Finite square well

2 types of states:

1) $0 < E < V_0$ "bound" states

$$\psi(x) \rightarrow \begin{cases} A_+ e^{iK_1 x} + A_- e^{-iK_1 x}, & 0 < x < a \quad (K_1 = \sqrt{2m(E-V)/\hbar^2}) \\ B_+ e^{iK_2 x} + B_- e^{-iK_2 x}, & x < 0 \text{ or } x > a \quad (K_2 = \sqrt{2m(E-V)/\hbar^2} \rightarrow \text{imaginary}) \end{cases}$$

So bound states decay as $B_+ e^{iK_2 x}$ or $B_- e^{-iK_2 x}$ ($K_2 = \sqrt{2m(E-V)/\hbar^2}$) in "classically forbidden" region when $E < V_0$. (Only one coef is nonzero to maintain normalizable $\psi$)

2) $E > V_0$ "continuum" or "scattering" states

$$\psi(x) \rightarrow \begin{cases} A'_+ e^{iK_1 x} + A'_- e^{-iK_1 x}, & 0 < x < a \quad K_1 = \sqrt{2m(E)/\hbar^2} \\ B'_+ e^{iK_2 x} + B'_- e^{-iK_2 x}, & x < 0 \text{ or } x > a \quad K_2 = \sqrt{2m(E-V)/\hbar^2} \end{cases}$$

How to determine $A'$s and $B'$s to "stitch" wavefunction together?

$\Rightarrow$ We need boundary conditions!
Boundary Conditions

1. \( \psi(x) \) must be continuous at boundaries so \( \frac{d\psi}{dx} \) is finite. Then,

\[
J = \text{Im} \left\{ \frac{\hbar}{m} \psi^* \frac{d\psi}{dx} \right\}
\]
is finite + continuity holds.

2. \(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = (E-V) \psi\)

Suppose a boundary exists at \( x=0 \). Integrate from one side to the other:

\[
-\frac{\hbar^2}{2m} \left[ \int_{-\epsilon}^{0} \frac{d^2}{dx^2} \psi \, dx - \int_{0}^{\epsilon} (E-V) \psi \, dx \right] \xrightarrow{\epsilon \to 0} 0 \quad \text{for finite } V(x)
\]

By fundamental thm of Calculus, we then have:

\[
\left. \frac{d}{dx} \psi \right|_{x=-\epsilon} - \left. \frac{d}{dx} \psi \right|_{x=0} = 0 \quad \text{so} \quad \left. \frac{d}{dx} \psi \right|_{x=0} = \psi' \text{ is continuous at a boundary!}
\]

With these 2 boundary conditions per N interfaces, we need to solve a large system of \( 2N \) equations \( \rightarrow \) transcendental equations!

We can avoid this problem by numerically solving eigenvalues + eigenvectors!
Numerical Solution of time-independent Schrödinger Eqn

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x) \quad \Rightarrow \quad \hat{H} \psi = E \psi \]

"Hamiltonian"

Transform differential \( \hat{H} \) into matrix operator:

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) \rightarrow -\frac{\hbar^2}{2m \Delta x^2} \]

(just like classical operator!)

In actual calculations, I suggest the following system of units:

\[ h \sim 6.6 \times 10^{-16} \text{ eV s} \]
\[ m \sim 5 \times 10^{-5} \text{ eV/c}^2 \]
\[ C \sim 3 \times 10^{10} \text{ cm/s} \]
\[ \Delta x \sim 10^{-9} \text{ cm} \]
\[ N \sim \text{several hundred (matrix size)} \]

\[ \left[ \frac{\hbar^2}{2m \Delta x^2} \right] = \frac{eV^2 \Delta x^2}{e^2 \Delta x^2} = eV \]
Results: 1 nm-wide Infinite Quantum well

100 x 100 matrix Hamiltonian

**Figure 1**

1 nm-wide Infinite Quantum Well: particle density distribution from lowest-energy wavefunction.

\[ \propto \sin^2 k_n x \]

- Numerical 1st
- Numerical 2nd
- Analytic 1st
- Analytic 2nd

**Figure 2**

1 nm-wide Infinite Quantum Well: energy eigenvalues

\[ E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \]

Energy eigenvalue [eV]

Quantum number n
Results: 1 nm-wide, 1 eV-deep finite quantum well

**Figure 1**
Finite Quantum Well: 1 nm wide, 1 eV deep

**Figure 3**
Finite Quantum Well: Energy eigenvalues

Note:
- Bomb states localized to well!
- Exponential decay into "evanescent" "classically forbidden region!"
- Continuum states
- $E < 0$ "bound state!"