Chapter 3: Problems in One Dimension

Application of concept of quantum mechanics to simple systems in 1 dimension:

- An impenetrable box → only discrete energy eigenvalues exist
- Harmonic oscillator potential → zero-point energy & algebraic solution & coherent states
- A potential wall, steps → reflection & transmission into a potential well & tunneling
- δ-function potential → bound states and scattering eigenstates of the Hamiltonian operator

3.1 Particle in an Impenetrable Box

Consider particle trapped in a potential $V(x) = \begin{cases} 0 & ; 0 \leq x \leq L \\ \infty & ; x < 0 \text{ or } x > L \end{cases}$

We need to determine all possible energy eigenvalues and the corresponding eigenfunctions from the time-independent Schrödinger equation:

$$-\frac{h^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) = E \psi(x)$$

Infinite potential region: Consider $V(x) = \infty$ for $x \to \pm \infty$. The term $\frac{h^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2}$ is finite almost everywhere (i.e., everywhere except at exceptional and separated points) and we have $E < \infty$.

So $\psi(x)$ must vanish almost everywhere.

We can therefore conclude that $\psi(x) = 0$ in the region where $V(x) = \infty$.

Smoothness of $\psi(x)$ at boundary points $x = 0, L$. For any finite $L$ (with $L \to \infty$) $\psi(x)$ must be smooth, because if $\psi(x)$ were discontinuous (i.e., $\psi(x) \approx 0$ for $x$ close to zero) we had $\frac{\partial^2 \psi(x)}{\partial x^2} \approx 0$, which does not appear in the time-independent Schrödinger equation. So we must have $\psi(x) = 0$. $\psi(x)$ is also continuous everywhere in the region $0 < x < L$.

Zero potential region: We have to solve the following eigenvalue problem with boundary conditions:

$$-\frac{h^2}{2m} \frac{\partial^2 \phi(x)}{\partial x^2} + E \phi(x) = 0, \quad \phi(0) = \phi(L) = 0$$

This is the differential equation for trigonometric functions and the general solution without yet considering the boundary condition reads $\phi(x) = N \exp(i(kx))$ with $E = \frac{h^2 k^2}{2m}$ and $k, a, b \in \mathbb{R}$.

The boundary conditions further restrict the possible eigenvalues and the form of the eigenfunctions.

$\phi(0) = 0$: $\sin(kL) = 0 \Rightarrow L = \frac{\pi}{k} (n = 1, 2, \ldots)$

$\phi(L) = 0$: $\sin(n\pi) = 0 \Rightarrow kL = \frac{n\pi}{2} \Rightarrow E = \frac{\pi^2 n^2}{2mL^2}$, $n \in \mathbb{N}$.

We thus obtain as the energy eigenfunctions and the associated energy eigenvalues:

$$\phi_n(x) = N \sin \left( \frac{n\pi x}{L} \right) \text{ with } E_n = \frac{\pi^2 n^2}{2mL^2}$$
Normalization gives the condition:
\[ N^2 \int_0^L \sin^2 \left( \frac{n\pi}{L} x \right) \, dx = \frac{N^2}{2} \implies N^2 = \frac{2}{L} \]

4. Final result: \( \phi_n \): energy eigenfunctions; \( E_n \): energy eigenvalues

\[ \phi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right), \quad E_n = \frac{n^2 \pi^2}{L^2}, \quad n = 1, 2, 3, \ldots \quad (n \in \mathbb{N}) \]

\[ E_n = \frac{E_1}{2}, \quad \text{so} \quad E_n = \frac{1}{2n^2 \pi^2}, \quad E_2 = 4E_1, \quad \ldots \quad E_n = n^2 E_1 \]

\[ \langle \phi_n | \phi_m \rangle = \frac{1}{L} \int_0^L \phi_n^*(x) \phi_m(x) \, dx = \delta_{nm} \]

4. Completeness: Every continuous wave function \( \psi(x), \ x \in [0,L] \) with \( \psi(0) = \psi(L) = 0 \) can be expanded in the \( \phi_n \) within as a superposition of the energy eigenfunctions: (→ Fourier Analysis!)

\[ \psi(x) = \sum_{n=1}^\infty \phi_n(x) \, c_n, \quad c_n = \langle \phi_n | \psi \rangle = \frac{1}{L} \int_0^L \phi_n^*(x) \psi(x) \, dx \]

This implies the completeness relation

\[ \sum_{n=1}^\infty \phi_n(x) \phi_n(y) = \delta(x-y) \]

4. Time evolution:

\[ \psi(x,t) = e^{-\frac{iE_n t}{\hbar}} \sum_{n=1}^\infty c_n \phi_n(x) = \sum_{n=1}^\infty e^{-\frac{iE_n t}{\hbar}} c_n \phi_n(x) \]
Consider particle in the harmonic oscillator potential $V(x) = \frac{k}{2}x^2$.

Hamilton operator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$

We can easily see that the energy spectrum of $\hat{H}$ contains only real numbers $E \geq 0$, because

$$\langle 4 \mid \hat{H} \mid 4 \rangle = \frac{1}{2}m \langle 4 \mid \hat{p}^2 \rangle + \frac{m \omega^2}{2} \langle 4 \mid \hat{x}^2 \rangle$$

$$= \frac{1}{2}m \langle 4 \mid \hat{p}^2 \rangle + \frac{m \omega^2}{2} \langle 4 \rangle \langle 4 \rangle = 0$$

The ground state is the energy eigenstate with the lowest energy eigenvalue. Using Heisenberg's Uncertainty Principle, we can show that the ground state's energy is indeed $\geq 0$.

