

Chapter 2 Time-independent Schrödinger equation

2.1 Stationary state

From $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi$ (2.1)

Assume V is independent of t , use **separation of variables**

$$\Psi(x, t) = \psi(x)f(t)$$

have $\frac{\partial \Psi}{\partial t} = \psi(x) \frac{df}{dt}$, $\frac{\partial^2 \Psi}{\partial x^2} = f \frac{d^2 \psi}{dx^2}$

Deduce from equation (2.1), then

$$i\hbar \psi \frac{df}{dt} = -\frac{\hbar^2}{2m} f \frac{d^2 \psi}{dx^2} + V \psi f \quad \Rightarrow \quad i\hbar \frac{1}{f} \frac{df}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2 \psi}{dx^2} + V$$

$$\Rightarrow \begin{cases} i\hbar \frac{1}{f} \frac{df}{dt} = E \\ -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2 \psi}{dx^2} + V = E \end{cases} \quad \Rightarrow \begin{cases} f(t) = e^{\frac{iEt}{\hbar}} \\ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V \psi = E \psi \end{cases} \quad \text{.....(2.2)}$$

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

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

is **time-independent Schrödinger equation**

properties of Ψ

(i) **Stationary state**

$$|\Psi(x, t)|^2 = \psi^* e^{\frac{iEt}{\hbar}} \psi e^{-\frac{iEt}{\hbar}} = |\psi|^2$$

for every expectation value $\langle Q(x, \hat{p}) \rangle = \int \psi^* Q(x, \hat{p}) \psi dx$ is constant in time

(ii) Definite total energy

Classical mechanics : total energy is **Hamiltonian**

$$H(x, p) = \frac{p^2}{2m} + V(x)$$

Quantum mechanics : corresponding **Hamiltonian operator**

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

thus equation (2.2) $\hat{H} \psi = E \psi \quad \longrightarrow \quad \langle \hat{H} \rangle = \int \psi^* \hat{H} \psi dx = E$

$$\hat{H}^2 \psi = \hat{H}(\hat{H} \psi) = \hat{H}(E \psi) = E(\hat{H} \psi) = E^2 \psi$$

$\longrightarrow \quad \langle \hat{H}^2 \rangle = \int \psi^* \hat{H}^2 \psi dx = E^2$

$$\text{so } \sigma_H^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = 0$$

(iii) Linear combination of separable solution

$$\Psi_n(x, t) = \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$$

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

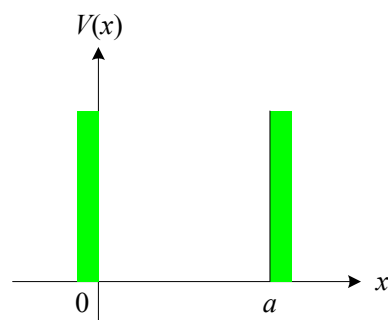
2.2 Infinite square well(one dimensional box)

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

and boundary conditions: $\Psi(0, t) = 0$
 $\Psi(a, t) = 0$

deduce:

outside the potential well $\psi(x) = 0$, probability is zero for finding the particle



inside the well $V=0$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \longrightarrow \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

$$E > 0 \quad \psi(x) = A \sin kx + B \cos kx \quad \text{and} \quad \psi(0) = \psi(a) = 0$$

