

Example (to go with Mathematica ~~is demo~~)



$$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Initial particle distribution:

step of width a in the center

$$\psi(x,t=0) = \begin{cases} A & \frac{L-a}{2} \leq x \leq \frac{L+a}{2} \\ 0 & \text{elsewhere} \end{cases}$$

$$\text{Normalization} \quad \int_{\frac{L-a}{2}}^{\frac{L+a}{2}} |\psi(x,t=0)|^2 dx = A \cdot a = 1 \Rightarrow A = 1/\sqrt{a}$$

$$\text{Decomposition} \quad \psi(x,t=0) = \sum_{n=1}^{\infty} c_n \psi_n = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$c_n = \int_0^L \psi(x,t=0) \psi_n(x) dx = \int_{\frac{L-a}{2}}^{\frac{L+a}{2}} \frac{1}{\sqrt{a}} \cdot \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} dx =$$

$$= \sqrt{\frac{2}{aL}} \frac{L}{\pi n} \left[\cos \left(\frac{n\pi}{2} - \frac{n\pi a}{2L} \right) - \cos \left(\frac{n\pi}{2} + \frac{n\pi a}{2L} \right) \right] = \sqrt{\frac{2}{aL}} \frac{2L}{\pi n} \sin \frac{n\pi a}{2L} \sin \frac{n\pi a}{2L}$$

(note: even states don't contribute due to the symmetry!)

$$\psi(x,t=0) = \sum_{n=1}^{\infty} \frac{1}{\sqrt{a}} \frac{4}{\pi n} \sin \frac{n\pi}{2} \sin \frac{n\pi a}{2L} \sin \frac{n\pi x}{L}$$

(if you want to be fancy $n \rightarrow 2k+1$)

$$\sin \frac{\pi n}{2} = \sin(\pi k + \frac{\pi}{2}) = (-1)^k$$

$$\psi(x,t=0) = \sum_{k=0}^{\infty} \frac{1}{\sqrt{a}} (-1)^k \frac{4}{\pi(2k+1)} \sin \frac{\pi(2k+1)a}{2L} \times$$

$$\times \sin \frac{\pi(2k+1)x}{L}$$

Time evolution

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} =$$

$$= \sum_{n=1}^{\infty} \frac{1}{\sqrt{a}} \frac{4}{\pi n} \sin \frac{n\pi}{2} \sin \frac{n\pi a}{2L} \sin \frac{n\pi x}{L} e^{-iE_n t/\hbar}$$

The exact solution requires infinite number of states. The more you include, the more accurate it is.