We may assume that the ground state $\mid 1_0 \rangle$ has the classical property $\langle \hat{X} \rangle = 0$, $\langle \hat{P} \rangle = 0$.

Since it should be the state that simply stays at the minimum and does not move.

$$\langle \hat{X}^2 \rangle = \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2$$

Hence $\langle \hat{X}^2 \rangle = \langle \hat{P}^2 \rangle = \frac{\hbar^2}{2m}$ (Heisenberg's Uncertainty Principle)

We can now look for the minimum of the function $E(\mu) = \frac{\hbar^2}{8m} \mu + \frac{m \omega^2}{4} \mu^2$

$$\mu_{\text{min}} = -\frac{\hbar^2}{2m \omega^2} \implies E(\mu_{\text{min}}) = \frac{\hbar^2}{8m} \mu_{\text{min}} = -\frac{\hbar^2}{2m \omega^2} \implies E(\mu_{\text{min}}) - V(\mu_{\text{min}}) = 0$$

So the ground state energy has the property $E_0 = \langle \hat{H} \rangle = \frac{\hbar^2}{2m \omega^2}$.

It turns out that the ground state is the Gaussian wave packet from Chap. 29. With $\mu_0 = 0$:

$$\psi_0(x) = (2\pi)^{\frac{1}{4}} \frac{1}{\sqrt{\mu_0}} \exp\left(-\frac{x^2}{2\mu_0}\right)$$

We check:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_0(x) - \frac{m \omega^2}{2} x^2 \psi_0(x)$$

$$\implies -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_0(x) + \frac{m \omega^2}{2} \psi_0(x) = \frac{\hbar^2}{8m \omega^2} \psi_0(x) + \frac{\hbar^2}{4m \omega^2} \psi_0(x)$$

So we must have $\mu_0 = \left(\frac{\hbar}{2m \omega}\right)^2$ and get $E_0 = \frac{\hbar^2}{2m \omega^2}$ as the ground state energy.

Note that $\frac{1}{2m} \langle \hat{P}^2 \rangle = \frac{m \omega^2}{2} \langle \hat{X}^2 \rangle$, so kinetic and potential energy average values are equal in the ground state.

Note: The ground state wave function is unique (up to a global phase factor).
Ladder operators:

From Chp. 2.8 (generalized uncertainty relation) and the fact that the ground state \( |\phi_0\rangle \) minimizes the Heisenberg's uncertainty relation it follows that

\[
\left( \frac{\hbar^2}{2m} \right)^{\frac{1}{4}} \left( \frac{\hbar}{\Delta x} \right)^{\frac{1}{4}} \Delta x = \frac{\hbar}{2} \text{ and } \Delta P = \frac{\hbar}{2} \Delta x
\]

It turns out to be extremely useful to define the ladder operators

\[
a : = \left( \frac{m \hbar^2}{2} \right)^{\frac{1}{4}} X + i \left( \frac{1}{2 \hbar m \omega} \right)^{\frac{1}{4}} P, \quad a^+ = \left( \frac{m \hbar^2}{2} \right)^{\frac{1}{4}} X - i \left( \frac{1}{2 \hbar m \omega} \right)^{\frac{1}{4}} P
\]

\[
\Rightarrow X = \left( \frac{m \hbar^2}{2} \right)^{\frac{1}{4}} (a + a^+) \quad \text{and} \quad P = \left( \frac{\hbar m \omega}{2} \right)^{\frac{1}{4}} i(a^+ - a)
\]

The commutation relation of the \( a \) and \( a^+ \) reads:

\[
[a, a^+] = 1 \quad \Rightarrow \quad N = a a^+ - 1
\]

We also have that the Hamiltonian operator \( N = a a^+ \) called number operator can be written as

\[
\hat{N} = \frac{m \hbar^2}{2m} X^2 + \frac{1}{2m \omega} P^2 + \frac{i}{\hbar \omega} [X, P] = \frac{1}{\hbar \omega} \left( \frac{1}{2m \omega} P^2 + \frac{m \hbar \omega}{2} X^2 \right) - \frac{1}{2} = \frac{1}{\hbar \omega} \hat{H} - \frac{1}{2}
\]

such that the Hamiltonian can be expressed as

\[
\hat{H} = \hbar \omega \left( a^+ a + \frac{1}{2} \right) = \hbar \omega \left( N + \frac{1}{2} \right)
\]

We also have the following commutation relations:

\[
[a, a^+] = 1, \quad [N, a^+] = -a
\]

\[
\Rightarrow \quad [\hat{H}, a^+] = \hbar \omega a^+, \quad [\hat{H}, a] = -\hbar \omega a
\]

Algebraic construction of the energy eigenstates:

We know that \( a |\phi_0\rangle = 0 \) with \( |\phi_0\rangle \) being unique and so we also have \( \hat{N} |\phi_0\rangle = 0 \), i.e. \( |\phi_0\rangle \) is an eigenstate to \( \hat{N} \) with eigenvalue 0.