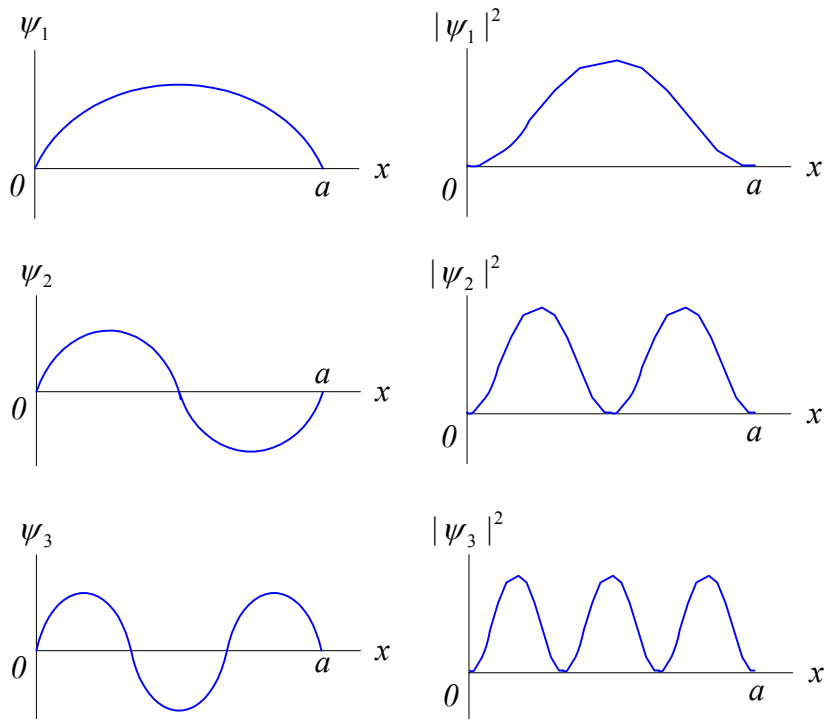
$$\psi_n(x) = A \sin k_n x \quad \text{where} \quad k_n = \frac{n\pi}{a}, \quad n=1,2,3,\dots$$

$$\text{thus} \quad \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}}$$

$$\text{normalize } \psi(x), \quad \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_0^a |A|^2 \sin^2(kx) dx = |A|^2 \frac{a}{2} = 1, \quad A = \sqrt{\frac{2}{a}}$$

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

$$\text{general solutions :} \quad \boxed{\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right) e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}}$$



first three states and probability density
of infinite square well

2.3 Harmonic oscillator

Classical treatment :

$$F = -kx = m \frac{d^2 x}{dt^2} \quad \longrightarrow \quad \frac{d^2 x}{dt^2} = -\frac{k}{m} x$$

$$\text{solution } x(t) = A \sin(\omega t) + B \cos(\omega t) \quad , \quad \omega = \sqrt{\frac{k}{m}}$$

$$\text{potential energy } V \text{ is related to } F : \quad F = -\frac{dV}{dx}$$

$$V = \frac{1}{2} kx^2 = \frac{1}{2} m \omega^2 x^2$$

Quantum treatment :

$$V(x) = \frac{1}{2} m \omega^2 x^2$$

$$\hat{H}(x, p) \psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi$$

$$\longrightarrow \quad \frac{1}{2m} \left[\left(-i\hbar \frac{d}{dx} \right)^2 + (m\omega x)^2 \right] \psi = E \psi \dots\dots\dots(2.3)$$

solve equation (2.3) by use **ladder operator** (a_+ , a_-)

$$a_+ = \frac{1}{\sqrt{2m}} \left(-i\hbar \frac{d}{dx} + im\omega x \right) \quad , \quad a_+ : \text{ is **raising operator** }$$

$$a_- = \frac{1}{\sqrt{2m}} \left(-i\hbar \frac{d}{dx} - im\omega x \right) \quad , \quad a_- : \text{ is **lowering operator** }$$

equation (2.3) rewrite by ladder operator :

$$\begin{aligned} (a_- a_+) f(x) &= \frac{1}{2m} \left(-i\hbar \frac{d}{dx} - im\omega x \right) \left(-i\hbar \frac{d}{dx} + im\omega x \right) f(x) \\ &= \frac{1}{2m} \left[-\hbar^2 \frac{d^2 f}{dx^2} + \hbar m \omega \frac{d}{dx} (xf) - \hbar m \omega x \frac{df}{dx} + (m\omega x)^2 f \right] \\ &= \frac{1}{2m} \left[\left(-i\hbar \frac{d}{dx} \right)^2 + \hbar m \omega + (m\omega x)^2 \right] f(x) \end{aligned}$$

compare equation(2.3)

$$\rightarrow (a_- a_+ - \frac{1}{2} \hbar \omega) \psi = E \psi$$

similarly $(a_+ a_- + \frac{1}{2} \hbar \omega) \psi = E \psi$

$$a_- a_+ - a_+ a_- = \hbar \omega$$

discussion

(i) :

