Infinite square well in 1D, part 3.

$$\psi(x) = A \cdot \sin(kx)$$

$$\underbrace{\psi(x=0)=0}_{\text{condition \#1}} \quad \text{and} \quad \underbrace{\psi(x=L)=0}_{\text{condition \#2}}$$

Condition #1 is always true for sine functions.

Condition #2 means:

$\psi(x=L) = A \cdot \sin(kL) = 0$ which leads to

$kL = n \cdot \pi$ where $n = 1, 2, 3, \ldots$

$$k = \frac{n\pi}{L}$$

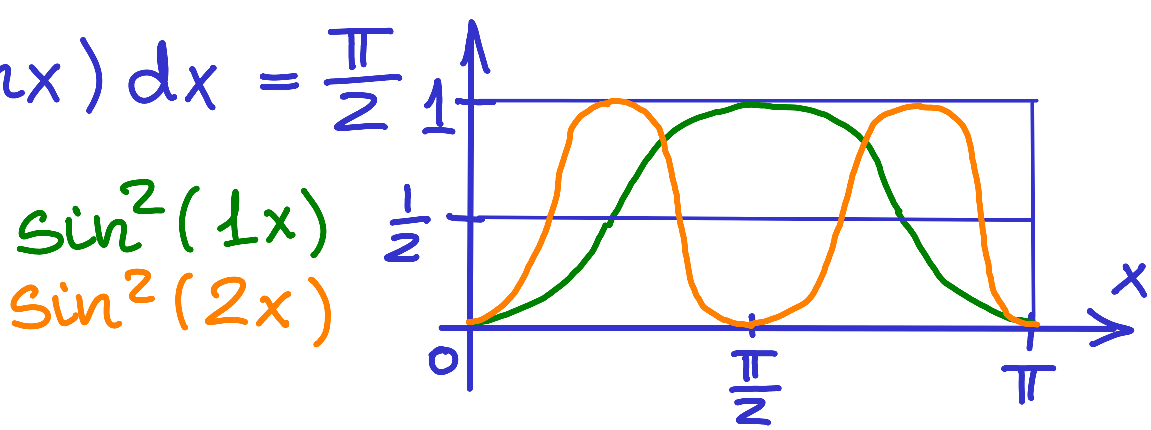
$$\boxed{\psi_n(x) = A \cdot \sin\left(\frac{n\pi x}{L}\right); \quad A = \sqrt{\frac{2}{L}}; \quad n = 1, 2, 3, \ldots}$$

Normalization:

$$1 = \int_0^L \rho_n(x)\,dx = \int_0^L \psi_n^*(x) \cdot \psi(x)\,dx = \int_0^L \psi_n^2(x)\,dx$$