\[
\begin{align*}
\hat{N} a^{\dagger} |\phi_0\rangle &= [\hat{N}, a^+] |\phi_0\rangle = a^+ a |\phi_0\rangle = a^+ |\phi_0\rangle, \\
\hat{H} a^{\dagger} |\phi_0\rangle &= [\hat{H}, a^+] |\phi_0\rangle = (\hat{E} + \frac{\hbar \omega}{2}) a^+ |\phi_0\rangle \quad \Rightarrow \quad <a^+ |\phi_0\rangle = \frac{\hat{E} + \frac{\hbar \omega}{2}}{\hbar \omega} \end{align*}
\]

\[
N a^{\dagger} |\phi_0\rangle = [N, a^+] |\phi_0\rangle = a^+ a |\phi_0\rangle = 0
\]

\[
(a a^+) |\phi_0\rangle = \frac{\hat{E} + \frac{\hbar \omega}{2}}{\hbar \omega} a |\phi_0\rangle = (a a^+) |\phi_0\rangle = \frac{\hat{E} + \frac{\hbar \omega}{2}}{\hbar \omega} |\phi_0\rangle
\]

So \( |\phi_0\rangle = a^+ |\phi_0\rangle \) is a normalized eigenstate of \( \hat{N} \) to the eigenvalue 1 and energy eigenstate with the eigenvalue \( \frac{\hbar \omega}{2} \), and we have \( a |\phi_0\rangle = |\phi_0\rangle \).
$\hat{N} a^\dagger \hat{\psi} = [N, a^\dagger] \hat{\psi} = a^\dagger N \hat{\psi} = 2 a^\dagger \hat{\psi}$

$\quad H a^\dagger \hat{\psi} = [H, a^\dagger] \hat{\psi} = a^\dagger H \hat{\psi} = (E_0 + \omega) a^\dagger \hat{\psi}$

$\langle \psi, a^\dagger \hat{\psi} \rangle = \langle \psi, a a^\dagger \hat{\psi} \rangle = \langle \psi, (N+1) \hat{\psi} \rangle = 2 \langle \psi, \hat{\psi} \rangle = 2$

$\quad N a^\dagger \hat{\psi} = a a^\dagger N \hat{\psi} = a a^\dagger \hat{\psi} = (N+1) \hat{\psi} = 2 \hat{\psi}$

$\langle \psi, a a^\dagger \hat{\psi} \rangle = \langle \psi, a \lambda a^\dagger \hat{\psi} \rangle = \langle \psi, \lambda^2 a^\dagger \hat{\psi} \rangle = 2 \langle \psi, \lambda \hat{\psi} \rangle = 2 \langle \psi, (N+1) \hat{\psi} \rangle = 4 \langle \psi, \hat{\psi} \rangle = 4$

So $\langle \hat{\psi}, \lambda \rangle = \frac{1}{\sqrt{2}} \frac{a^\dagger}{\sqrt{\lambda^2}} = \frac{1}{\sqrt{2}} \frac{a^\dagger}{\sqrt{\lambda^2}}$ is a normalized eigenstate of $\hat{N}$ to the eigenvalue 2 and energy eigenstate to the eigenvalue $\frac{\sqrt{2}}{\sqrt{\lambda}}$, and we have $a^\dagger \hat{\psi} = \sqrt{\lambda} \hat{\psi}$.

Proof: exercise

With this method we can (indeed!) construct a GNS of eigenstates of
the number operator $\hat{N}$ and the Hamilton operator $H$:

$\quad a^\dagger \hat{\psi}_0 = 0 \quad \langle \psi_0, a^\dagger \hat{\psi}_0 \rangle = 1$

$\quad a^\dagger \hat{\psi}_n = \frac{1}{\sqrt{n+1}} (\sqrt{n+1} \hat{a}^\dagger \hat{\psi}_n)$

$\quad a^\dagger \hat{\psi}_n = \sqrt{n+1} \hat{a}^\dagger \hat{\psi}_n \quad \langle \hat{\psi}_n, a^\dagger \hat{\psi}_n \rangle = \langle \hat{\psi}_n, \sqrt{n+1} \hat{a}^\dagger \hat{\psi}_n \rangle = n + 1$

$\quad \langle \hat{\psi}_n, a \hat{\psi}_n \rangle = \langle \hat{\psi}_n, \sqrt{n} \hat{a} \hat{\psi}_n \rangle = \frac{1}{\sqrt{n+1}} \langle \hat{\psi}_n, (n+1) \hat{\psi}_n \rangle = 1 + \frac{1}{\sqrt{n+1}}$

$\quad N \hat{\psi}_n = n \hat{\psi}_n \quad \langle \hat{\psi}_n, a^\dagger \hat{\psi}_n \rangle = \langle \hat{\psi}_n, \sqrt{n+1} \hat{a}^\dagger \hat{\psi}_n \rangle = n + 1$

$\quad H \hat{\psi}_n = \hbar \omega (n + \frac{1}{2}) \hat{\psi}_n \quad \langle \hat{\psi}_n, a^\dagger \hat{\psi}_n \rangle = \langle \hat{\psi}_n, \sqrt{n+1} \hat{a}^\dagger \hat{\psi}_n \rangle = n + 1$

Due to property (x) we call $a^\dagger$ creation operator and $a$ annihilation operator.
The state $\hat{\psi}_n$ is called the $n$-th excited state.

