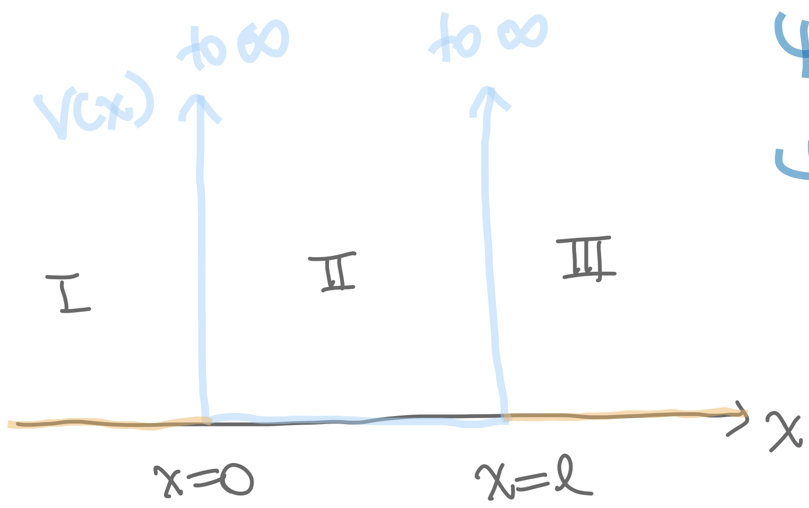
Lecture 3

Tuesday, September 17, 2024 11:31

Particle in a Box Continued



$\psi_I = 0$

$\psi_{III} = 0$

Last time:

$$\psi_{II} = A\cos\left[\frac{(2mE)^{\frac{1}{2}}}{\hbar}x\right] + B\sin\left[\frac{(2mE)^{\frac{1}{2}}}{\hbar}x\right]$$

To find A and B, we need to apply boundary conditions.

Condition: the wavefunction must be continuous.

$$\lim_{x\to 0}\psi_I = \lim_{x\to 0}\psi_{II}$$

$$0 = \lim_{x\to 0}\left\{A\cos\left[\frac{(2mE)^{\frac{1}{2}}}{\hbar}x\right] + \cancel{B\sin\left[\frac{(2mE)^{\frac{1}{2}}}{\hbar}x\right]}\right\}$$

$\cos 0 = 1$ $\quad\quad$ $\sin 0 = 0$

$$0 = A$$

$$\psi_{II} = B \sin\left[\frac{(2mE)^{\frac{1}{2}}}{\hbar} x\right] \qquad \hbar = \frac{h}{2\pi}$$

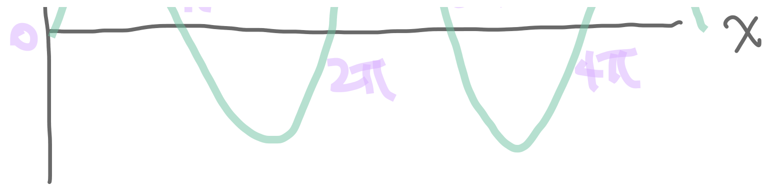
$$\psi_{II} = B \sin\left[\frac{2\pi (2mE)^{\frac{1}{2}}}{h} x\right]$$

$$\lim_{x \to l} \psi_{III} = \lim_{x \to l} \psi_{II}$$

$$0 = \lim_{x \to l} B \sin\left[\frac{2\pi (2mE)^{\frac{1}{2}}}{h} x\right]$$

We don't want to set B to zero: we would get a wavefunction that is everywhere zero — no particle!