$$\begin{aligned} (a_+ a_- + \frac{1}{2} \hbar \omega)(a_+ \psi) &= (a_+ a_- a_+ + \frac{1}{2} \hbar \omega a_+) \psi \\ &= a_+ (a_- a_+ + \frac{1}{2} \hbar \omega) \psi = a_+ [(a_- a_+ - \frac{1}{2} \hbar \omega) \psi + \hbar \omega \psi] \\ &= a_+ (E \psi + \hbar \omega \psi) = (E + \hbar \omega)(a_+ \psi) \end{aligned}$$

and

$$\begin{aligned} (a_- a_+ - \frac{1}{2} \hbar \omega)(a_- \psi) &= a_- (a_+ a_- - \frac{1}{2} \hbar \omega) \psi \\ &= a_- [(a_+ a_- + \frac{1}{2} \hbar \omega) \psi - \hbar \omega \psi] = a_- (E \psi - \hbar \omega \psi) \\ &= (E - \hbar \omega)(a_- \psi) \end{aligned}$$

(ii)

$$\begin{aligned} (a_+ a_- + \frac{1}{2} \hbar \omega)(a_+)^2 \psi &= (a_+ a_- a_+ + \frac{1}{2} \hbar \omega a_+) (a_+ \psi) \\ &= a_+ (a_- a_+ + \frac{1}{2} \hbar \omega)(a_+ \psi) = a_+ (a_+ a_- + \hbar \omega + \frac{1}{2} \hbar \omega)(a_+ \psi) \\ &= a_+ [(E + \hbar \omega)(a_+) \psi + \hbar \omega(a_+) \psi] \\ &= (E + 2\hbar \omega)(a_+)^2 \psi \end{aligned}$$

and

$$\begin{aligned} (a_- a_+ - \frac{1}{2} \hbar \omega)(a_-)^2 \psi &= (a_- a_+ a_- - \frac{1}{2} \hbar \omega a_-)(a_- \psi) \\ &= a_- (a_+ a_- - \frac{1}{2} \hbar \omega)(a_- \psi) = a_- (a_- a_+ - \hbar \omega - \frac{1}{2} \hbar \omega)(a_- \psi) \\ &= a_- [(E - \hbar \omega)(a_-) \psi - \hbar \omega(a_-) \psi] \\ &= (E - 2\hbar \omega)(a_-)^2 \psi \end{aligned}$$

(iii) there must exist a min state with $a_- \psi_0 = 0$

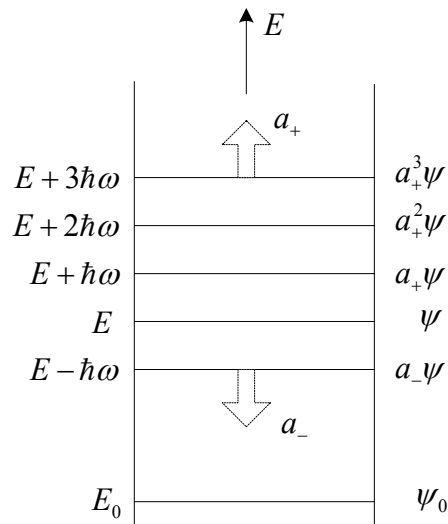
$$\frac{1}{\sqrt{2m}} (-i\hbar \frac{d\psi_0}{dx} - im\omega x \psi_0) = 0$$

$$\rightarrow \psi_0(x) = A_0 e^{-\frac{m\omega}{2\hbar} x^2}$$

and from $(a_+ a_- + \frac{1}{2} \hbar \omega) \psi_0 = E_0 \psi_0$

$\rightarrow E_0 = \frac{1}{2} \hbar \omega$

so the ladder of states can illustrate :



the ladder of stationary states

$$\psi_n(x) = A_n (a_+)^n e^{-\frac{m\omega}{2\hbar}x^2}, \quad E_n = (n + \frac{1}{2})\hbar\omega, \quad n = 0, 1, 2, \dots$$

