Boundary Conditions

(i) Normalizable: \[ \lim_{x \to \infty} \psi(x) = 0 \]

(ii) Continuity of \( \psi(x) \): PDF defined for all \( x \)

(iii) Continuity of \( \psi'(x) \): everywhere \( V(x) \) finite, ensure \[ \frac{\hbar^2}{2m} \text{ continuous and } \frac{\hbar^2}{2m} \text{ finite} \]

Finite square well

\[ \begin{array}{c}
-\frac{V_0}{2} \quad x = 0 \\
E = 0 \quad E < 0
\end{array} \]

Usually take \( V = 0 \) at \( \infty \)

(Sum particle)

\[ |a| < \frac{a}{2} \quad \psi''_1 = -k^2 \psi_1 \quad k = \sqrt{2m(V_0 - E)}/\hbar \]

\[ |a| > \frac{a}{2} \quad \psi''_2 = q^2 \psi_2 \quad q = \sqrt{2m|E|}/\hbar \]

QM particle penetrates (tunnel) into classically forbidden region

\[ k^2 + q^2 = \frac{2m}{\hbar^2} \left[ V_0 + E - E \right] = \frac{2mV_0}{\hbar^2} \text{ constant} \]
(i) implies exponential decay \( |x| > \frac{a}{2} \)

\[
\begin{align*}
  x < -\frac{a}{2} & \quad \psi_I = C e^{\alpha x} \\
  x > \frac{a}{2} & \quad \psi_I = D e^{-\beta x}
\end{align*}
\]

\(-\frac{a}{2} < x < \frac{a}{2} \quad \psi_I = A \sin kx + B \cos kx\)

because \( V(x) = V(-x) \) solutions will be even or odd. Three constants determined by (ii), (iii).

\[\psi(x)\]

**Sketch of**

good and
first excited stat, \(-\frac{a}{2}\)

even \quad \psi_E = B \cos kx

\[
\begin{align*}
  B \cos \frac{k a}{2} &= 0 \\
  -k \cos k \frac{a}{2} &= 0 \quad \alpha &> \frac{a}{2} \\
  \tan \left( \frac{k a}{2} \right) &= \frac{q}{k} \\
  \cot \left( \frac{k a}{2} \right) &= -\frac{q}{k}
\end{align*}
\]

transcendental equation

define \( \gamma = \frac{k a}{2}, \beta = \frac{q a}{2}, \gamma = \frac{q}{2} \sqrt{2m V_0} \)

all dimensionless, \( \gamma \) = constant characterizing strength of well.

\[
\gamma^2 + \beta^2 = \gamma^2
\]
Graphical Solution

Always at least 1 solution in IP. $g_2$ is example with 2 solutions.

$$E_n = -V_0 + \frac{k^2}{2m} b^2 = -V_0 + \frac{\hbar^2}{2ma^2} (2\alpha n)^2$$

Recover $\infty$ well in limit $V_0 \to \infty$ (redefine as zero of potential) $g \to \infty$, $\alpha \to \frac{n\pi}{2}$.

$$E_n \to \frac{\hbar^2}{2ma^2} (n\pi)^2.$$
Free particle wave packet

Expand in terms of plane waves.

\[ E = \frac{(\hbar k)^2}{2m} \quad \text{non-relativistic energy} \]

Dispersion relation: \[ \omega(k) = \frac{1}{\hbar} \left( \frac{\hbar^2 k^2}{2m} \right) \]

Plane wave state, choose normalization:

\[ \phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \]

Fourier transform of \( \Psi(x) \rightarrow \tilde{\Psi}(k) \)

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

\[ \tilde{\Psi}(x,t) = \int_{-\infty}^{\infty} \tilde{\Psi}(k) \frac{1}{\sqrt{2\pi}} e^{i(kx - \omega(k)t)} \, dk \]

Because there is no confining potential, over time \( \Delta x \) will increase.
If we take $\psi(x,0)$ to be Gaussian:

$$\psi(x,0) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2}$$

you will find on the

$$\psi(x,t) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{at}} e^{-\frac{x^2}{2at}}$$

where $\alpha = 1 + \frac{2i\hbar a t}{m}$ (complex) and

as $t$ increases with time, wave packet has multiple momentum components that propagate with different speeds.

