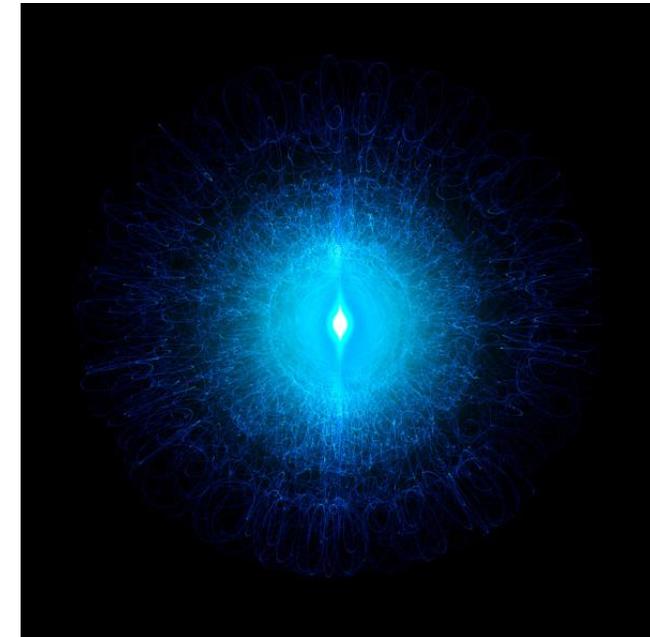
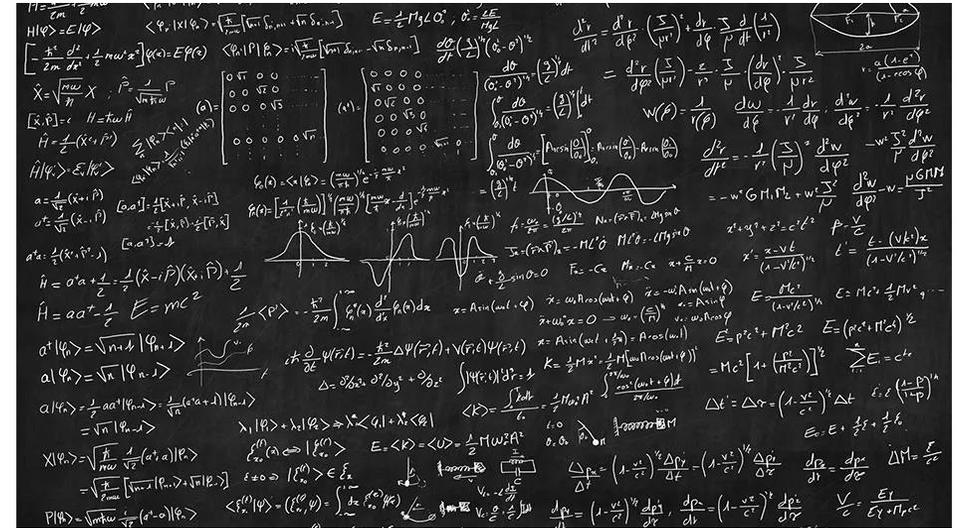


PARTÍCULA NUMA CAIXA

Equação de Schrödinger

Índice

- Significado físico da equação
- Definição do problema
- Resolução da equação analiticamente
- Porque é que queremos usar o computador?
- Método
- Conclusão