Therefore, $\sin\left[\frac{2\pi (2mE)^{\frac{1}{2}}}{h} l\right] = 0$



$$\frac{2\cancel{\pi}(2mE)^{\frac{1}{2}}}{h}\ell = \boxed{\pm n\cancel{\pi}}$$

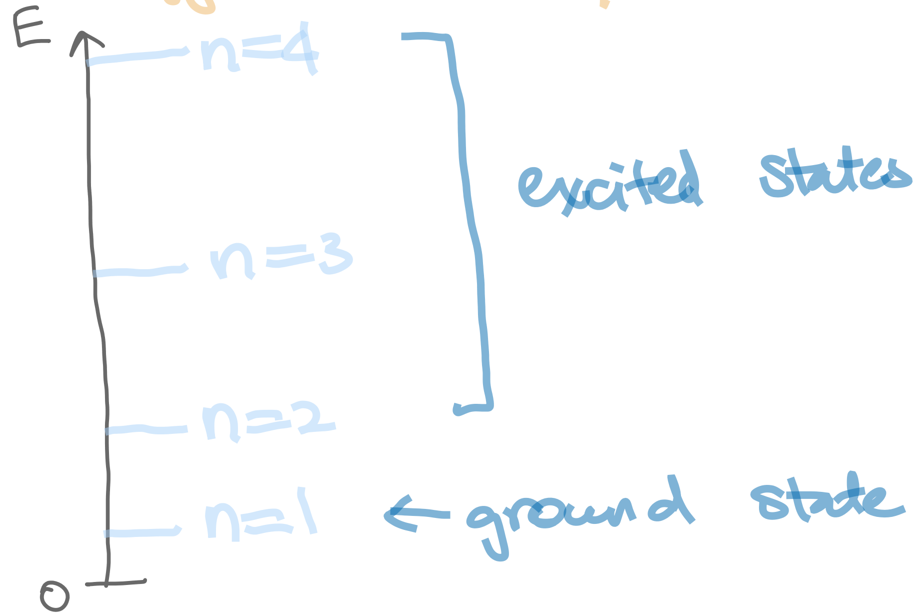
n cannot be 0 ; now, solve for E

$$(2mE)^{\frac{1}{2}} = \pm\frac{nh}{2\ell}$$

$$2mE = \frac{n^2h^2}{4\ell^2}$$

$$\boxed{E = \frac{n^2h^2}{8m\ell^2}\ , \ n = 1, 2, 3, \ldots}$$

the energy levels are quantized



Why can n not be 0 ?

If $n=0$, $E=0$

$$a = \pm i(2mE)^{\frac{1}{2}}/\hbar$$ ← previously found roots of auxiliary equation

We do not obtain two distinct roots.

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2mE}{\hbar^2}\psi_{II} = 0$$ Use original Schrödinger equation

$$\frac{d^2\psi_{II}}{dx^2} = 0$$

Integrate twice:

$$\frac{d\psi_{II}}{dx} = c \quad \text{and} \quad \psi_{II} = cx + d$$

$$\lim_{x\to 0}\psi_{I} = \lim_{x\to 0}\psi_{II}$$

$$0 = \lim_{x\to 0} cx + d, \quad d = 0$$

$$\lim_{x\to L}\psi_{III} = \lim_{x\to L}\psi_{II}$$

$x \to \ell \qquad\qquad x \to \ell$

$$0 = \lim_{x \to \ell} cx \quad , \quad c = 0$$

Empty box... n cannot be 0.

Compare to a classical system: zero energy simply means the particle is motionless inside the box. Also, no restriction on energy levels (non-quantized).

$$\psi_{II} = B \sin\left[\frac{2\pi}{h}(2mE)^{\frac{1}{2}} x\right]$$

$$\frac{2\pi}{h}(2mE)^{\frac{1}{2}} \ell = \boxed{\pm n\pi} \quad , \text{ when } \sin(x) = 0$$

$$\boxed{\psi_{II} = B \sin\left(\frac{n\pi x}{\ell}\right)}$$

$\sin(-x) = -\sin(x)$

$n = 1, 2, 3, \ldots$

Still need to find B!

$$\int_{-\infty}^{\infty} |\psi|^2 \, dx = 1$$

$$\underbrace{\int_{-\infty}^{0} |\psi_{I}|^2 dx}_{0} + \int_{0}^{l} |\psi_{II}|^2 dx + \underbrace{\int_{l}^{\infty} |\psi_{III}|^2 dx}_{0} = 1$$

$$\int_{0}^{l} |\psi_{II}|^2 dx = 1$$

$$|B|^2 \int_{0}^{l} \sin^2\left(\frac{n\pi x}{l}\right) dx = 1$$

Integral Table :

