equivrac{|F|^2}{|A|^2}=rac{1}{1+eta}=rac{1}{1+(mlpha^2/2\hbar^2E)}$$

Discussion:

$$ullet$$
 If  $E>V_{
m max}$  , then  $T=1$  and  $R=0$ 

$$ullet$$
 If  $E < V_{
m max}$  , then  $T=0$  and  $R=1$ 

$$\circ$$
 if  $T 
eq 0$ , tunneling

Show

$$\delta(x) = rac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} \, dk$$

Proof

$$F(k) = rac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = rac{1}{\sqrt{2\pi}}$$

# 2.6 The Finite Square Well

$$V(x) = egin{cases} -V_0, & -a \leq x \leq a \ 0, & |x| > a \end{cases}$$

(1) bound state E < 0

$$x < -a, V(x) = 0$$

$$rac{d^2\psi}{dx^2}=\kappa^2\psi, \quad ext{where} \quad \kappa\equivrac{\sqrt{-2mE}}{\hbar} \ \psi(x)=Be^{\kappa x}$$

$$-a < x < a, V(x) = -V_0$$

$$rac{d^2\psi}{dx^2} = -l^2\psi, \quad ext{where} \quad l \equiv rac{\sqrt{2m(E+V_0)}}{\hbar} \ \psi(x) = C\sin(lx) + D\cos(lx)$$

$$x > a, V(x) = 0$$

$$\psi(x) = Fe^{-\kappa x}$$

· even solutions

$$\psi(x) = egin{cases} Fe^{-\kappa x}, & (x > a) \ D\cos(lx), & (0 < x < a) \ \psi(-x), & (x < 0) \end{cases}$$

• boundary condition at x = a

$$\begin{cases} Fe^{-\kappa a} = D\cos(la) \\ -\kappa Fe^{-\kappa a} = -lD\sin(la) \end{cases} \Rightarrow \kappa = l\tan(la)$$

$$\begin{cases} z \equiv la & z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0} \\ (\kappa^2 + l^2) = 2mV_0/\hbar^2 \end{cases} \Rightarrow \tan z = \sqrt{(z_0/z)^2 - 1}$$

#### Discussion:

· Wide, deep well

$$egin{align} z_0 o \infty &\Rightarrow z_n = n\pi/2 &\Rightarrow \ E_n + V_0 &pprox rac{n^2\pi^2\hbar^2}{2m(2a)^2} & (n=1,3,5,\cdots) \end{array}$$

- Shallow, narrow well
  - $\circ$  for  $z_0 < \pi/2$ , only one remains
- (2) scattering state E>0

When wave come from left

$$\psi(x) = egin{cases} Ae^{ikx} + B^{-ikx}, & x < -a \ C\sin(lx) + D\cos(lx) & -a < x < a \ Fe^{ikx} & x > a \end{cases}$$

Boundary conditions

$$egin{aligned} Ae^{-ika}+B^{ika}&=-C\sin(la)+D\cos(la)\ ik[Ae^{-ika}-B^{ika}]&=l[C\cos(la)+D\sin(la)]\ C\sin(la)+D\cos(la)+Fe^{ika}\ l[C\cos(la)-D\sin(la)]&=ikFe^{ika} \end{aligned}$$

Eliminate

$$B=irac{\sin(2la)}{2kl}(l^2-k^2)F \ F=rac{e^{-2ika}A}{\cos(2la)-irac{(k^2+l^2)}{2kl}\sin(2la)} 
ightarrow$$

Transmission coefficient

$$T^{-1} = 1 + rac{V_0^2}{4E(E+V_0)} \sin^2\left(rac{2a}{\hbar}\sqrt{2m(E+V_0)}
ight)$$

 $\qquad \text{ when } T=1$ 

$$rac{2a}{\hbar}\sqrt{2m(E+V_0)}=n\pi \qquad \Rightarrow E_n+V_0=rac{n^2\pi^2\hbar^2}{2m(2a)^2}$$