We can obtain the configuration space energy eigenfunctions by applying the creation operator $a^\dagger$:

$\quad \phi_n(x) = (\sqrt{2\pi} \hbar)^{-n} \exp \left\{ -\frac{1}{2} \left( \frac{\hbar}{\sqrt{2\pi} \xi} \right)^2 \right\} \quad \varepsilon = \left( \frac{\hbar}{2\pi \xi} \right)^2 = \frac{\hbar^2}{2\pi^2} \Delta x$

$\quad \phi_n(x) = (\sqrt{2\pi} \hbar)^{-n} \exp \left\{ -\frac{1}{2} \left( \frac{\hbar}{\sqrt{2\pi} \xi} \right)^2 \right\} \quad a^\dagger = \frac{1}{\sqrt{2\pi} \xi} \left( \frac{\sqrt{\hbar}}{\sqrt{2\pi} \xi} \right)^2 \left( \sqrt{2\pi} \xi \right)^2 \frac{\hbar}{\sqrt{2\pi} \xi} \Delta x$

$\quad \phi_n(x) = (\sqrt{2\pi} \hbar)^{-n} \exp \left\{ -\frac{1}{2} \left( \frac{\hbar}{\sqrt{2\pi} \xi} \right)^2 \right\} \quad \phi_n(x) = (\sqrt{2\pi} \hbar)^{-n} \exp \left\{ -\frac{1}{2} \left( \frac{\hbar}{\sqrt{2\pi} \xi} \right)^2 \right\} \quad H_n \left( \frac{\hbar}{\sqrt{2\pi} \xi} x \right)$

Hermite polynomials:

$\quad H_n(x) = e^{-x^2} \left( \frac{\hbar^2}{2\pi^2} \frac{\hbar}{\sqrt{2\pi} \xi} \right)^n \frac{d^n}{dx^n} \left( e^{x^2} \right)$

$\quad H_0(x) = 1 \quad H_3(x) = 8x^3 - 12x$

$\quad H_1(x) = 2x \quad H_4(x) = 16x^4 - 40x^2 + 12$

$\quad H_2(x) = 4x^2 - 2 \quad H_5(x) = 32x^5 - 160x^3 + 120x$
Orthogonality: \[ \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \sqrt{\pi} 2^n n! \delta_{nm} \]

Generating function: \[ e^{t^2+2tx} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) \]

Differential equation: \[ \left( \frac{d^2}{dx^2} - 2x \frac{d}{dx} + 2n \right) H_n(x) = 0 \]

→ Multiparticle state interpretation:

The energy eigenstates \( |k\rangle \) with \( E_k = \hbar \omega (\frac{k}{\hbar} + 1) \) also provide the quantum mechanical description of states with \( n \) identical Bose particles each having energy \( E_k \).

Example: Photons (light particles) with a fixed direction and a fixed frequency \( \omega \).

1|0\rangle: zero photon state, "vacuum" with vacuum energy \( E_0 = \frac{1}{2} \hbar \omega \).

1|n\rangle: n photon state with energy \( E_n = E_0 + n \hbar \omega \).

\( a \): operator that annihilates one photon.

\( a^* \): operator that creates one photon.

→ Coherent States:

The energy eigenstates \( |n\rangle \) do not at all resemble at all a classical particle oscillating in the harmonic oscillator potential with \( x(t) = x_0 \cos(\omega t - \phi) \) because we have at any time \( t \):

\[ \langle t | x | t \rangle = x_0 \cos(\omega t - \phi) \quad \text{and} \quad \langle t | x^2 | t \rangle = \frac{1}{2} (x_0)^2 + \frac{(\hbar \omega)^2}{2} (\cos^2(\omega t - \phi) - 1) \]

We want to construct a solution of the time-dependent Schrödinger equation that describes an oscillating behavior.

\[ \frac{d}{dt} \langle \psi | \psi \rangle = 0 \quad \text{at} \quad t = 0 \]

A solution with \( \langle \psi | \psi \rangle = \langle \psi_0 | \psi_0 \rangle = 1 \) at \( t = 0 \) may have the correct property, so we may look for a wave function

\[ \frac{1}{2} \left( \frac{\Delta x}{\Delta x} + i \frac{\Delta p}{\Delta p} \right) | \psi_0 \rangle = 0 , \quad \Delta x = \frac{\hbar}{2\omega} \frac{1}{\Delta p} = \frac{\hbar}{2\omega} \frac{1}{\Delta p} \text{ from the ground state } |0\rangle \]

\[ a | \psi_0 \rangle = \frac{1}{2} \left( \frac{\Delta x}{\Delta x} + i \frac{\Delta p}{\Delta p} \right) | \psi_0 \rangle = 0 | \psi_0 \rangle , \quad z \in \Delta \]

\[ a | \psi_0 \rangle = z | \psi_0 \rangle \quad z \in \Delta \]

→ The eigenvalue equation \( a | \psi_0 \rangle = z | \psi_0 \rangle \), \( z \in \Delta \), is an example of a coherent state.

* \( | \psi_0 \rangle \) is obviously a superposition of states with different particle number.

* Destroying one photon from state \( | \psi_0 \rangle \) gives \( | \psi_0 \rangle \) = \( \sum_{n=0}^{\infty} z^n | n \rangle \).

* Important for the quantum mechanical description of coherent light.