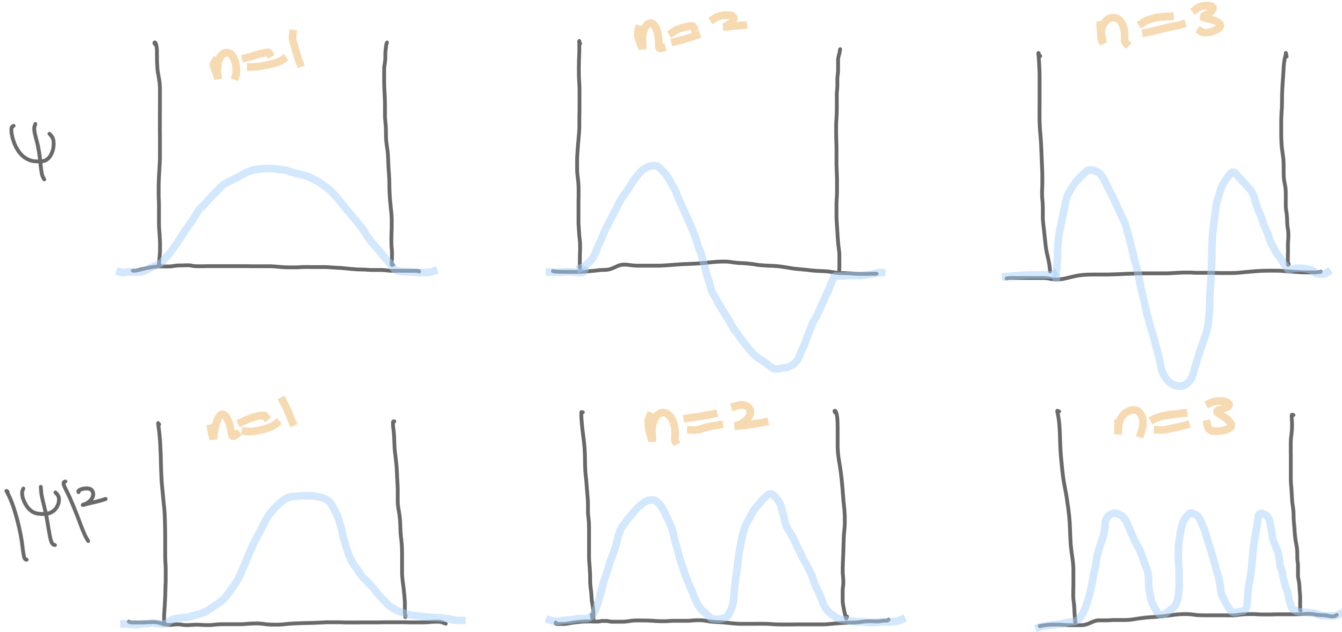
$$\int \sin^2(bx)dx = \frac{x}{2} - \frac{1}{4b}\sin(2bx)$$

$$|B|^2 \left[\frac{x}{2} - \frac{l}{4n\pi}\sin\left(\frac{2n\pi x}{l}\right)\right]_0^l = 1$$

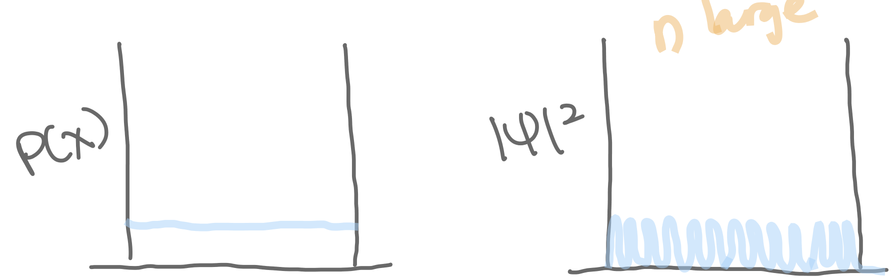
$$|B|^2 \left(\frac{l}{2}\right) = 1$$

$$|B| = \left(\frac{2}{l}\right)^{\frac{1}{2}}$$

$$\boxed{\psi_{II} = \left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{\ell}\right), \quad n = 1, 2, 3, \ldots}$$



Classical Result



The quantum mechanical result approaches the classical one when n is very large.

