Kinetic Energy Operator in Quantum Mechanics

The kinetic energy operator in one dimension is defined as:

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$

where:

- $\hbar$: Reduced Planck's constant.
- m: Mass of the particle.
- $\frac{d^2}{dx^2}$: The second derivative with respect to position, representing how the wavefunction $\psi(x)$ changes curvature.

In the **Schrödinger equation**, this operator appears as part of the Hamiltonian, which governs the total energy of the system:

$$\hat{H}\psi(x) = E\psi(x), \quad \hat{H} = \hat{T} + \hat{V},$$

where $\hat{T}$ is the kinetic energy operator, and $\hat{V}$ is the potential energy operator.

In the problem of the particle in a box with an infinite potential well, the potential energy $V(x)$ inside the box is zero. Thus, the Hamiltonian simplifies to:

Discretizing the Kinetic Energy Operator

To solve the Schrödinger equation numerically, we need to approximate the second derivative $\frac{d^2}{dx^2}$ using **finite difference methods**.

1. **Finite Difference Approximation**

The second derivative of a function $\psi(x)$ at a grid point x_i can be approximated using the central difference formula:

$$\left.\frac{d^2\psi}{dx^2}\right|_{x_i} \approx \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\Delta x^2},$$

where:

- $\psi_i = \psi(x_i)$ is the value of the wavefunction at the i-th grid point.
- Δx: Spacing between adjacent grid points.

This formula results in a **tridiagonal matrix** when applied to all grid points in the domain.

2. **Constructing the Laplacian Matrix**

The finite difference approximation for the second derivative leads to the **Laplacian operator** (a matrix representation of $\frac{d^2}{dx^2}$):

$$L = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -2 \end{bmatrix}.$$

Here:

- The main diagonal contains -2 (representing the $-2\psi_i$ term).
- The sub- and superdiagonals contain 1 (representing the ψ_{i-1} and ψ_{i+1} terms).

The second derivative of a function $\psi(x)$ is central to many physical problems, including the Schrödinger equation. Using the finite difference method, we approximate the second derivative at a point x_i as:

$$\left.\frac{d^2\psi}{dx^2}\right|_{x_i} \approx \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\Delta x^2}.$$

Here:

- ψ_{i-1}: The value of the function at the point to the **left** of x_i.
- ψ_i: The value of the function at x_i (the point of interest).
- ψ_{i+1}: The value of the function at the point to the **right** of x_i.
- Δx: The spacing between adjacent grid points.

This formula comes from a Taylor expansion around x_i and is accurate to second order ($O(\Delta x^2)$).

Representing the Second Derivative as a Matrix

For a discretized domain with N points, the second derivative operator is represented by a tridiagonal matrix acting on a vector of function values. Let's build this step by step.

1. **Matrix Form of the Second Derivative**

For a grid with N points, let $\psi = [\psi_1, \psi_2, \ldots, \psi_N]^T$ represent the wavefunction values at the grid points. The second derivative operator can be written as a matrix multiplication:

$$\frac{d^2\psi}{dx^2} \approx \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-1} \\ \psi_N \end{bmatrix}.$$

2. **Components of the Matrix**

- **Main Diagonal** (-2): Represents the $-2\psi_i$ term for each grid point.
- **Off-Diagonals** (1): Represent the ψ_{i-1} and ψ_{i+1} contributions from the neighboring points.
- **Boundary Conditions**: At the edges ($x = 0$ and $x = L$), the wavefunction $\psi(x)$ is zero for an infinite potential well. This means the boundary points are implicitly excluded from the matrix.