Waves: traveling wave

\[ y(x,t) = A \sin \left( 2\pi ft - \frac{2\pi}{\lambda_x} x \right) \]

\[ = A \sin \left( \omega t - k x \right) \]

- \( A \) - amplitude
- \( \omega \) - angular frequency \( 2\pi f \)
- \( k \) - wave vector: counts the number of nodes per unit distance along the direction of travel

\[ k = \frac{2\pi}{\lambda_x} \ast \vec{x} = k_x \ast \vec{x} \text{ generally a vector} \]

Constant phase plane \( \omega t - k_x x = \text{constant} \) propagates at a velocity called "phase velocity"

\[ v_{ph} = \frac{dx}{dt} = \frac{\omega}{k_x} = \lambda_x f \]

For constant velocity (such as light \( v = c \)) we have \( \omega = c k_x \)
This is not true in general (in crystals, esp. for electrons \& phonons) which have "dispersion" \( \omega(k) \)

- Complex representation:

\[ \Psi = A e^{i(\omega t - k_x x)} \]

- Standing wave

Superposition of two waves in opposite directions with equal speed

\[ \Psi = A \left[ \sin(\omega t - k_x x) + \sin(\omega t + k_x x) \right] \]

\[ = 2A \cos(\omega t) \sin(k_x x) \]

Nodes where \( \Psi = 0 \) are fixed in space.

Ex: \( \Psi = 0 \) at \( x = 0 \) and \( x = D \)
\[ \sin \left( \frac{2\pi}{\lambda_n} D \right) = 0 \]

\[ D = \frac{n \lambda}{2} \quad (n = 1, 2, 3, 4, \ldots) \]

D is a multiple of half-wave length.

- Schrödinger Equation

Wave-particle duality \( E = h\omega \), \( \vec{p} = \hbar \vec{k} \)

\[ \psi = A e^{i(E\cdot\vec{r} - \omega t)} = A e^{i(\vec{p}\cdot\vec{r} - E t)\hbar} \]

\[ \nabla \psi = \frac{i}{\hbar} \vec{p} \psi = \frac{i}{\hbar} \vec{p} A e^{i(\vec{p}\cdot\vec{r} - E t)\hbar} = \frac{i}{\hbar} \vec{p} \psi \]

\[ \Rightarrow \text{Define (postulate)} \quad \rho = \frac{\hbar}{i} \nabla \psi \]

where the gradient operator is

\[ \vec{D} = \frac{\hbar}{2x} \frac{\partial}{\partial x} + \frac{i}{2\hbar} \left( \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right) \]

\[ \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi e^{i(\vec{p}\cdot\vec{r} - E t)\hbar} = -\frac{iE}{\hbar} \psi \]

\[ \Rightarrow E = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} \]

Total energy is kinetic + potential \( \rightarrow \)
\[ E = \frac{1}{2} m v^2 + U = \frac{p \cdot p}{2m} + U \]

\[ \frac{p \cdot p}{2m} \Psi + V \Psi = E \Psi \]

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi = i\hbar \frac{\partial \Psi}{\partial t} \]

\[ \Rightarrow \text{Hamiltonian} \quad H = \frac{\hat{p} \cdot \hat{p}}{2m} + U \]

Laplacian : 
\[ \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \]

Time independent Schrödinger Eqn:
\[ H \Psi = E \Psi \]

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi + (U - E) \Psi = 0 \]

- Normalization Condition
\[ \begin{align*}
\text{1D} & & \int_{-\infty}^{\infty} \Psi^* \Psi \, dx = 1 \\
\text{3D} & & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* \Psi \, d^3r = 1
\end{align*} \]
Expectation of an operator

\[ \langle H \rangle = \int_{-\infty}^{\infty} \psi^* H \psi \, dx \]

3D \[ \langle H \rangle = \iiint \psi^* H \psi \, d^3r \]

Standard deviation

\[ \Delta H = \int \left( \psi^* H^2 - \langle H \rangle^2 \right) \psi \, dx \]

Satisifies \[ \Delta E \cdot \Delta x \geq \hbar/2 \quad \Delta p \cdot \Delta x \geq \hbar/2 \]

1D Potential Well

\[ V = 0 \quad \text{for} \quad 0 < x < D \quad \text{and} \quad V = \infty \quad \text{elsewhere} \]

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + (U - E) \psi = 0 \]

BC \[ \psi(0) = 0, \quad \psi(D) = 0 \]