Significado físico da equação

Constante de Planck reduzida

Segunda derivada da função de onda

$$\frac{\hbar^2 d^2 \psi(x)}{2m dx^2} + V(x)\psi(x) = E\psi(x)$$

Energia Cinética

Energia Potencial

Energia Total

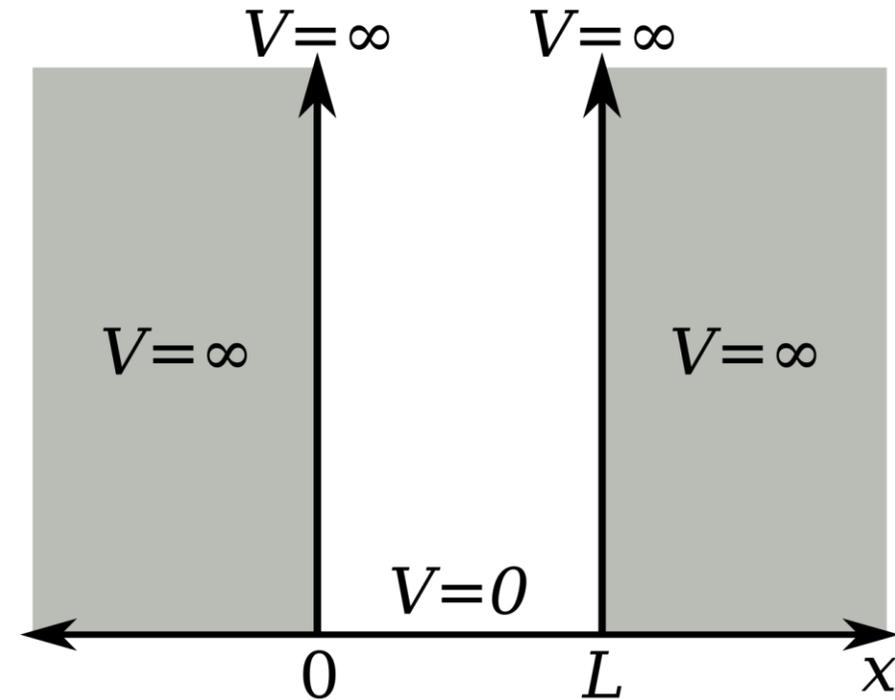
The diagram illustrates the physical meaning of the Schrödinger equation. It shows the equation $\frac{\hbar^2 d^2 \psi(x)}{2m dx^2} + V(x)\psi(x) = E\psi(x)$ with three boxed terms. The first term, $\frac{\hbar^2 d^2 \psi(x)}{2m dx^2}$, is labeled 'Energia Cinética' (Kinetic Energy) with an arrow pointing from the label below to the term. The second term, $V(x)\psi(x)$, is labeled 'Energia Potencial' (Potential Energy) with an arrow pointing from the label below to the term. The third term, $E\psi(x)$, is labeled 'Energia Total' (Total Energy) with an arrow pointing from the label below to the term. Above the equation, two labels with arrows point to the first two terms: 'Constante de Planck reduzida' (Reduced Planck constant) points to \hbar^2 , and 'Segunda derivada da função de onda' (Second derivative of the wave function) points to $d^2 \psi(x)$.

Definição do problema

Função de onda

- $\Psi(x)$ é contínua
- $\frac{d}{dx} \Psi(x)$ é contínua
- $\int_0^L |\Psi(x)|^2 dx = 1$

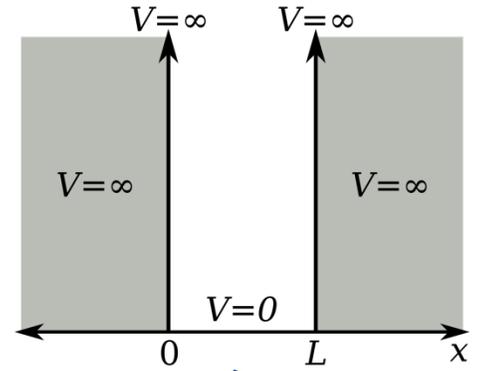
Como definir a caixa matematicamente



Resolução da Equação Analiticamente

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

$$\frac{d^2\psi(x)}{dx^2} = -E'\psi(x)$$



$$\psi(x) = a \cos(kx) + b \sin(kx)$$

Condições de fronteira

$$\begin{cases} \psi(0^+) = \psi(0^-) \Rightarrow a = 0 \\ \psi(L^+) = \psi(L^-) \Rightarrow E_n = \frac{\hbar^2}{2m} \left(\frac{\pi n}{L}\right)^2, n \in \mathbb{N} \end{cases}$$

