

## Particle in a box (Potential barrier)

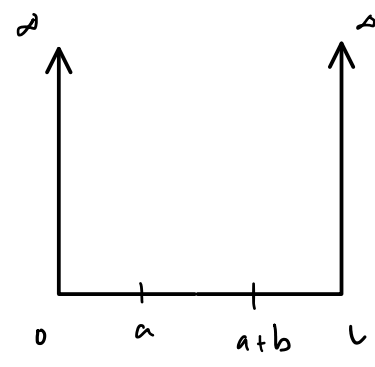
For particle in a box of side  $L$ :

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad E = \frac{n^2 h^2}{8mL^2}$$

Q1

1. \* For a particle in a 1-D box of side  $L$ , show that the probability of finding the particle between  $x = a$  and  $x = a + b$  approaches the classical value  $b/L$ , if the energy of the particle is very high.

1-D box of side  $L$ .



Prob of particle from  $a \rightarrow a+b$

$$\begin{aligned} \int_a^{a+b} \psi^* \psi &= \frac{2}{L} \int_a^{a+b} \sin^2 \frac{n\pi x}{L} dx \\ &= \frac{1}{L} \int_a^{a+b} 1 - \cos \frac{2n\pi x}{L} dx \\ &= \frac{1}{L} \left[ x - \sin \frac{n\pi x}{L} \times \frac{1}{n\pi} \right]_a^{a+b} \\ &= \frac{1}{L} \left[ b - \frac{1}{n\pi} \left( \sin \frac{2n\pi(a+b)}{L} - \sin \frac{2n\pi a}{L} \right) \right] \end{aligned}$$

$\therefore \text{prob} = b/L$  [as expected classically]

Q2

2. Consider a particle confined to a 1-D box. Find the probability that the particle in its ground state will be in the central one-third region of the box.

Required prob  $\Rightarrow \frac{2}{L} \int_{L/3}^{2L/3} \sin^2 \frac{\pi x}{L} dx$

Ans =  $\frac{1}{3} + \frac{\sqrt{3}}{2\pi}$

$$\begin{aligned} \frac{1}{L} \left[ \int_{L/3}^{2L/3} 1 - \cos \frac{2\pi x}{L} dx \right] &= \frac{1}{L} \left( \frac{L}{3} - \sin \frac{2\pi x}{L} \times \frac{1}{2\pi} \right)_{L/3}^{2L/3} \\ &= \frac{1}{3} + \frac{\sqrt{3}}{2\pi} \end{aligned}$$

Q3

3. Consider a particle of mass  $m$  moving freely between  $x = 0$  and  $x = a$  inside an infinite square well potential.  
(a) Calculate the expectation values  $\langle \hat{X} \rangle_n$ ,  $\langle \hat{P} \rangle_n$ ,  $\langle \hat{X}^2 \rangle_n$ , and  $\langle \hat{P}^2 \rangle_n$ , and compare them with their classical counterparts.  
(b) Calculate the uncertainties product  $\Delta x_n \Delta p_n$ .  
(c) Use the result of (b) to estimate the zero-point energy.

Infinite square well  $\Rightarrow$  particle in a box

Explanat<sup>n</sup> from the sol<sup>n</sup>.

Q4

4. Consider a one dimensional infinite square well potential of length  $L$ . A particle is in  $n = 3$  state of this potential well. Find the probability that this particle will be observed between  $x = 0$  and  $x = L/6$ . Can you guess the answer without solving the integral? Explain how.

from the sol<sup>n</sup>  $\Rightarrow$  good method [nodes]

Q5

5. \* Consider a one-dimensional particle which is confined within the region  $0 \leq x \leq a$  and whose wave function is  $\Psi(x, t) = \sin(\pi x/a) \exp(-i\omega t)$ .  
(a) Find the potential  $V(x)$ . ↪ stationary state with energy  $\hbar\omega$   
(b) Calculate the probability of finding the particle in the interval  $a/4 \leq x \leq 3a/4$ .

Use TISE

a)  $\psi(0, t) = 0, \quad \psi(a, t) = 0$

for  $0 < x < a$ , TISE

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\frac{\hbar^2}{2m} \left( \frac{\pi}{a} \right)^2 \psi + V \psi = \hbar\omega \psi$$

$$V = \hbar\omega - \frac{\hbar^2}{2m} \left( \frac{\pi}{a} \right)^2$$

Normalisation const =  $\sqrt{2/a}$

$$\begin{aligned} \text{prob} &= \frac{2}{a} \int_{a/4}^{3a/4} \sin^2 \frac{\pi x}{a} dx = \frac{1}{a} \left[ x - \sin \frac{2\pi x}{a} \times \frac{a}{2\pi} \right]_{a/4}^{3a/4} \\ &= \frac{1}{a} \left[ \frac{a}{2} + \frac{a}{\pi} \right] = \frac{1}{2} + \frac{1}{\pi} > \frac{1}{2} \end{aligned}$$

Classical prob

Q6

6. An electron is moving freely inside a one-dimensional infinite potential box with walls at  $x = 0$  and  $x = a$ . If the electron is initially in the ground state ( $n = 1$ ) of the box and if we suddenly quadruple the size of the box (i.e., the right-hand side wall is moved instantaneously from  $x = a$  to  $x = 4a$ ), calculate the probability of finding the electron in:  
(a) the ground state of the new box and  
(b) the first excited state of the new box.

The total wave func<sup>n</sup> of new box stays same as old one

$$\psi(x)_{\text{in}} = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \quad (n=1)$$

$$\Rightarrow \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) = \sum_{i=1}^{\infty} c_i \sqrt{\frac{2}{4a}} \sin\left(\frac{i\pi x}{4a}\right)$$

integrate with conjugate of  $i^{\text{th}}$  func<sup>n</sup> to obtain  $c_i$

Q7

7. Solve the time independent Schrodinger equation for a particle in a 1-D box, taking the origin at the centre of the box and the ends at  $\pm L/2$ , where  $L$  is the length of the box.

Q8

8. \* Consider a particle of mass  $m$  in an infinite potential well extending from  $x = 0$  to  $x = L$ . Wave function of the particle is given by

$$\psi(x) = A \left[ \sin\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right) \right]$$

where  $A$  is the normalization constant

- (a) Calculate  $A$   
(b) Calculate the expectation values of  $x$  and  $x^2$  and hence the uncertainty  $\Delta x$ .  
(c) Calculate the expectation values of  $p$  and  $p^2$  and hence the uncertainty  $\Delta p$ .  
(d) What is the probability of finding the particle in the first excited state, if an energy measurement is made?

(given,  $\int_0^L x \cos\left(\frac{n\pi x}{L}\right) dx = 0$ ,  $\int_0^L x^2 \cos\left(\frac{n\pi x}{L}\right) dx = 0$ , for all  $n$ )

from Sol<sup>n</sup>.