Particle in a Box

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$|\leftarrow \quad a \quad \rightarrow|$

$\mathcal{H}\Psi = E\,\Psi$

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

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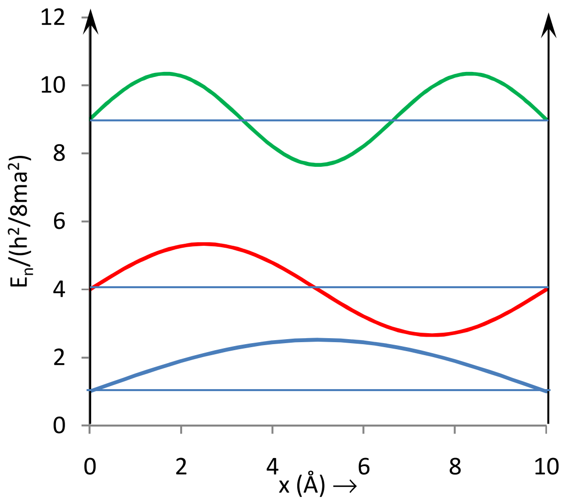
for $0 \le x \le a$



A sin kx : $\frac{d\Psi}{dx} = A\,k\cos kx$ $\qquad$ $\frac{d^2\Psi}{dx^2} = -A\,k^2\sin kx$

B cos kx : $\frac{d\Psi}{dx} = -B\,k\sin kx$ $\qquad$ $\frac{d^2\Psi}{dx^2} = -B\,k^2\cos kx$

LHS: $\qquad$ RHS:

$$\frac{-\hbar^2}{2m}(-A\,k^2\sin kx) = E\,A\sin kx$$

$$E = \frac{\hbar^2k^2}{2m} \qquad k = \frac{(2mE)^{1/2}}{\hbar}$$

General Solution: $\qquad \Psi(x) = A\sin kx + B\cos kx$

Boundary Conditions: at $x = 0$: $\Psi(x) = 0$ $\quad \cos(0) = 1$ so $B = 0$

at $x = a$: $\Psi(x) = 0$

$\Psi(a) = A\sin ka = 0 \qquad$ so $\quad k = n\pi/a$

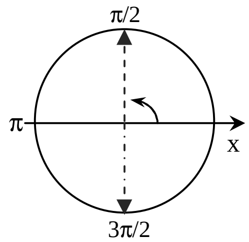
$n = 1 \qquad kx = \frac{n\pi x}{a}$ at a: $\qquad ka = \pi$

$n = 2 \qquad\qquad ka = 2\pi$

$$E = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

cos π/2 = 0
sin π/2 = 1

cos π = -1
sin π = 0



cos 0 = 1
sin 0 = 0
cos 2π = 1
sin 2π = 0

cos 3π/2 = 0
sin 3π/2 = -1

Normalization $\quad \int_{-\infty}^{\infty} \Psi^2\,dx = 1$

$$= A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$ for particle in the box.

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let $y = \frac{n\pi x}{a}$ then $\frac{dy}{dx} = \frac{n\pi}{a}$ and rearranging gives $x = \frac{a}{n\pi} y$ and $dx = \frac{a}{n\pi} dy$
and when x = 0 to a, then y = 0 to nπ.

Substituting to change variables gives:

$$A^2 \left(\frac{a}{n\pi}\right) \int_0^{n\pi} \sin^2(y)\, dy = 1$$

Looking up the integral in the CRC: $\int \sin^2(x)\, dx = -\tfrac{1}{2} \sin x \cos x + \tfrac{1}{2} x$

Substituting gives:

$$A^2 \left(\frac{a}{n\pi}\right) \left(-\tfrac{1}{2} \sin y \cos y + \tfrac{1}{2} y \right|_0^{n\pi} = 1$$

Note that sin(0) = 0 and sin(nπ)=0.
Evaluating the result at the endpoints gives:

$$A^2 \left(\frac{a}{n\pi}\right)\left(\frac{n\pi}{2}\right) = A^2 \frac{a}{2} = 1$$

$$A = \left(\frac{2}{a}\right)^{1/2}$$

$$\Psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$$