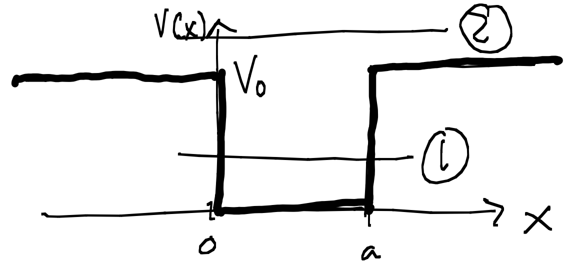
Finite square well



In each piecewise const. region,

$$\psi'' = -k^2 \psi$$

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}}, \quad V = 0 \text{ or } V_0$$

2 types of states:

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

$$\psi(x) \rightarrow \begin{cases} A_+ e^{+ik_1 x} + A_- e^{-ik_1 x}, & 0 < x < a \quad \left(k_1 = \sqrt{\frac{2mE}{\hbar^2}}\right) \\ B_+ e^{+ik_2 x} + B_- e^{-ik_2 x}, & x < 0 \text{ or } x > a \quad \left(k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \rightarrow \text{imaginary!}\right) \end{cases}$$

So bound states decay as $B_+ e^{+\kappa_2 x}$ or $B_- e^{-\kappa_2 x}$ $\left(\kappa_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\right)$ in "classically forbidden" region where $E < V_0$. (Only one coef is nonzero to maintain normalizable ψ)

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

$$\psi(x) \rightarrow \begin{cases} A'_+ e^{ik_1 x} + A'_- e^{-ik_1 x}, & 0 < x < a, \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ B'_+ e^{ik_2 x} + B'_- e^{-ik_2 x}, & x < 0 \text{ or } x > a \quad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \end{cases}$$

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

$\Longrightarrow$ We need Boundary conditions!

Boundary Conditions

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

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

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

Suppose a boundary exists @ $x=0$. Integrate from one side to the other:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2}{dx^2}\varphi\,dx = \int_{-\epsilon}^{\epsilon}(E-V)\varphi\,dx \xrightarrow{\lim_{\epsilon\to 0}} 0 \quad \text{for finite } V(x)$$

By fundamental Thm of Calculus, we then have:

$$\left.\frac{d}{dx}\varphi\right|_{x=\epsilon} - \left.\frac{d}{dx}\varphi\right|_{x=-\epsilon} = 0$$ so $\frac{d}{dx}\varphi \equiv \varphi'$ 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

$$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]}_{\text{"Hamiltonian"}}\psi(x) = E\psi(x) \Longrightarrow \hat{H}\psi = E\psi$$

Transform differential $\hat{H}$ into matrix operator:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \longrightarrow \frac{-\hbar^2}{2m\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & & \\ 1 & -2 & 1 & & & \\ 0 & 1 & -2 & 1 & & \\ \vdots & & 1 & -2 & 1 & \\ \vdots & & & & \ddots & \\ & & & & & \ddots \end{bmatrix}\begin{bmatrix}\psi(x_1)\\ \psi(x_2)\\ \vdots \\ \vdots \end{bmatrix}$$

(just like classical operator!)

$$V(x)\psi(x) \longrightarrow \begin{bmatrix} V(x_1) & 0 & \cdots & \\ 0 & V(x_2) & & \\ \vdots & & \ddots & \\ & & & \ddots \end{bmatrix}\begin{bmatrix}\psi(x_1)\\ \psi(x_2)\\ \vdots \\ \vdots \end{bmatrix}$$