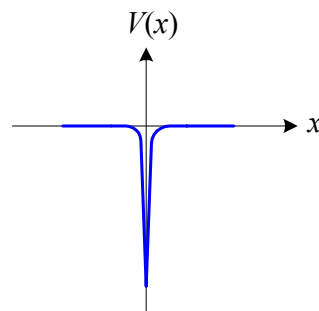
2.4 Delta-function potential

Energy E

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

Consider potential $V(x) = -\alpha\delta(x)$ $\alpha > 0$

$$\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases}$$



then $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$

(i) bound state : $E < 0$

$x < 0, V(x) = 0 \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi = k^2 \psi, \quad k = \frac{\sqrt{-2mE}}{\hbar}$

$\psi(x) = Ae^{-kx} + Be^{kx} \xrightarrow{\text{must } A=0, x \rightarrow -\infty, \psi=0} \psi(x) = Be^{kx}$

similarly, $x > 0 \quad \psi(x) = Ce^{-kx}$

use boundary condition : ψ is continuous in $\psi(0)$

$\xrightarrow{\text{blue arrow}} \psi(0) = B = C$

find k : from $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$

$\xrightarrow{\text{blue arrow}} -\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2} dx + \int_{-\epsilon}^{\epsilon} V(x)\psi(x) dx = E \int_{-\epsilon}^{\epsilon} \psi(x) dx$

$\xrightarrow{\text{blue arrow}} \Delta\left(\frac{d\psi}{dx}\right)\Big|_{x=0} = \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} V(x)\psi(x) dx$
 $= -\frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \alpha\delta(x)\psi(x) dx = -\frac{2m\alpha}{\hbar^2} \psi(0) = -\frac{2m\alpha}{\hbar^2} B \dots\dots\dots(2.4)$

and $\begin{cases} d\psi/dx = -Bke^{-kx}, & x > 0 \\ d\psi/dx = Bke^{kx}, & x < 0 \end{cases}$

$\xrightarrow{\text{blue arrow}} \frac{d\psi}{dx}\Big|_{x=0^+} - \frac{d\psi}{dx}\Big|_{x=0^-} = -2Bk = \Delta\left(\frac{d\psi}{dx}\right)$

so $k = \frac{m\alpha}{\hbar^2}, \quad \text{and} \quad E = -\frac{\hbar^2 k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$

normalize ψ : $B = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar}$

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}}, \quad E = -\frac{m\alpha^2}{2\hbar^2}$$

(ii) scattering state : $E > 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\rightarrow \begin{cases} \psi(x) = Ae^{ikx} + Be^{-ikx} & , \quad x < 0 \\ \psi(x) = Ce^{ikx} + De^{-ikx} & , \quad x > 0 \end{cases}$$

and $\begin{cases} \psi(0) = A + B = C + D & \dots\dots\dots(2.5) \\ \Delta\left(\frac{d\psi}{dx}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}(A + B) = ik(C - D - A + B) & \dots\dots\dots(2.6) \end{cases}$

for wave coming in from left ($D = 0$), equation (2.5),(2.6) rewrite

$$\begin{cases} A + B = C \\ C = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \beta = \frac{m\alpha}{\hbar^2 k} \end{cases}$$

$$\rightarrow B = \frac{i\beta}{1 - i\beta} A, \quad C = \frac{1}{1 - i\beta} A$$

Ae^{ikx} is **incident wave**, Be^{-ikx} is **reflected wave**, Ce^{ikx} is **transmitted wave**

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2} = \frac{1}{1 + \frac{2\hbar^2 E}{m\alpha^2}}, \quad T = \frac{|C|^2}{|A|^2} = \frac{1}{1 + \beta^2} = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}}$$

R is **reflection coefficient**, T is **transmission coefficient**

2.5 Free particle

$$V(x) = 0 \text{ everywhere}, \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\rightarrow \Psi(x, t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)} + Be^{-i(kx + \frac{\hbar k^2}{2m}t)}$$

$$\rightarrow \Psi_k(x, t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)} \quad \text{with} \quad \begin{cases} k > 0 \Rightarrow \text{traveling to right} \\ k < 0 \Rightarrow \text{traveling to left} \end{cases}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk \quad \text{is wave packet}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega t)} dk \quad , \quad \omega = \frac{\hbar k^2}{2m}$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk$$

Fourier transform $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$

wave packet moves along at **group velocity** $v_{group} = \frac{d\omega}{dk}$

and **phase velocity** $v_{phase} = \frac{\omega}{k}$

so $v_{group} = 2v_{phase}$