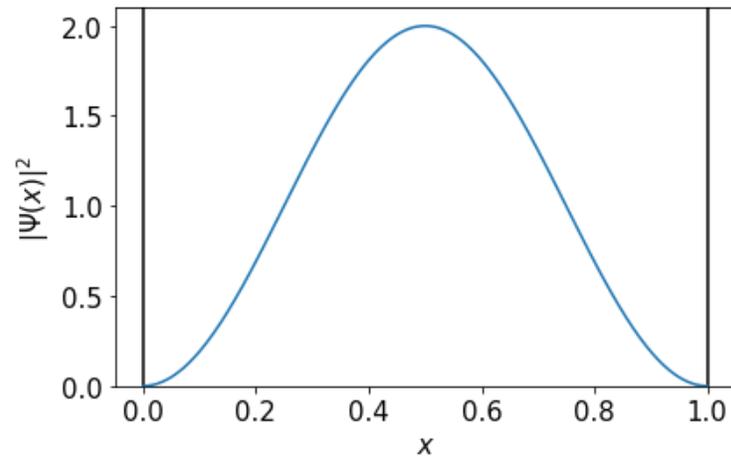
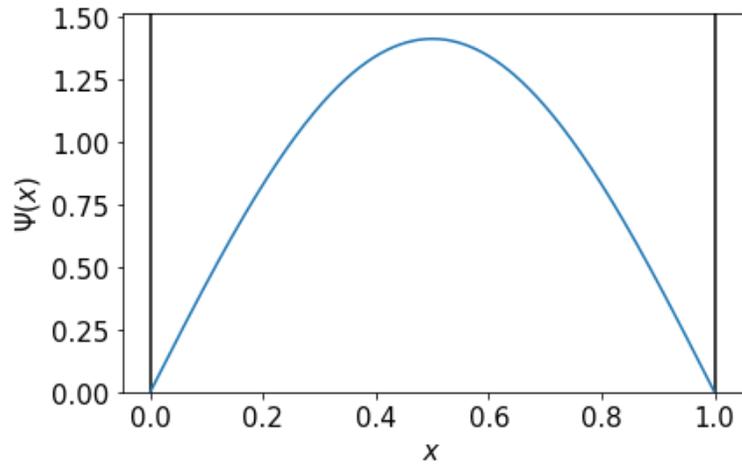
Quantização da Energia

Normalização da função de onda

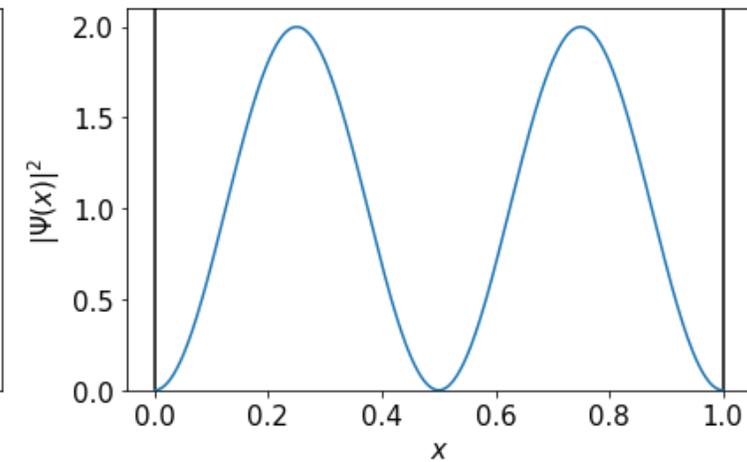
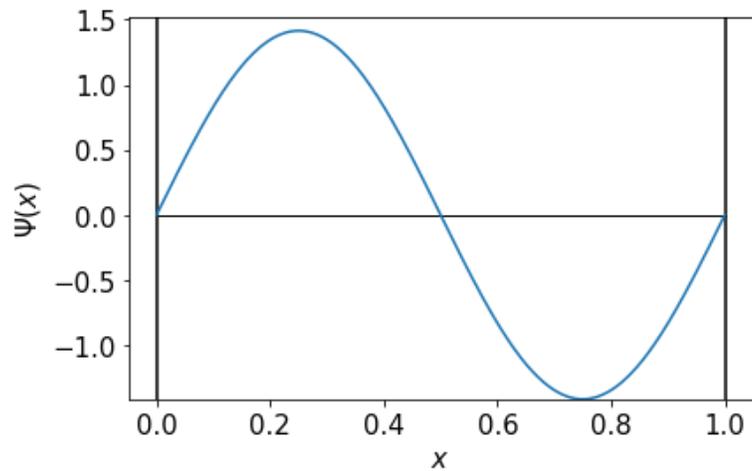
$$\int_0^L |\psi(x)|^2 dx = 1$$

$$\psi(x) = \begin{cases} 0, \text{ fora da caixa} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n}{L} x\right) \end{cases}$$

Gráficos



**Estado fundamental
n=1**



**1° estado excitado
n=2**



nodo

Porque é que queremos usar o computador?



