

6) Given the wavefunction for a particle in a 1D box (PIB) of length l ,

(5x1= 5 marks)

$$\psi(x) = \sqrt{\frac{2}{l}} \left[\sin \frac{\pi x}{l} + \frac{1}{2} \sin \frac{2\pi x}{l} + \frac{1}{3} \sin \frac{3\pi x}{l} \right]$$

Realize that the wavefunction is superposition of $n = 1, 2$ and 3 states.

a) Normalize the wavefunction

$$\begin{aligned} \int_0^l \psi^* \psi dx &= 1 \\ \Rightarrow \int_0^l \sqrt{\frac{2}{l}} \left[\sin \frac{\pi x}{l} + \frac{1}{2} \sin \frac{2\pi x}{l} + \frac{1}{3} \sin \frac{3\pi x}{l} \right] \times \sqrt{\frac{2}{l}} \left[\sin \frac{\pi x}{l} + \frac{1}{2} \sin \frac{2\pi x}{l} + \frac{1}{3} \sin \frac{3\pi x}{l} \right] dx \\ &= \int_0^l \frac{2}{l} \sin^2 \frac{\pi x}{l} dx + \frac{1}{4} \int_0^l \frac{2}{l} \sin^2 \frac{2\pi x}{l} dx + \frac{1}{9} \int_0^l \frac{2}{l} \sin^2 \frac{3\pi x}{l} dx \end{aligned}$$

(since the eigenfunctions are orthonormal)

$$\begin{aligned} &= 1 + \frac{1}{4} + \frac{1}{9} = \frac{36 + 9 + 4}{36} = \frac{49}{36} \\ \Rightarrow \sqrt{\frac{36}{49}} \left(\sqrt{\frac{2}{l}} \left[\sin \frac{\pi x}{l} + \frac{1}{2} \sin \frac{2\pi x}{l} + \frac{1}{3} \sin \frac{3\pi x}{l} \right] \right) \end{aligned}$$

is the normalized wavefunction.

b) Use the normalized wavefunction to:

i. Determine the probability of finding the particle in the first excited state of the PIB

Probability is $|C_i|^2$ when $\psi = c_1\phi_1 + c_2\phi_2 + \dots$. The first E.S. is when $n = 2$.

$$c_2 = \frac{1}{2} \sqrt{\frac{36}{49}} \Rightarrow |C_i|^2 = \frac{1}{4} \times \frac{36}{49} = \frac{9}{49}$$

ii. Determine the average energy of the particle

$$\begin{aligned}
\langle E \rangle &= \int_0^l \psi^* \hat{H} \psi dx = \int_0^l (c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3)^* \hat{H} (c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3) dx \\
&= \int_0^l (c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3)^* (c_1 E_1 \phi_1 + c_2 E_2 \phi_2 + c_3 E_3 \phi_3) dx \\
&= c_1^2 E_1 + c_2^2 E_2 + c_3^2 E_3 \text{ (orthonormal eigenfunctions)} \\
&= \frac{36}{49} \left(1 \times 1 + \frac{1}{4} \times 4 + \frac{1}{9} \times 9 \right) \frac{h^2}{8ml^2} = \frac{108}{49} \frac{h^2}{8ml^2}
\end{aligned}$$

c) Is the wavefunction orthogonal to the second excited state of the PIB? Show.

No, since it has the second excited state.

$$\begin{aligned}
&\int_0^l \sqrt{\frac{2}{l}} \sin \frac{3\pi x}{l} \left\{ \sqrt{\frac{36}{49}} \left(\sqrt{\frac{2}{l}} \left[\sin \frac{\pi x}{l} + \frac{1}{2} \sin \frac{2\pi x}{l} + \frac{1}{3} \sin \frac{3\pi x}{l} \right] \right) \right\} dx \\
&= 0 + 0 + \frac{1}{3} \times \sqrt{\frac{36}{49}}
\end{aligned}$$

d) Estimate the uncertainty in the momentum of the particle.

$$\sigma_{p_x} = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\langle 2mE \rangle - 0} = \sqrt{\frac{108}{49} \frac{h^2}{4l^2}}$$

(from $E = p^2/2m$ and the fact that the average value of momentum of a PIB moving in both directions is zero. Value of E is from part ii.)