Practice Problems

1. A particle of mass $\underline{2.00 \times 10^{-26}\,g}$ m is in a one-dimensional box of length 4.00 nm. Find

one-dimensional box of length

the $\boxed{\text{frequency and wavelength}}$ of the photon

$E=h\nu$

ℓ

emitted when the particle goes from the $n=3$ to the $n=2$ level.

$$E = \frac{n^2 h^2}{8m\ell^2}$$

$$\Delta E = h\nu = E_{n=3} - E_{n=2}$$

$$\cancel{h}\nu = (3^2 - 2^2)\frac{h^{\cancel{2}}}{8m\ell^2}$$

$$\nu = \frac{5}{8}\frac{h}{m\ell^2}$$

$$\nu = \frac{5}{8}\,\frac{6.626\times10^{-34}\ \cancel{kg}\cdot \cancel{m^2}\cdot s^{-1}}{(2.00\times10^{-29}\ \cancel{kg})(4.00\times10^{-9}\ \cancel{m})^{\cancel{2}}}$$

$$\boxed{\nu = 1.29\times10^{12}\ s^{-1}}$$

$$c = \lambda\nu\ ,\quad \lambda = \frac{c}{\nu}$$

$$\boxed{\lambda = 2.32\times10^{-4}\ m}$$

2. For an electron in a certain one-dimensional box, the longest wavelength transition occurs at 400 nm. Find the length of the box.

m_e $n=1$ to $n=2$ λ l

$$\cancel{h}\nu = (2^2 - 1^2)\frac{h^{\cancel{2}}}{8ml^2}$$

$$8ml^2 = 3\frac{h}{\nu}$$

$$\nu = \frac{c}{\lambda}$$

$$l^2 = \frac{3}{8}\frac{h}{\nu m}$$

$$l = \left(\frac{3}{8}\frac{h}{\nu m}\right)^{\frac{1}{2}}$$

$$l = \left(\frac{3}{8}\frac{h\lambda}{cm}\right)^{\frac{1}{2}}$$

$$l = \left[\frac{3}{8}\frac{(6.626\times10^{-34}\,\cancel{kg}\cdot m^2\cdot \cancel{s^{-1}})(400\times10^{-9}\,\cancel{m})}{(2.998\times10^{8}\,\cancel{m}\,\cancel{s^{-1}})(9.11\times10^{-31}\,\cancel{kg})}\right]^{\frac{1}{2}}$$

$$l = 6.03\times10^{-10}\ m$$

$$\boxed{l = 0.603\ nm}$$

Orthonormality

$$\psi_i = \left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n_i \pi x}{\ell}\right), \quad 0 < x < \ell$$

$\psi_i = 0$ elsewhere

$$\int_{-\infty}^{\infty} \psi_i^* \psi_j \, dx = 1 \quad \text{if } i = j$$

$$\int_{-\infty}^{\infty} \psi_i^* \psi_j \, dx = \int_0^{\ell} \left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n_i \pi x}{\ell}\right) \left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n_j \pi x}{\ell}\right) dx$$

$i \neq j$

Integral Table

$$\int \sin(ax)\sin(bx)\,dx = \frac{\sin[(a-b)x]}{2(a-b)} - \frac{\sin[(a+b)x]}{2(a+b)},$$

$a^2 \neq b^2$

$$\left(\frac{2}{\ell}\right)\left[\frac{\overset{0}{\cancel{\sin(n_i - n_j)\pi}}}{2(n_i - n_j)\pi/\ell} - \frac{\overset{0}{\cancel{\sin(n_i + n_j)\pi}}}{2(n_i + n_j)\pi/\ell}\right] = 0$$

$$\int_{-\infty}^{\infty} \psi_i^* \psi_j \, dx = 0 \qquad i \neq j$$

$$\int_{-\infty}^{\infty} \psi_i^* \psi_j \, dx = \delta_{ij}$$

$$\boxed{\delta_{ij} \equiv \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}}$$