We define for convenience: \( |1\rangle = |1\rangle \) and \( |2\rangle = |1\rangle \).

We can make the ansatz \( |z\rangle = f(a^*) |0\rangle \) and because \( \left[ a, f(a^*) \right] = f(a^*) |0\rangle = \frac{1}{2} f(a^*) |0\rangle \)

...
We see that $|z\rangle = c \sum_{n=0}^{\infty} \frac{(z)^n}{n!} |n\rangle = c \sum_{n=0}^{\infty} \frac{(2z)^n}{n!} |0\rangle$

Norm: $1 = \langle z | z \rangle = |c|^2 \sum_{n=0}^{\infty} \frac{(2z)^n}{n!} \langle n | n \rangle = |c|^2 \sum_{n=0}^{\infty} \frac{1}{n!} |z|^n = |c|^2 e^{\frac{|z|^2}{2}} \Rightarrow |c| = e^{-\frac{|z|^2}{2}}$

We set $c = |c|$. 

$\textbf{Time-dependent solution:}$

$\psi(x,t) = e^{-i\frac{1}{2}x^2} \sum_{n=0}^{\infty} \frac{(-i e^{-i\frac{1}{2}x^2})^n}{n!} \phi_n(x) = e^{-i\frac{1}{2}x^2} \phi(x)$

$\psi(x,t) = e^{-i\frac{1}{2}x^2} \phi(x)$

$\text{with } z(t) = 2 e^{i\omega t}$

$\text{Location and momentum expectation value:}$

$\langle x \rangle = \frac{\langle \psi(x) | x \psi(x) \rangle}{\langle \psi(x) | \psi(x) \rangle} = \frac{\frac{1}{\sqrt{2}} \langle \psi(x) | (a + a^\dagger) \psi(x) \rangle}{\frac{1}{2} \langle \psi(x) | (a - a^\dagger) \psi(x) \rangle}$

$= \frac{\frac{1}{\sqrt{2}} \langle \psi(x) | (a + a^\dagger) \psi(x) \rangle}{\frac{1}{2} \langle \psi(x) | (a - a^\dagger) \psi(x) \rangle} = \frac{\frac{1}{\sqrt{2}} \langle \psi(x) | (a + a^\dagger) \psi(x) \rangle}{\frac{1}{2} \langle \psi(x) | (a - a^\dagger) \psi(x) \rangle} = \frac{1}{\sqrt{2}}$ $2 \pi \hbar \omega \sin(\omega t - \frac{\pi}{2})$ 

$\Rightarrow$ Exactly corresponds to the motion of a classical particle in the harmonic oscillator potential with the amplitude $x_0 = \frac{\hbar \omega}{2} \pi \sin(\omega t - \frac{\pi}{2})$.

$\textbf{Explicit expression for wave function:}$

$\psi_2(x,t) = e^{-i\frac{1}{2}x^2} \sum_{n=0}^{\infty} \frac{(-i e^{-i\frac{1}{2}x^2})^n}{n!} \phi_n(x) = e^{-i\frac{1}{2}x^2} e^{i(\hbar \omega t - \frac{\pi}{2})} \phi(x)$

$\text{valid if } [a, a^\dagger] = [a^\dagger, a] = 0$

$\text{Use: } e^x = e^{a + b} = e^a e^b = e^{a^\dagger} e^a$

$\Rightarrow a^\dagger = \frac{1}{\sqrt{2}} \left( \frac{x}{\hbar \omega} - \frac{\hbar \omega}{2} \frac{d}{dx} \right), a = \frac{1}{\sqrt{2}} \left( \frac{x}{\hbar \omega} + \frac{\hbar \omega}{2} \frac{d}{dx} \right)$

$\Rightarrow$ 

$\psi_2(x,t) = e^{-i\frac{1}{2}x^2} e^{-i(\frac{\hbar \omega}{2}) \frac{d}{dx}} \int e^{i(\hbar \omega t - \frac{\pi}{2})} \phi(x) dx$

$\Rightarrow$ 

$|\phi_n(\psi_2)|^2 = \frac{1}{\frac{\hbar \omega}{2}} \exp \left\{ -\frac{1}{\frac{\hbar \omega}{2}} (x - x_0 \cos(\omega t - \frac{\pi}{2}))^2 \right\}$

$x_0 = \frac{\hbar \omega}{2} \pi \sin(\omega t - \frac{\pi}{2})$ 

This is exactly a Gaussian wave packet oscillating with frequency $\omega$, that does not broaden with time.

This does completely agree with our classic notion of a coherent light beam.
Energy expectation value:

\[
\langle H \rangle = \frac{\hbar}{2} \langle [a, a^+ + \frac{1}{2}] \rangle = \frac{\hbar}{2} \langle a^+ a + \frac{1}{2} \rangle + \hbar \langle [a^+, a] \rangle = \frac{\hbar}{2} + \hbar \langle a^+ a \rangle = \frac{\hbar}{2} + \hbar \langle \phi_{2n} | a^+ a | \phi_{2n} \rangle
\]

= \frac{\hbar}{2} + \hbar \langle |2n+1\rangle^2 - \hbar \omega (2n+1) = \hbar \omega \left( \frac{x_0^2}{2} + \frac{1}{2} \right)
\]

= \frac{\hbar \omega}{2} \langle x_0^2 \rangle + \frac{\hbar}{2}

\]

We see that the classical limit is obtained for \( |x_0| \to 1 \).

