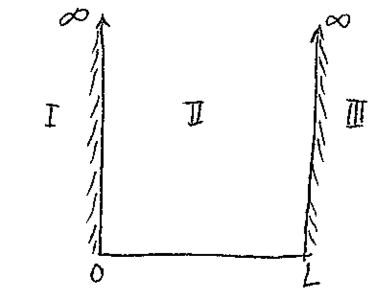
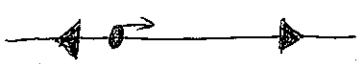
Translational motion

Particle on a line (particle in a 1-D box)



Let examine a system where a ~~mass~~ particle of mass m moving freely along the x-axis between $x=0$ and $x=L$, i.e. the particle is subjected to the potential

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & x < 0 \ , \ x > L \end{cases} \tag{23.1}$$



Note: Classically, one may relate this problem to a frictionless bead moving along a string between two points.

From classical mechanics, we can write down the total energy of the system

$$\frac{p_x^2}{2m} + V = E \tag{23.2}$$

To convert to quantum mechanics, we use the postulate #3

$$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx} \Rightarrow p_x^2 = -\hbar^2 \frac{d^2}{dx^2} \tag{23.3}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\,\psi(x) \tag{23.4}$$

(23.4) is the time independent Schrödinger equation, where

$\psi(x)$ is the coordinate eigenfunction and E is the energy eigenvalue.

To solve this problem, we divide the x-axis into three regions

Region I : $x < 0$
Region II : $0 \leq x \leq L$
Region III : $L < x$

From classical mechanics, we know that the particle would not be in regions I and III. In quantum mechanics, we need to examine the behavior of the wavefunction in those regions.

In regions I and III, eq. (23.4) becomes

$$\frac{d^2\psi}{dx^2} - \lim_{V\to\infty} \frac{2mV}{\hbar^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) \tag{24.1}$$

From one of the postulates, $\psi(x)$ must be finite. Hence, for a finite E, the right hand side of (24.1) must be finite, yet the left hand side is infinite unless $\psi(x) = 0$

$$\psi^{I}(x) = \psi^{III}(x) = 0 \tag{24.2}$$

In region II, since $V = 0$, we need to worry only the kinetic energy term

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x) \tag{24.3}$$

where $$k^2 = \frac{2mE}{\hbar^2} \tag{24.4}$$

The general solution to eq. (24.3) is

$$\psi^{II}(x) = A \sin(kx) + B \cos(kx) \qquad (25.1)$$

For $\psi(x)$ to be continuous at $x = 0$ and $x = L$, we must impose the boundary conditions

$$\psi^{I}(0) = \psi^{II}(0) = 0 \qquad (25.2)$$
$$\psi^{II}(L) = \psi^{III}(L) = 0 \qquad (25.3)$$

From (25.2) $\Rightarrow$ $\psi^{II}(0) = B = 0$ $\quad \therefore \quad$ $\psi^{II}(x) = A \sin(kx)$ $\quad$ (25.4)

From (25.3) $\Rightarrow$ $\psi^{II}(L) = A \sin(kL) = 0$ $\quad$ (25.5)

This means $\quad kL = n\pi \qquad n = 1, 2, \ldots$

($n=0$ is ruled out, since it implies $\psi^{II}(x) = 0$)

From (24.4) $\Rightarrow$

$$E = \frac{\hbar^2 k^2}{2m} \qquad (25.6)$$

Substitute $kL = n\pi$ into eq. (25.6), we obtain

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} = \frac{h^2 n^2}{8mL^2} \qquad n = 1, 2, \ldots \qquad (25.7)$$

E_n is <u>the energy level</u> and n is <u>the quantum number</u>

Thus, the energy quantization arises from the boundary condition.

