Lecture1:
Eigen solver

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Today's goal

- Understand the Schrodinger equation.
  - Compare your simulation results with the analytic solution.
- First exposure to the discretization

Infinite potential well (1)

- A particle in the infinite potential well
  - Schrödinger equation in this example

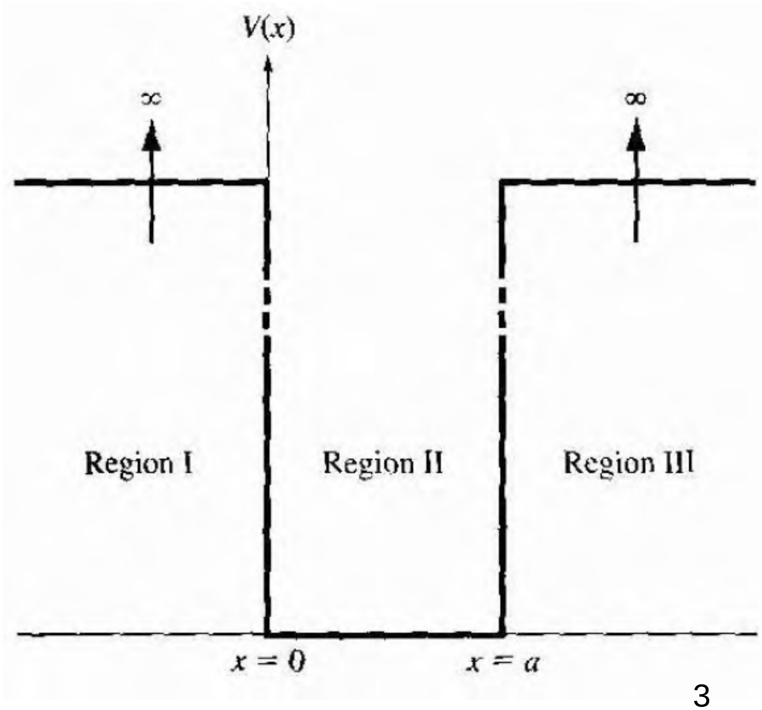
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x), \qquad 0 < x < a$$

  - Boundary conditions:

$$\psi(0) = \psi(a) = 0$$

  - It's an eigenvalue problem.

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)$$



Infinite potential well (2)

- Sine and cosine functions can be solutions.

$$\psi(x) = A_1 \cos kx + A_2 \sin kx$$

  - Cosine term cannot satisfy the boundary condition at $x = 0$.