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

$\hbar \sim 6.6\times10^{-16}\ eV\cdot s$

$m \sim 5\times10^{5}\ eV/c^2$

$c \sim 3\times10^{10}\ cm/s$

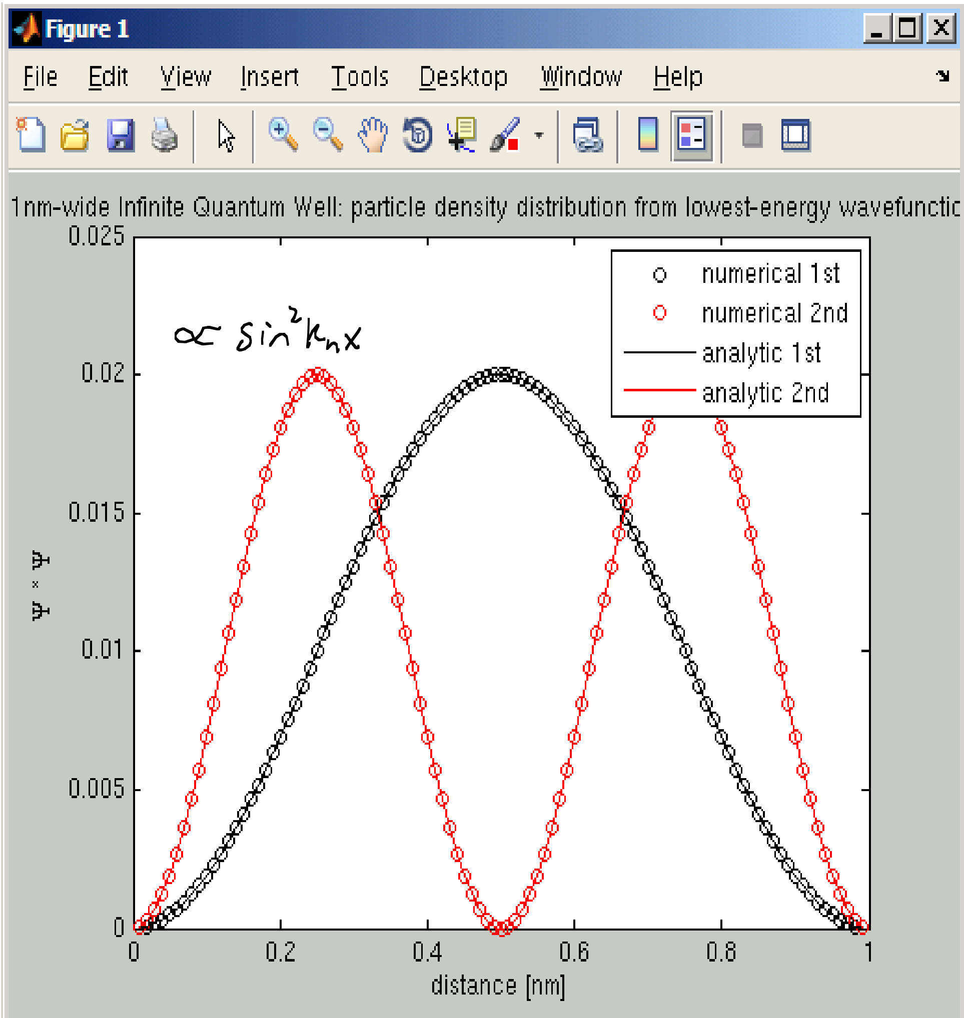
$\Delta x \sim 10^{-9}\ cm$

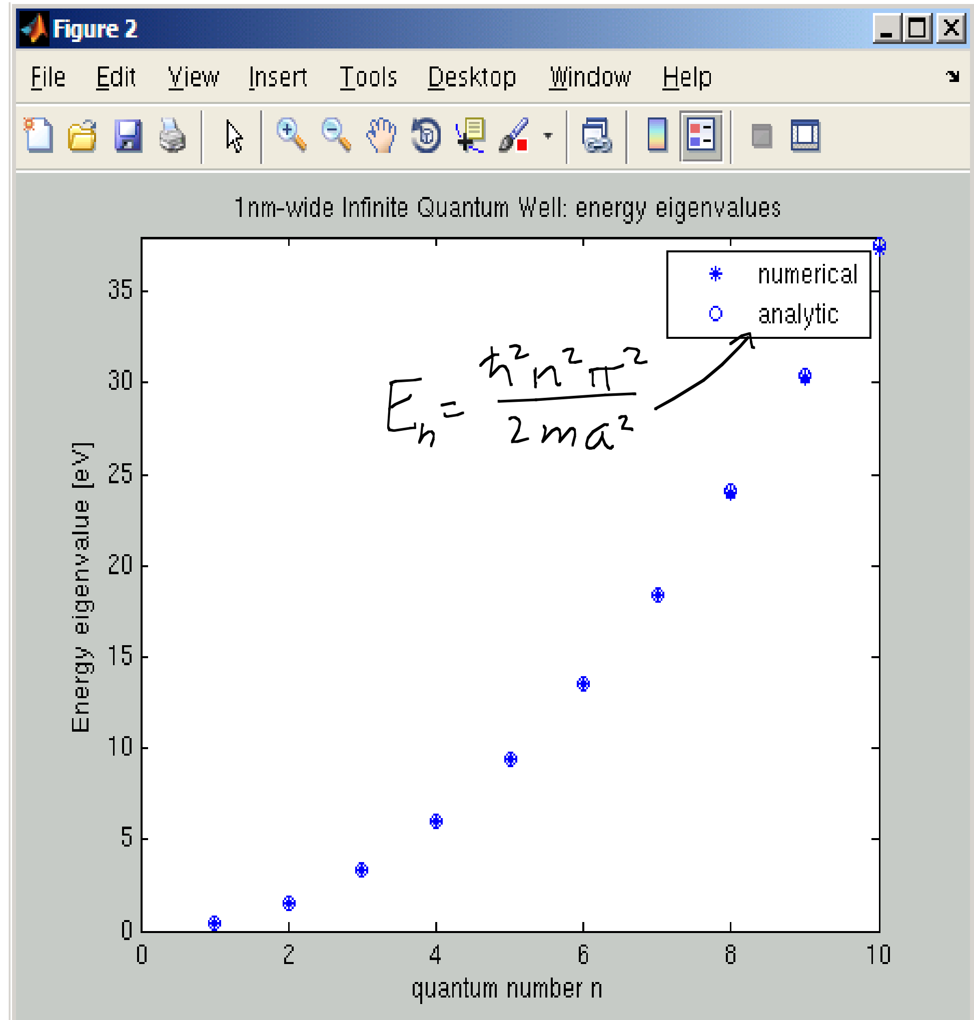
$N \sim$ several hundred
(matrix size)

$$\left[\frac{\hbar^2}{2m\Delta x^2}\right] = \frac{eV^{\cancel{2}}\cdot \cancel{s^2}}{\cancel{eV}\frac{\cancel{s^2}}{\cancel{cm^2}}\cancel{cm^2}} = eV!$$

Results: 1nm-wide Infinite Quantum well

100 x 100 matrix Hamiltonian





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