Lecture 3

Monday, September 18, 2023 12:39

Linear homogeneous second-order differential equation with constant coefficients :

$$y'' + p y' + q y = 0 \qquad (2.6)$$

To solve (2.6), assume a solution of the form $y = e^{ax}$

$$a^2 e^{ax} + p a e^{ax} + q e^{ax} = 0$$

$$(a^2 + pa + q) e^{ax} = 0$$

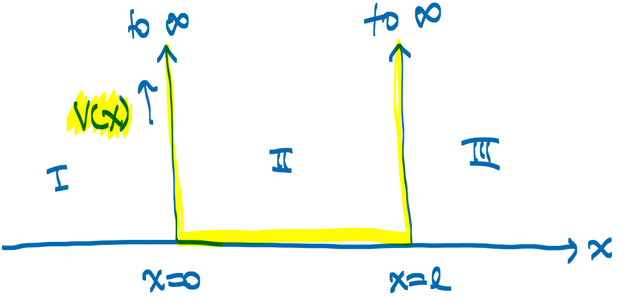
$$\boxed{a^2 + pa + q = 0}$$

auxiliary equation

quadratic equation with two roots a_1 and a_2; if $a_1 \neq a_2$, we will have two independent solutions to (2.6).

$$\boxed{y = c_1 e^{a_1 x} + c_2 e^{a_2 x}} \qquad (2.8)$$

2.2 Particle in a One-Dimensional Box



$\psi_{I} = 0$, $\psi_{III} = 0$ (previously determined)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + \underset{\underset{0}{\uparrow}}{V(x)}\,\psi_{II} = E\psi_{II}$$

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2} E \psi_{II} = 0$$

$$y'' + \frac{2mE}{\hbar^2} y = 0$$

write auxiliary equation:

$$a^2 + \frac{2mE}{\hbar^2} = 0$$

$$a^2 = -\frac{2mE}{\hbar^2}$$

$$a = \pm\sqrt{-\frac{2mE}{\hbar^2}}$$

$$a = \pm\frac{\sqrt{2mE}}{\hbar} i$$

$$\psi_{II} = c_1 e^{(2mE)^{\frac{1}{2}}/\hbar \cdot ix} + c_2 e^{-(2mE)^{\frac{1}{2}}/\hbar \cdot ix}$$

$$\text{Let } \theta \equiv \boxed{\frac{(2mE)^{\frac{1}{2}}}{\hbar} x}$$

$$\psi_{II} = c_1 e^{i\theta} + c_2 e^{-i\theta}$$

Euler's formula:

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$e^{-i\theta} = \cos\theta - i\sin\theta$$

$$\psi_{II} = c_1\left[\cos\theta + i\sin\theta\right] + c_2\left[\cos\theta - i\sin\theta\right]$$

$$\psi_{II} = c_1\cos\theta + ic_1\sin\theta + c_2\cos\theta - ic_2\sin\theta$$

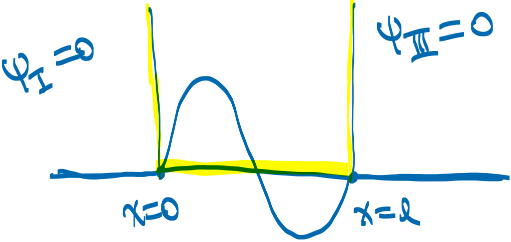
$$\psi_{II} = \overbrace{(c_1+c_2)}^{A}\cos\theta + \overbrace{i(c_1-c_2)}^{B}\sin\theta$$

$$\boxed{\psi_{II} = A\cos\theta + B\sin\theta}$$

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

Next: find A and B by applying boundary conditions.

Postulate that the wavefunction will be continuous :



If ψ is continuous at $x = 0$, then ψ_I and ψ_{II} must approach the same value at $x = 0$.

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

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

$$\therefore\ 0 = A$$

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

$\hbar = \frac{h}{2\pi}$ ← Planck's constant

$$\psi_{II} = B\sin\left[\frac{2\pi(2mE)^{\frac{1}{2}}}{h}x\right] \qquad (2.17)$$

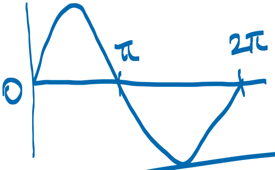
Now, apply the continuity condition at $x = l$.