$$\psi(a) = A_2 \sin ka = 0$$

  - Then, we have

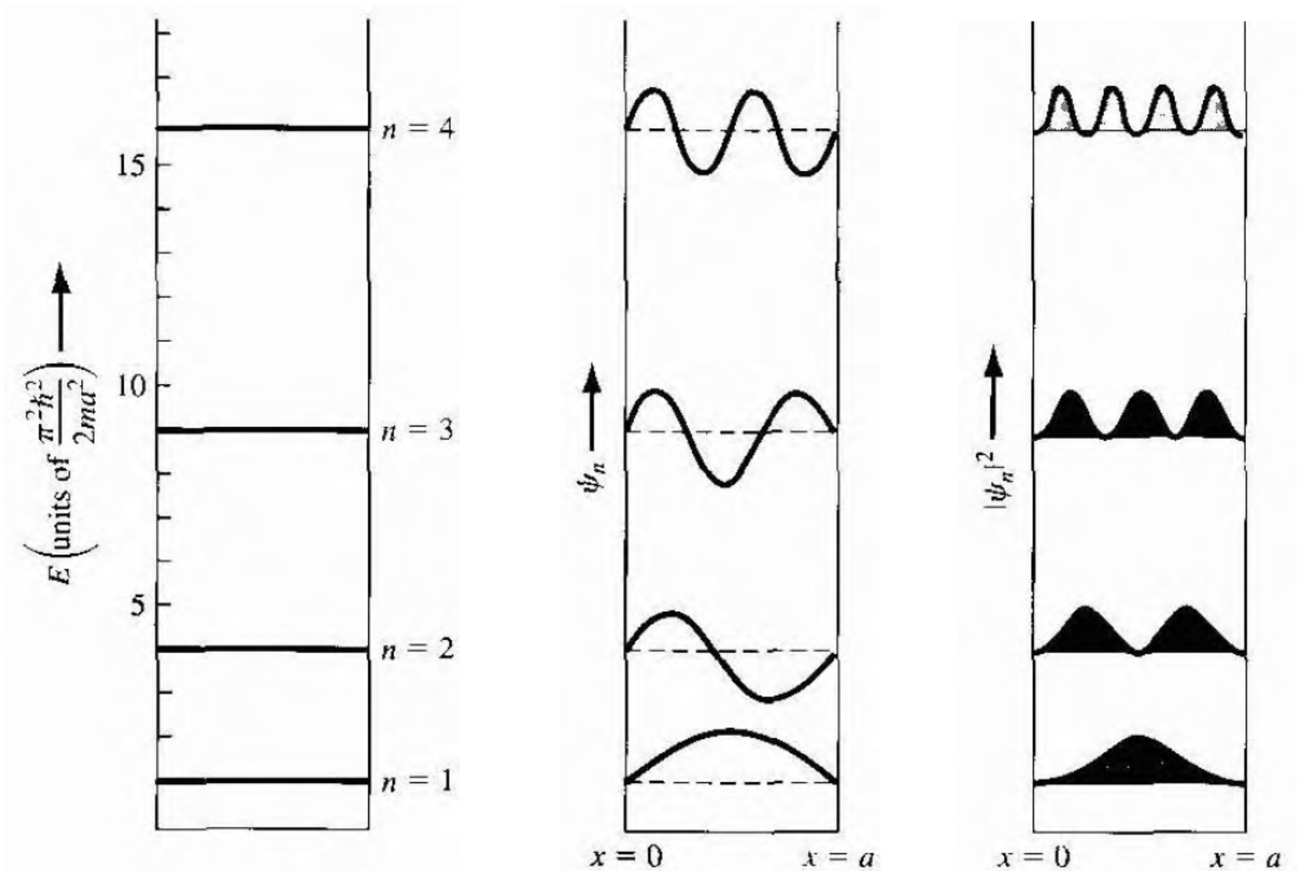
$$ka = \pi n$$

An integer

  - Therefore, allowed values of k are quantized.

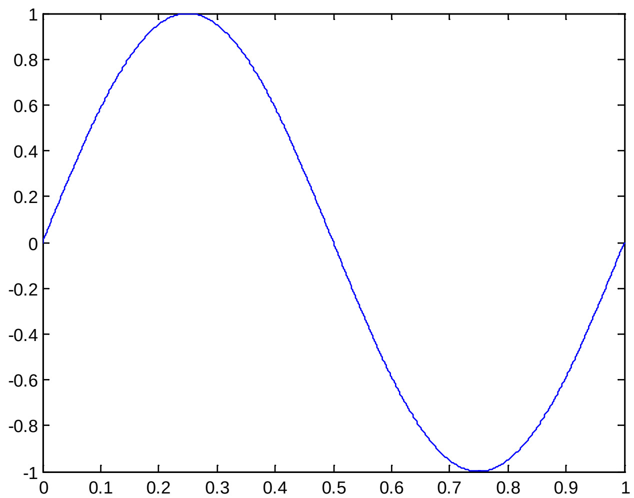
Infinite potential well (3)

- Energy levels
  - Total energy is written as $E_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$

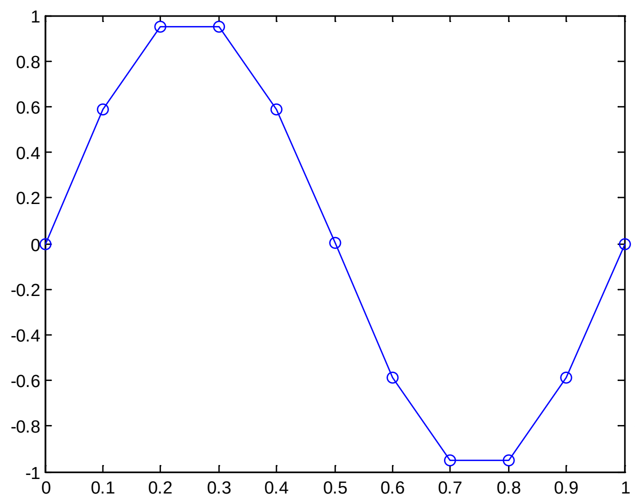


How to solve it numerically

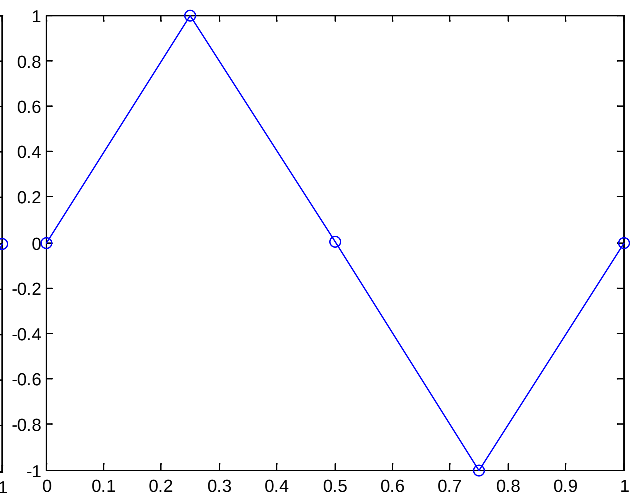
- In principle, we have to know $\psi(x)$ at any point.
  - Of course, we cannot do that. (Limited computer memory)
  - "Smoothness" should be assumed.
  - Example) A sine function



1000 points per period



10 points per period



4 points per period

Discretization

- Let us assume that we have N points.
  - Unformly distributed, therefore,

$$x_i = \frac{i-1}{N-1} a = (i-1)\Delta x$$

  - Then, 1st and Nth points are boundaries.

$$\psi(x_1) = 0, \qquad \psi(x_N) = 0$$

  - All other points are not.
  - We need to solve the Schrodinger equation.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x), \qquad 0 < x < a$$

Second derivative

- Discretization of the second derivative
  - For a uniformly spaced grid,

$$\left.\frac{d^2\psi}{dx^2}\right|_{x=x_i} \approx \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{\Delta x^2}$$

  - With the above approximation, the Schrodinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{\Delta x^2} = E\psi(x_i)$$

Matrix form

- In a matrix form,
  - It is written as

$$-\frac{\hbar^2}{2m\Delta x^2}\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \cdots & \\ & & 1 & -2 \end{bmatrix}\begin{bmatrix} \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-1} \end{bmatrix} = E\begin{bmatrix} \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

Homework#1

- Due: September 6 (This Wednesday)
- Solve the infinite potential well problem numerically.
  - Compare your simulation results with the analytic solution.
  - Change the number of points, N. Observe the solution.