Método

Discretizar as derivadas:

$$\frac{d\Psi}{dx} = \frac{1}{2\Delta x} [\Psi_{n+1} + \Psi_{n-1}]$$



$$\frac{d^2\Psi}{dx^2} = \frac{1}{2\Delta x^2} [\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n]$$

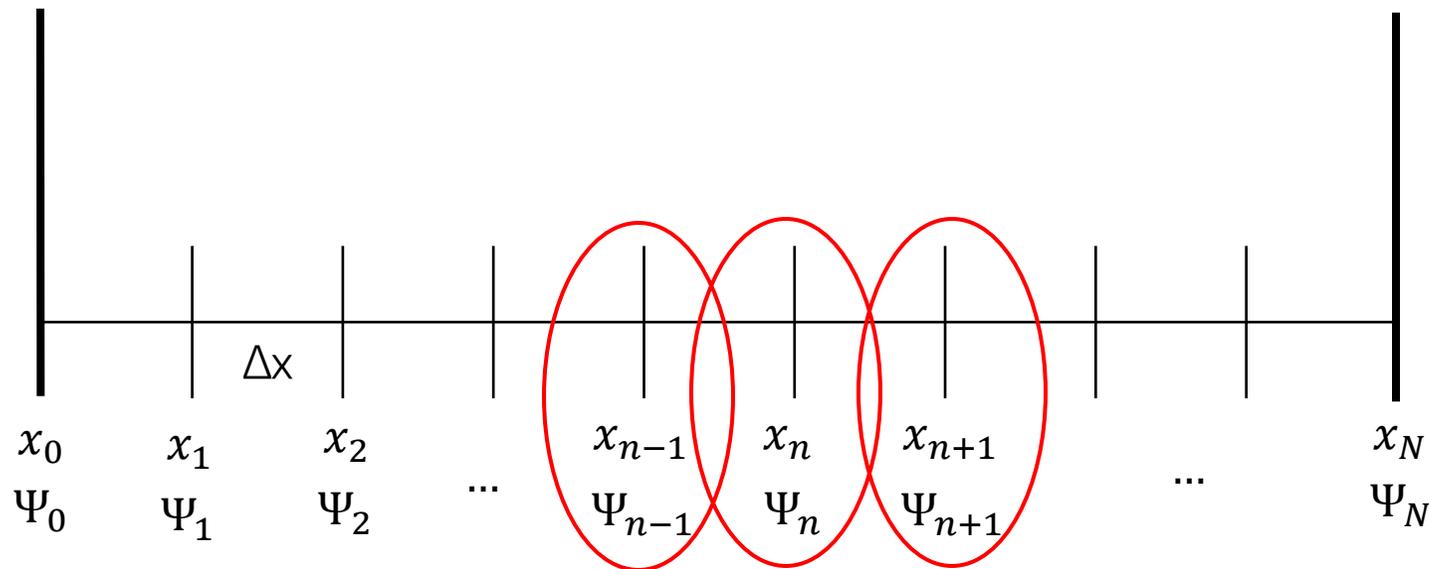


$$\frac{d^2\psi(x)}{dx^2} = -E'\psi(x)$$

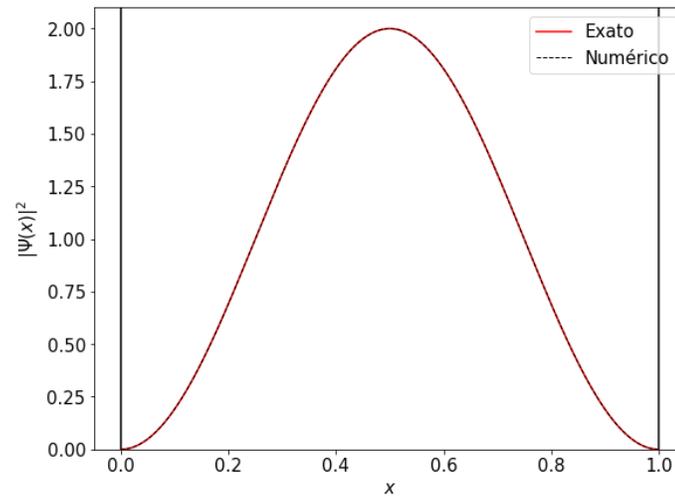
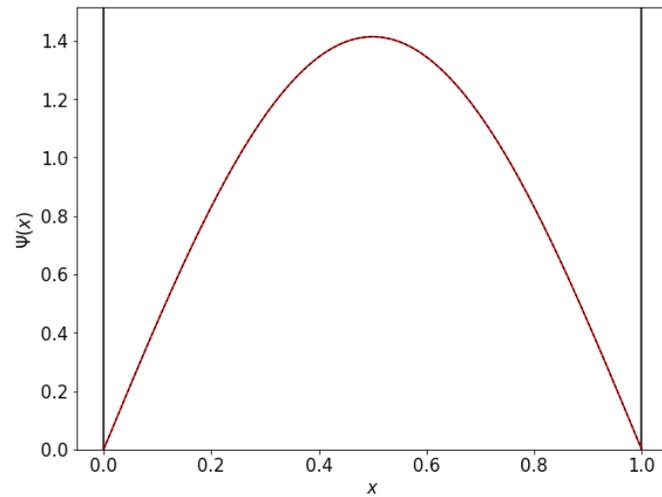