This is consistent with the following derivation:

We have \( \langle \phi_{2n} | \phi_{2m} \rangle = e^{-i\pi m} \sum_{\mu=0}^{\infty} \frac{1}{\mu!} \langle \phi_{2n} | \phi_{\mu} \rangle \).

The function \( f_2(x) = \frac{|e^{i\pi n}|}{n!} \) has its maximum at \( n = |x| \), so the states \( |\phi_n \rangle \) with \( n = |x| \) dominate the coherent state for \( |x| \gg 1 \).
3.3. Potential With a Step

Consider a particle that experiences a very localized force at $x=0$ of the form $F_0(x) = -V_0 \delta(x)$.

So the particle moves in a potential of the form $V(x) = V_0 \theta(x)$,

and the force acts to the left.

Hamilton operator: $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0 \theta(x)$

We have to find all solutions of the eigenvalue problem $H \phi_0(x) = E \phi_0(x)$.

We have $\langle H \rangle \geq 0$ for any state, so $E \geq 0$ as well.

Region $x < 0$: We have to solve the free particle Schrödinger equation $-\frac{\hbar^2}{2m} \phi_0(x) = E \phi_0(x)$

The solution has the form: $A e^{ikx} + B e^{-ikx}$, $p = \hbar k$, $E = \frac{\hbar^2 k^2}{2m}$, $k \in \mathbb{R}$

Note that $p e^{ikx} = -\hbar e^{-ikx}$, so $e^{ikx}$ describe a right/left moving particle.

Region $x > 0$: We solve the eigenvalue equation $-\frac{\hbar^2}{2m} \phi_0(x) = (E-V_0) \phi_0(x)$

$(E-V_0)$ can be positive or negative, so we must consider 2 cases.

Case $0 \leq E \leq V_0$: Solution has the form: $C e^{-kx}$, $k > 0$

with $\frac{\hbar^2 k^2}{2m} = V_0 - E - V_0 = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$, $k \in \mathbb{R}$

Note that the solution $e^{-kx}$ is not allowed since it diverges for large $x$.

Case $E > V_0$: Solution has the form: $C e^{ikx} + D e^{-ikx}$

with $\frac{\hbar^2 k^2}{2m} = E - V_0 = \frac{\hbar^2 k^2}{2m} - V_0 \Rightarrow k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$, $k \in \mathbb{R}$

Continuity at $x = 0$: $\phi_0(x)$ and $\phi_1(x)$ must be continuous at $x = 0$, because otherwise $\phi(x)$ would contain terms $\delta(x)$ or $\delta(x)$, which however do not appear in the Schrödinger equation.

Construction of a complete set of energy eigenfunctions

We want to identify the eigenfunctions $\phi_k(x)$ with: $H \phi_k(x) = E_k \phi_k(x)$

(1) Right-moving incoming particle with $E_k < V_0$:

\[
\phi_k(x) = \begin{cases}
  e^{ikx} + R e^{-ikx}, & x < 0 \\
  C e^{-kx}, & x > 0
\end{cases}
\]

with $0 < k = \sqrt{\frac{2m(E_k - V_0)}{\hbar^2}}$. 

05/01/2016
Continuity of \( \phi_h(x) \) at \( x = 0 \): \( A + R = C \)

Continuity of \( \phi_h(x) \) at \( x = 0 \): \( \left\{ \begin{array}{ll}
    i k (e^{i k x} - R e^{-i k x}), & x < 0 \\
    - R - i k C e^{-i k x}, & x > 0
  \end{array} \right. \) at \( x = 0 \) gives \( i k (1-R) = -ikC \)

\[ C = \frac{2k}{k + ik}, \quad R = \frac{k - ik}{k + ik} \quad \text{with} \quad |C| = \frac{2k}{\sqrt{k^2 + k^2}} < 1 \]

\[ L = C = \frac{2k}{k + ik} e^{i \delta_0} = \frac{2}{\sqrt{k^2 + k^2}} \left( \sqrt{k^2 + k^2} \right) e^{i \delta_0}, \quad \delta_0 = -\arctan \left( \frac{k}{k} \right) \quad (-\pi < \delta_0 < 0) \]

\[ R = e^{i \delta_0}, \quad \delta_0 = -2 \arctan \left( \frac{k}{k} \right) \quad (-\pi < \delta_0 < 0) \]

\[ P \text{ Physical interpretation:} \quad \text{with sharp monochromatic } p = ik \]

\[ + e^{i k x} \Theta(x): \text{increasing wave, coming from left, with probability current } \Delta = \frac{ik}{2im} e^{i k x} \Delta x = \frac{4k}{2im} \]

\[ * R e^{-i k x} \Theta(x): \text{totally reflected wave, going left, with probability current } \Delta = \frac{4k}{2im} e^{-i k x} \Delta x = \frac{4k}{2im} \Delta x \]

\[ * L e^{-i k x} \Theta(x): \text{wave function penetrating into the classically forbidden zone } x > 0 \text{, with probability} \]

\[ \text{current amplitude } \Delta = \frac{4k}{2im} e^{i k x} \Delta x = 0 \quad \text{Quantum effect} \]

\[ \text{Note: The reflected wave (as well as the penetrating wave) obtains an additional phase shift } e^{i k x} \text{ which can be physically observed by a time delay of the reflected particle.} \]