Solution: \[ \psi = A \exp \left[ -i \frac{\sqrt{2mE}}{\hbar} x \right] + B \exp \left[ i \frac{\sqrt{2mE}}{\hbar} x \right] \]

\[ \text{for} \quad 0 < x < D, \quad 0 \text{ elsewhere} \]
Apply BCs: at $x=0$ we have $A+B=0$

at $x=0$:

$$A \exp \left[-i D \sqrt{\frac{2mE}{\hbar}} \right] + B \exp \left[i D \sqrt{\frac{2mE}{\hbar}} \right] = 0$$

$$\sin \left(D \sqrt{\frac{2mE}{\hbar}} \right) = 0 \Rightarrow D \sqrt{\frac{2mE}{\hbar}} = n\pi$$

so that

$$E_n = \frac{1}{2m} \left( \frac{n \pi \hbar}{D} \right)^2 \quad (n=1,2,3,\ldots)$$

Q: Why is $n=0$ not a solution?

- $n$ is called a quantum number.

Normalizing $\int x_n x_n^* \, dx = 1$

gives:

$$x_n = \sqrt{\frac{2}{D}} \sin \left( \frac{n\pi x}{D} \right)$$

Example

Q: What is the solution for a finite potential well?

\[ V \]

\[ V \]

\[ U=0 \]

\[ D \]

Answer: electron "leaks" out exponentially depending on the height of the $V$
Example: 2D potential well

\[ y = D \]

\[ \begin{array}{c}
\text{Inside the quantum well} \\
- \frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - E \psi(x, y) = 0
\end{array} \]

Separation of variables

\[ \psi(x, y) = X(x) Y(y) \] gives

\[ \frac{1}{X} \frac{d^2X}{dx^2} + \frac{1}{Y} \frac{d^2Y}{dy^2} + \frac{2mE}{\hbar^2} = 0 \]

Since \( E_{1m} > 0 \), set

\[ \frac{1}{X} \frac{d^2X}{dx^2} = -\lambda^2 \quad \frac{1}{Y} \frac{d^2Y}{dy^2} = -\beta^2 \]

which has solutions

\[ X(x) = A \sin(\lambda x) + B \cos(\lambda x) \]

Applying BCs: \( \psi(0) = 0 \), \( \psi(D) = 0 \) for \( x, y \)
\[ d = \frac{n \pi}{D} \quad \Rightarrow \quad x_n(x) = A_n \sin \left( \frac{n \pi x}{D} \right) \]
\[ \beta = \frac{m \pi}{D} \quad \Rightarrow \quad y_n(y) = B_m \sin \left( \frac{m \pi y}{D} \right) \]

Energy levels:
\[ E_{nm} = \frac{(n^2 + m^2) \pi^2 \hbar^2}{2mD^2} \]

\[ Y_{nm} = \frac{2}{D} \sin \left( \frac{n \pi x}{D} \right) \sin \left( \frac{m \pi y}{D} \right) \]

from normalization.

- Very useful solution used widely for silicon nanowires and other 1D systems

- Degeneracy: \( Y_{12} \neq Y_{21} \)
  but \( E_{12} = E_{21} \)

In 3D systems, many states (unique wave functions) have the same energy level — said to be degenerate.
Example 2: Harmonic Oscillator

Potential around equilibrium position $x_0$ is approximately quadratic.

$$U(x') = U(x_0) + \frac{1}{2} \left[ \frac{d^2 U}{dx'^2} \right] (x'-x_0)^2 + 0 \left[ (x'-x_0)^3 \right]$$

Around $x_0 \Rightarrow x' = x - x_0$

$$F = -\frac{dU}{dx} \Rightarrow F(x_0) = 0$$

$$F(x') = -K(x'-x_0) \quad \text{with} \quad K = \frac{d^2 U}{dx'^2} \bigg|_{x' = 0}$$

$$= -Kx \quad \text{for} \quad x = x' - x_0$$

- Schrödinger Equation for this system

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \left( \frac{Kx^2}{2} - E \right) \psi = 0$$

with BCs $\psi(x \to \infty) = \psi(x \to -\infty) = 0$
Solutions are

\[ E_n = (n + \frac{1}{2})\hbar \omega \quad (n = 0, 1, 2, \ldots) \]

\[ \psi_n (x) = \left( \frac{1}{2^n n! \sqrt{\pi\hbar}} \right)^{1/2} H_n \left[ \left( \frac{\sqrt{m\omega x^2}}{\hbar} \right) \right] \times \exp \left( - \frac{\sqrt{m\omega x^2}}{2\hbar} \right) \]

where \( \omega = \sqrt{\frac{K}{m}} \) — same as the mass-spring system

*Energy is quantized in steps of two with \( E_0 = \frac{1}{2} \hbar \omega \) being "zero-point" energy, a consequence of the uncertainty principle*