$$\Psi_{n+1} = 2\left[1 - \frac{2mE_m}{\hbar^2}\right] \Psi_n - \Psi_{n-1}$$

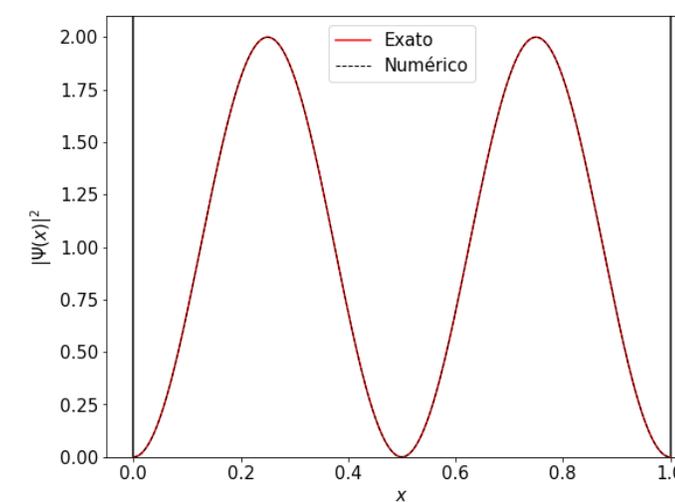
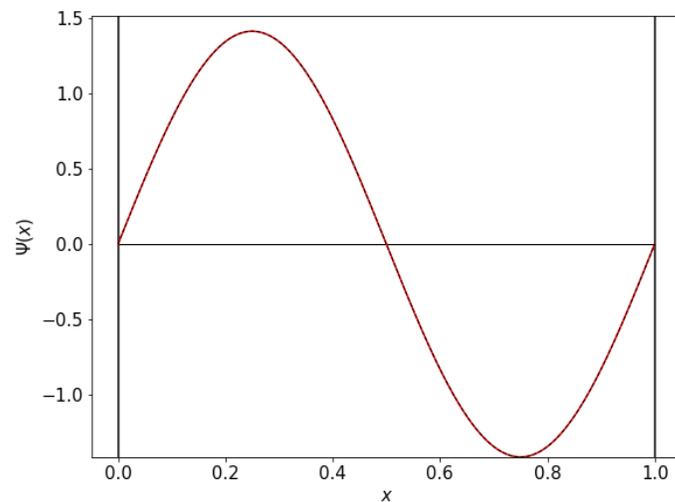
$$\begin{aligned} \Psi_0 &= 0 \\ \Psi_1 &= 1 \end{aligned}$$