Important: This physical interpretation is further supported by the fact that the interference between incoming and reflected waves vanishes:

\[ j_{xx} = \frac{k}{2im} \left[ i k (e^{-i k x} - R e^{i k x}) \right] \]

\[ = \frac{k}{2im} \left[ i k (1 - 1R^2 - R e^{2ikx} + R e^{-2ikx}) \right] \]

\[ = \frac{k}{2im} (1 - 1R^2) \quad \text{The net current } j_{xx} = 0, \text{ due to } 1R^2 = 1. \]

\[ \text{Limit of infinitely high potential wall } \left( V_0 \to -\infty \right): \quad k \to \infty, \quad C \to 0, \quad R \to -1 = e^{-i \pi} \]

\[ \text{Phase shift of reflected wave!} \]

(2) Right-moving incoming particle with \( E(k) > V_0 \):

\[ \phi_h(x) = \frac{e^{i k x} + R e^{-i k x}}{Te^{i k x}}, \quad x < 0 \quad \text{with} \quad L > \frac{2 \pi \sqrt{V_0}}{k} \]

\[ L = \frac{\sqrt{k^2 - 2 \pi \sqrt{V_0}}}{k} < k \]

Continuity of \( \phi_h(x) \) and \( \phi_h(x) \) at \( x = 0 \) gives: \( A + R = T \) and \( i k (1-R) = ikT \)

\[ T = \frac{2k}{k + ik}, \quad R = \frac{k - ik}{k + ik} \quad \text{with} \quad |T| < 2 \quad \text{and} \quad 0 < R < 1 \]
Physical interpretation: with sharp momentum p=t k

* $e^{i k x} \theta(x)$: incoming wave coming from left as in (1) with $\theta(0) = \begin{cases} 1 & \text{for } x < 0 \\ 0 & \text{for } x > 0 \end{cases}$

* $R e^{-i k x} \theta(-x)$: partially reflected wave going left with $\theta(x) = -1 - \frac{|R|^2 + i k}{2m} \quad \text{Quantum effect!}$

* $T e^{i k x} \theta(x)$: transmitted wave going right with $\theta(x) = \frac{|T|^2 + i k}{2m}$

with sharp momentum $p=t k$

1. Probability that incoming particle is reflected:
   \[ \frac{\text{inc}}{\text{in}} = \frac{|R|^2}{|T|^2 + |R|^2} \quad \text{Probability conservation} \]

2. Probability that incoming particle is transmitted:
   \[ \frac{\text{trans}}{\text{in}} = \frac{|T|^2}{|T|^2 + |R|^2} \quad \text{Particle number conservation} \]

3. Limit of infinite energy ($E \to V_0$): $k' \to k, R \to 0, T \to 1$

4. Left-moving incoming particle with $E(k) > V_0$: only $k > \frac{2 \pi V_0}{\hbar}$ is possible

5. Continuity of $\phi_1(x)$ and $\phi_2(x)$ at $x=0$ gives: $A + B' = T$ and $i k (T + B') = -i k T$

6. Exactly the same result for the reflected and the transmitted wave amplitudes as for case (2)!

7. Construction of scattered wave packets:
   * start a $x=x_0$ at $t=0$
   * has group velocity $v_g = \frac{E}{m}$ (right-moving incoming)

8. We take a superposition of $\phi$ states with a strongly peaked wave function $\frac{1}{2 \pi} e^{-i k x} \phi(x)$ shifted to $x = \frac{k}{2 \pi} t$ and an additional phase $\phi \psi(x) = \frac{1}{2 \pi} e^{-i k x} \phi(x)$ such that the wave packet is located at $x_0$ at $t=0$ ($x_0 < 0$).

9. Case $E(k) < V_0$: We have to take $\psi(x)$ from case (1)

10. $\psi(x) = \begin{cases} e^{i k x} + \frac{R}{C} e^{-i k x}, & x < 0 \\ C e^{-i k x}, & x > 0 \end{cases}$ with $0 < k < \frac{2 \pi V_0}{\hbar}$

    \[ C = \frac{2 \pi}{\hbar} \frac{V_0}{k} \quad \text{phase shifting packet at } x_0 \text{ at } t=0 \]

    \[ R = e^{i \delta}, \quad \delta = -i \arctan \left( \frac{k}{k} \right) \quad (-\pi < \delta < 0) \]

    \[ C = - i \frac{2 \pi}{\hbar} V_0 \quad \text{velocity} \quad \frac{V_0}{\hbar} = \frac{k_0}{m} \]

    \[ (-\pi < \delta < 0) \]
\( t=0 \): Wave packet located at \( x_0 \), moves right with \( v_0 = \frac{p_0}{m} \).

\( t=t_1 \): Wave packet broadens, located at \( x_0 + v_0 t \).

\( t=t_2 \): Packet hits potential barrier, penetration into zone \( x>0 \), continued broadening.

Packet passes a bit at barrier due to \( k \)-dependence of complex phases \( \xi_r \) and \( \xi_e \).

\( t=t_3 \): Reflected wave moves left with \( v_0 = \frac{p_0}{m} \), further broadening. Wave is a bit behind the classic reflected particle due to \( k \)-dependence of complex phase \( \xi_e \). \( \rightarrow \) phase shift.

\( t=t_4 \): Further broadening, phase shift remains constant.