⑤

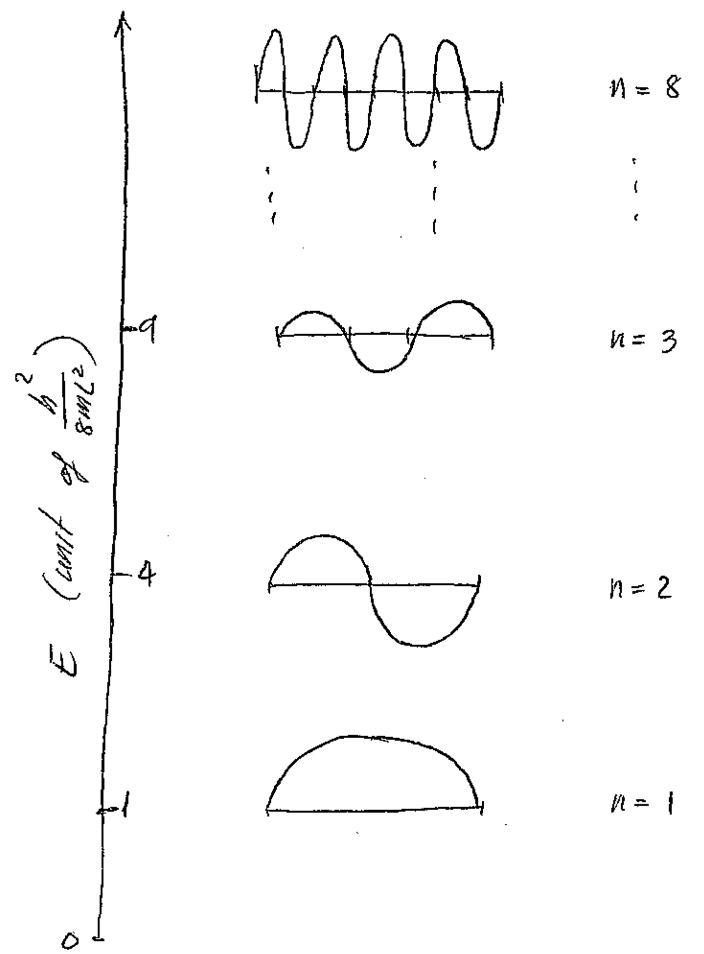
To determine the coefficient A, we use the normalization condition

$$1 = \int_{-\infty}^{\infty} \psi^* \psi \, dx = A^2 \int_0^L \sin^2(kx)\, dx \qquad \sin^2 x = \frac{1}{2}(1-\cos 2x)$$

$$1 = \frac{1}{2} A^2 L \quad \rightarrow \quad A = \left(\frac{2}{L}\right)^{1/2}$$

The complete solution is

$$\boxed{\begin{aligned} E_n &= \frac{h^2 n^2}{8mL^2} \qquad n = 1, 2, \ldots \\ \psi_n &= \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right) \end{aligned}}$$



Observations:

① The lowest energy of the system is not zero

$E_1 = \dfrac{h^2}{8mL^2}$ is called the zero-point energy

There are two possible explanations

a) From the uncertainty principle

Since the location of the particle is not completely indefinite (it is localized between $0 \le x \le L$), $\Delta x = L$, its momentum cannot be precisely zero.

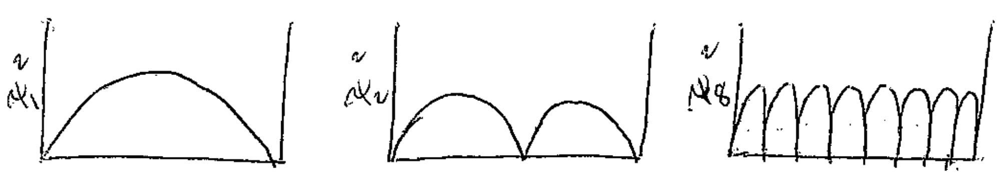
b) From the continuity condition of the wavefunction

Since $\psi^{I} = \psi^{III} = 0$ and ψ^{II} is not zero everywhere, the continuity condition of the wavefunction force ψ to curve, and the curvature of ψ, $\dfrac{d^2\psi}{dx^2}$, implies the non-zero kinetic energy.

② Probability density

$\psi^2 = \dfrac{2}{L}\sin^2\left(\dfrac{n\pi x}{L}\right)$ is not uniform.

However, ψ^2 becomes more uniform as n increases and reflects the classical results.



The corresponding principle As the quantum number increases to infinity, quantum mechanics approaches the classical mechanics limit.