Aplicação do método



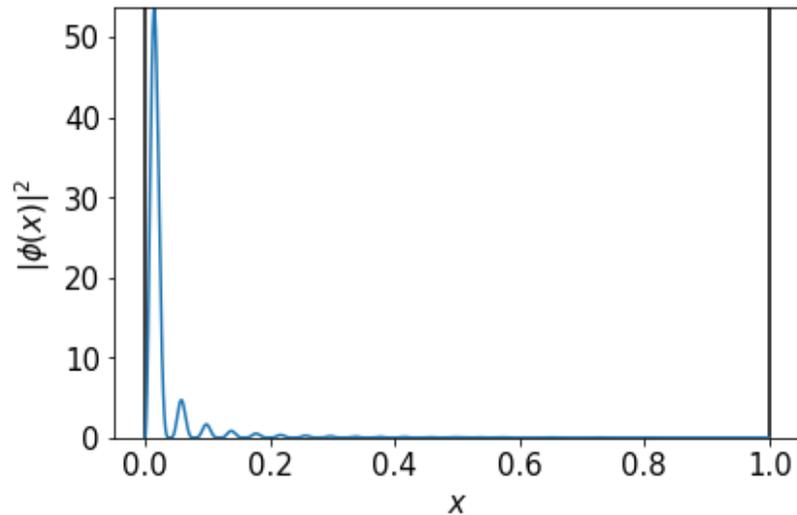
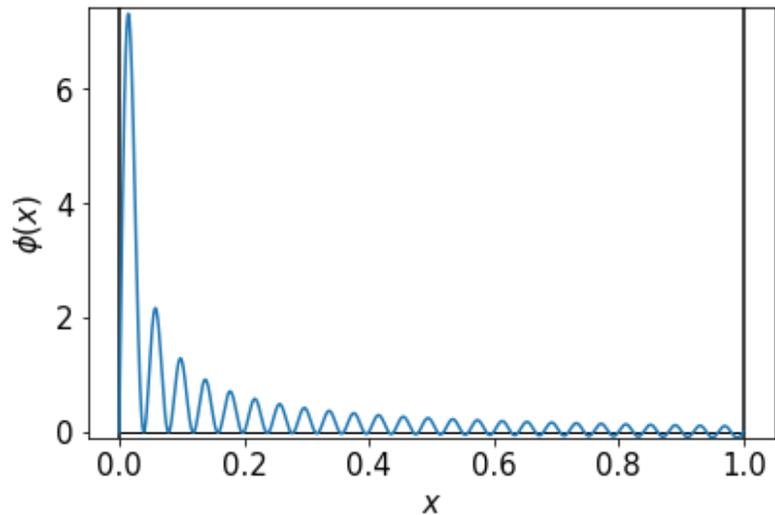
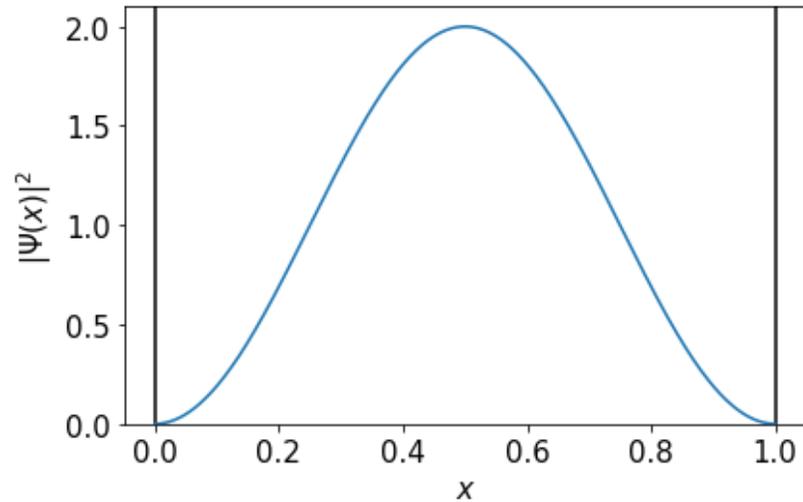
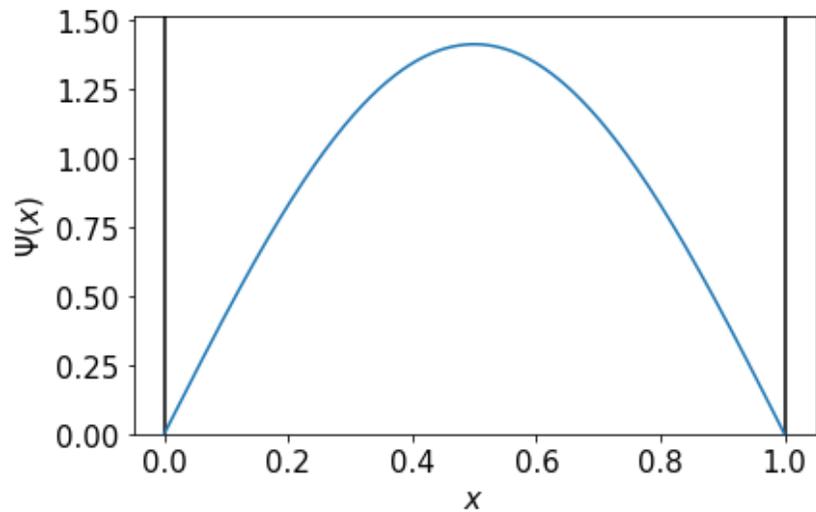
Comparação dos resultados



Curvas sobrepostas



Princípio de incerteza de Heisenberg



Não sabemos a posição



$$E = \frac{\hbar^2 \pi^2}{2m L^2}$$

Sabemos a posição



$$\varphi(x) = \frac{1}{\sqrt{N}} \sum_{n=1}^N \Psi_n(x)$$

CONCLUSÃO