Plane wave normalization:

$$\int_{-\infty}^{\infty} \Phi_{k'}^* \Phi_k \, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i(k-k')x} \, dx$$

$$\equiv \delta(k-k')$$

Dirac "delta function". Technically not a function.

Analogous to kronecker $\delta$ in limit of continuous domain.
\textit{\textbf{Δelta Function}}

Dirac delta function defined by
\[ \int_{a}^{b} f(x) \delta(x-a) \, dx = \begin{cases} f(a) & x = a \\ 0 & \text{otherwise} \end{cases} \]

Picture unit-area spike at \( x = a \)

Mathematically, "\textit{function}" is distributed with many representations.

\( \delta(x) \) has dimensions \( \frac{1}{\text{dim} x} \)

Important representation:

\[ \delta(x) = \lim_{\Delta \to 0} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} e^{ikx} \, dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \, dk \]

\[ = \lim_{\Delta \to \infty} \frac{\sin(kx)}{kx} \]

\( x \to \infty \)

\( \sin(kx) \)

Sketched:

\[ \sin(kx) \]
\[
\text{Note: 1) } \lim_{x \to 0} \left[ \lim_{x \to 0} \frac{\sin (\alpha x)}{\pi x} \right] = \lim_{x \to 0} \frac{\alpha \sin (\alpha x)}{\pi x} = \frac{\alpha}{\pi} \quad \lim_{x \to 0} \frac{\alpha}{\pi} \to \infty
\]

\[
\text{2) } \int_{-\infty}^{\infty} \left[ \lim_{x \to 0} \frac{\sin (\alpha x)}{\pi x} \right] = \lim_{x \to 0} \frac{2}{\pi} \int_{0}^{\infty} \sin u \, du = \frac{2}{\pi} \int_{0}^{\infty} \sin u \, du = \frac{2}{\pi} \left[ \cos u \right]_{0}^{\infty} = \frac{2}{\pi} \cdot 0 = 1
\]
$\delta$-function potential

$$V(x) = -\frac{\hbar^2}{2m} \frac{\lambda}{b} \delta(x)$$

where $\delta(x)$ is a length

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

$$\psi'' = -\frac{\hbar^2}{b^2} \delta(x) \psi + \frac{2mE\psi}{\hbar^2}$$

When you see $\delta$, integrate! In $\mathbb{R}^3$, we look for bound states ($E < 0$).

$$\psi_{\pm}(x) = A e^{\pm kx}, \quad k = \sqrt{2m|E|}/\hbar$$

Must decay exponentially.

Integrate over infinitesimal neighborhood of $x = 0$:

$$\int_{-\epsilon}^{\epsilon} \psi'' dx = -\frac{\hbar^2}{b^2} \int \delta(x) \psi dx + k^2 \int \psi dx \bigg|_{-\epsilon}^{\epsilon}$$

$$\frac{d\psi}{dx} \bigg|_{-\epsilon}^{\epsilon} = -\frac{\hbar^2}{b^2} \psi(0) + k^2(2\epsilon) \psi(0)$$

Let $\epsilon \to 0$:

$$\frac{d\psi}{dx} \bigg|_{0^+} - \frac{d\psi}{dx} \bigg|_{0^-} = -\frac{\hbar^2}{b^2} \psi(0)$$

$$-2kA = -\frac{2}{b^2} A$$
\[ k = \frac{\lambda}{2b} \]

\[ E = -\frac{1}{2m} \left( \frac{\hbar \lambda}{2b} \right)^2 \] bound state

normalization:

\[ 2k = \int_0^\infty e^{-2kx} \, dx = \frac{|\lambda|^2}{\hbar} \int_0^\infty e^{-y} \, dy \]

= \frac{|\lambda|^2}{\hbar} \Rightarrow \lambda = \sqrt{\frac{\hbar}{2k}} \Rightarrow \text{choosing real}

\[ \Psi_{\pm}(x) = \left( \frac{\lambda}{2b} \right)^{\frac{1}{2}} e^{\mp \frac{\lambda}{2b} x} \]