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

$\uparrow$

$B \neq 0$; if $B = 0$, we would have an empty box. Therefore :

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



The zeros of the sine function occur at ⓪, $\pm\pi$, $\pm 2\pi$, ... $= \pm n\pi$. Therefore :

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

Special case : $n = 0$; $E = 0$

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2} E\psi_{II} = 0$$

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

$$\frac{d\psi_{II}}{dx} = c \quad \text{and} \quad \psi_{II} = c\overset{(\ell)}{x} + d$$

(where c and d are constants)

Apply boundary conditions :

$\psi_{II}(0) = 0$: $d = 0$

$\psi_{II}(\ell) = 0$: $c = 0$ $\quad \psi_{II} = \boxed{c \cdot \ell}$

$\psi_{II} = 0$ for $E = 0$ Thus : $E = 0$ is not an allowed energy value.

Going back to non-zero values for n, we solve for E :

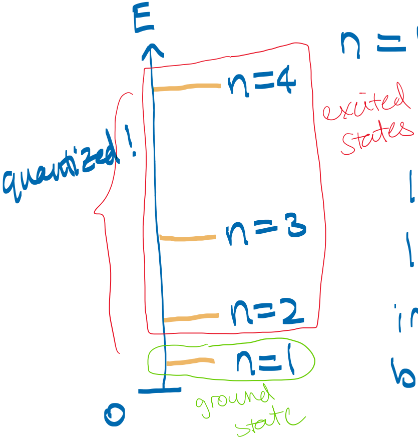
$$\frac{2\cancel{\pi}(2mE)^{\frac{1}{2}}}{h}\ell = \pm n\cancel{\pi}$$

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

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

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

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



lowest four energy levels for the particle in a one-dimensional box

-in contrast to the classical result where the particle can have any non-negative energy

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

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

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

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

$\sin(-x) = -\sin x$ ← not an independant solution

To determine B, apply the requirement of normalization

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

$$\cancel{\int_{-\infty}^{0} |\overset{0}{\psi_{I}}|^2 dx} + \int_{0}^{\ell} |\psi_{II}|^2 dx + \cancel{\int_{\ell}^{\infty} |\overset{0}{\psi_{III}}|^2 dx}$$

$$= 1$$

$$\int_0^\ell \left|B\sin\left(\frac{n\pi x}{\ell}\right)\right|^2 dx = 1$$

$$B^2 \boxed{\int_0^\ell \sin^2\left(\frac{n\pi x}{\ell}\right) dx} = 1$$

Integral table: $\qquad k = \frac{n\pi}{\ell}$

$$\int \sin^2 kx\, dx = \frac{x}{2} - \frac{1}{4k}\sin(2kx)$$

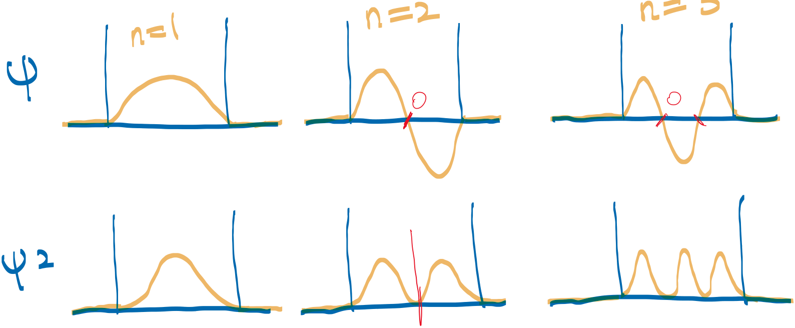
$$B^2 \left| \overset{0}{\frac{x}{2}} - \frac{1}{4}\cdot\frac{\ell}{n\pi}\sin\left(\frac{\overset{0}{2n\pi x}}{\ell}\right) \right|_0^\ell = 1$$

$$B^2 \left[\frac{\ell}{2} - \overbrace{\frac{1}{4}\frac{\ell}{n\pi}\sin\left(\frac{2n\pi \cancel{\ell}}{\cancel{\ell}}\right)}^{0}\right] = 1$$

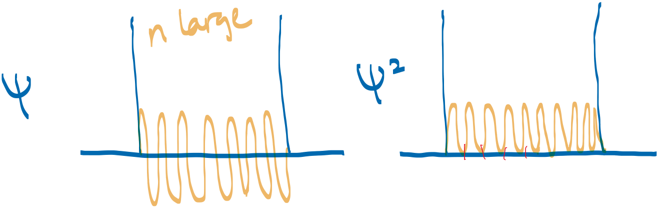
$$B^2 \cdot \frac{\ell}{2} = 1$$

$$B = \sqrt{\frac{2}{\ell}}$$

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



point at which the value of ψ is zero: node ; number of nodes = n − 1.



approaches classical result
when n is large

apparent paradox: particle can travel from one side of the box to the other without ever being found in the centre; microscopic particles cannot be understood in the same way that we understand macroscopic objects.

Kronecker delta (next lecture)

2.3