$$1 = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \cdot \frac{L}{2}$$

$$\int_0^{\pi} \sin^2(nx)\,dx = \frac{\pi}{2}$$

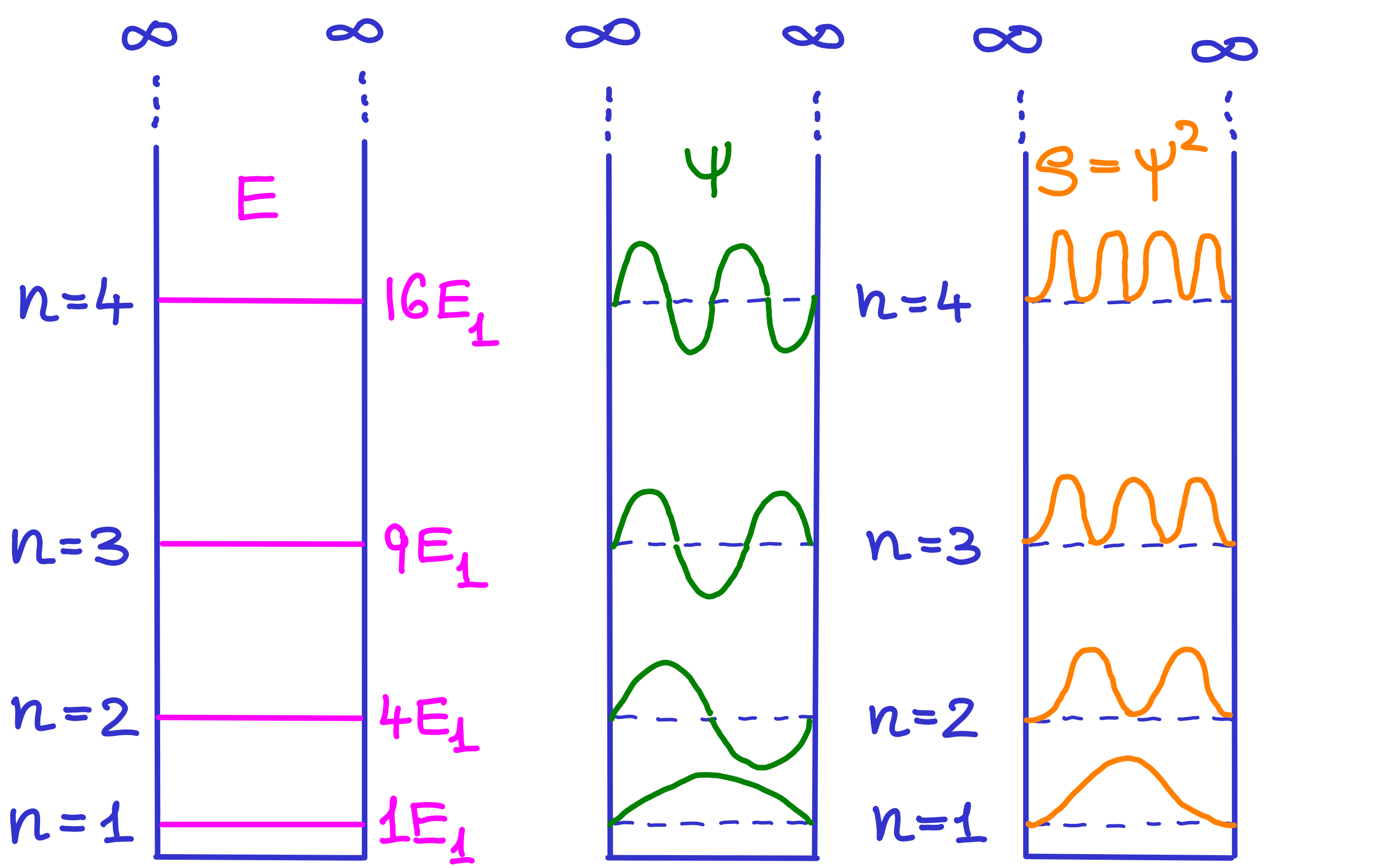


Infinite square well in 1D, part 4.

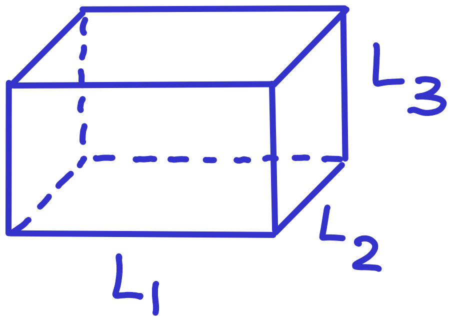
$$\left.\begin{aligned} k &= \frac{\sqrt{2mE}}{\hbar} \\ kL &= n\pi \end{aligned}\right\} \quad \frac{\sqrt{2mE}}{\hbar} L = n\pi$$

$$\boxed{E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 \frac{h^2}{8mL^2}}$$

Energy spectrum of the infinite square well : $\boxed{E_n \propto n^2 \, ; \; E_n = n^2 E_1 \, ; \; E_1 = \frac{h^2}{8mL^2}}$



Infinite potential well in 3D



The three coordinates x, y and z are independent.

$$\Psi(x,y,z) = A \cdot \sin(k_1 x) \cdot \sin(k_2 y) \cdot \sin(k_3 z)$$

$$k_1 = \frac{n_1 \pi}{L_1} \; ; \; k_2 = \frac{n_2 \pi}{L_2} \; ; \; k_3 = \frac{n_3 \pi}{L_3}$$

$n_1, n_2, n_3 = 1, 2, 3, \ldots$ independently

$$E_{n_1,n_2,n_3} = \frac{h^2}{8m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right)$$

Cubical box : $L_1 = L_2 = L_3 = L$

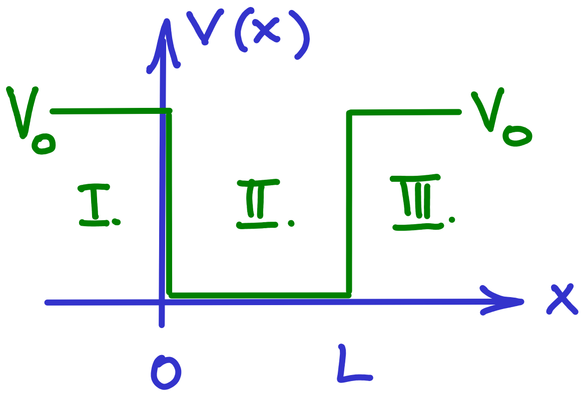
$$E_{n_1,n_2,n_3} = \frac{h^2}{8mL^2}\left(n_1^2 + n_2^2 + n_3^2\right)$$

Ground state: $E_{gs} = \frac{3h^2}{8mL^2}$

1st excited state: $E_{1st xs} = \frac{6h^2}{8mL^2}$

<u>Degeneracy</u>: several different states have the same energy: (2, 1, 1); (1, 2, 1); (1, 1, 2).

Finite square-well potential



$$V(x) = \begin{cases} V_0 & \text{if } x < 0 \\ 0 & \text{if } 0 \leq x \leq L \\ V_0 & \text{if } L < x \end{cases}$$

Regions I and III:

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} + V_0 \cdot \psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2} \cdot \psi$$

$$\frac{d^2\psi}{dx^2} = \alpha^2 \cdot \psi \; ; \quad \alpha^2 = \frac{2m(V_0 - E)}{\hbar} > 0$$

$$\psi_I = A \cdot e^{\alpha x} + \cancel{B \cdot e^{-\alpha x}} \; ; \quad \psi_{III} = \cancel{C \cdot e^{\alpha x}} + D \cdot e^{-\alpha x}$$

$\psi(x = -\infty) = 0$ $\quad$ $\psi(x = \infty) = 0$

Region II:

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \cdot \psi$$

$$\frac{d^2\psi}{dx^2} = -k^2 \cdot \psi \; ; \quad k^2 = \frac{2mE}{\hbar^2} > 0$$

$$\psi_{II} = E \cdot e^{ikx} + F \cdot e^{-ikx}$$

Finite square-well potential 2.

$$\sin(kx) = \frac{e^{ikx} - e^{-ikx}}{2i}$$

$$\cos(kx) = \frac{e^{ikx} + e^{-ikx}}{2}$$

$$e^{ikx} = \cos(kx) + i \cdot \sin(kx)$$

$$e^{-ikx} = \cos(kx) - i \cdot \sin(kx)$$