**Case \( E(k) > V_0 \):** We have to take \( \phi_e(x) \) from case (2).

\[
\phi_e(x) = \begin{cases} 
  e^{ikx} + R e^{-ikx}, & x < 0 \\
  T e^{ikx}, & x > 0 
\end{cases}
\]

with \( k > \frac{2 \mu V_0}{p_0^2} \), \( v_0 = \frac{p_0}{m} = \frac{k_0}{\mu} \), \( v_0' = \frac{k_0'}{\mu} < v_0 \).

\[
T = \frac{2k}{k+k'} \quad R = \frac{k-k'}{k+k'}
\]

with \( 1 < T < 2 \) and \( 0 < R < 1 \), \( T, R \in \mathbb{R} \).

\( t=0 \): Wave packet located at \( x_0 \), moves right with \( v_0 = \frac{p_0}{m} \).

\( t=t_1 \): Wave packet broadens, located at \( x_0 + v_0 t \).

\( t=t_2 \): Packet hits potential barrier, continued broadening, transmitted and reflected wave packets separate.

\( t=t_3 \): Reflected wave moves left with \( v_0 = \frac{p_0}{m} \), further broadening. \( \rightarrow \) Bounced back without delay.

Transmitted wave moves right with \( v_0' = \frac{k_0'}{\mu} < v_0 \), further broadening. \( \rightarrow \) Follows classic motion.

\( t=t_4 \): Further broadening.
3.4. Potential Wall

Consider a particle experiencing a force related to a potential wall of the form

\[ V(x) = V_0 \Theta(x) \Theta(a-x) \]

\[ = \begin{cases} 0, & x < 0 \text{ or } x > a \\ V_0, & 0 \leq x \leq a \end{cases}, \quad V_0 > 0 \]

From our considerations for the potential step we expect that an incoming particle with \( E \leq V_0 \) (coming from the left) can penetrate into the classically forbidden zone \( 0 \leq x \leq a \) and with some finite probability emerge for \( x > a \).

We only consider energy eigenfunctions representing incoming particles from the left.

1. Right-moving incoming particle with \( E(k) \leq V_0 \):

\[ \phi_k(x) = \begin{cases} e^{ikx} + \frac{1}{2} e^{-ikx}, & x < 0 \quad \text{with} \quad 0 \leq k \leq \frac{2\sqrt{V_0}}{a} \\ \frac{A e^{ikx} + B e^{-ikx}}{T e^{-ikx}}, & 0 \leq x \leq a \\ \frac{C e^{ikx} + D e^{-ikx}}{T e^{-ikx}}, & x > a \end{cases} \]

We have:
- partial reflection towards \( x < 0 \), phase shift
- penetration into classically forbidden zone \( 0 \leq x \leq a \)
- classically forbidden transmission into \( x > a \)

**\( \Rightarrow \) quantum effect that does not exist classically**

2. Right-moving incoming particle with \( E(k) > V_0 \):

\[ \phi_k(x) = \begin{cases} e^{ikx} + \frac{1}{2} e^{-ikx}, & x < 0 \quad \text{with} \quad k > \frac{2\sqrt{E}}{a} \\ \frac{A e^{ikx} + B e^{-ikx}}{T e^{-ikx}}, & 0 \leq x \leq a \\ \frac{C e^{ikx} + D e^{-ikx}}{T e^{-ikx}}, & x > a \end{cases} \]

We have:
- partial reflection towards \( x < 0 \)
- quantum effect
- transmission into \( x > a \), like classic particle

**\( \Rightarrow \) Nature's application of the tunnel effect — d-Decay**

\( \Rightarrow \) d-particle = \( \alpha \) the nucleus

Heavy nuclei are unstable and can decay by the emission of d-particles

**Mechanism:** Inside the nucleus \( R < 10^{-15} \text{m} = 10^{-15} A^{\frac{1}{3}} \) the nuclear force provides an attractive potential for the d-particle generated by the other protons and neutrons. Outside the nucleus \( r > R \) the nuclear force is screened and the Coulomb-force provides a repulsive potential \( V(r) \sim \frac{2(2-2)e^4}{r} \) for the d-particle.
$^{238}_{92} \text{U} \rightarrow ^{234}_{90} \text{Th} + a$, $E_{\text{th}} = 4.2 \text{ MeV}$, $E_{\text{barrier}} = 28 \text{ MeV}$, $T_{1/2} = 4.5 \times 10^9 \text{ a}$

$^{232}_{90} \text{Th (Thorium)}$, $E_{\text{th}} = 4.0 \text{ MeV}$, $T_{1/2} = 1.4 \times 10^6 \text{ a}$

$^{226}_{88} \text{Ra (Radium)}$, $E_{\text{th}} = 4.8 \text{ MeV}$, $T_{1/2} = 1600 \text{ a}$

$^{212}_{84} \text{Po (Polonium)}$, $E_{\text{th}} = 8.8 \text{ MeV}$, $T_{1/2} = 2 \times 10^{-7} \text{ s}$

→ Physical application of the tunnel effect: Scanning Tunneling Microscopy ("Tunnel-microscopist")

† Nobel prize 1986 for Gerd Binnig and Heinrich Rohrer

Tunnel current depends exponentially on distance $d$. One can picture the form of the conducting surface by scanning the surface (by moving the tip).