Chapter 5: Quantum Mechanics in One Dimension

#5.5

$$\psi(x) = A\,x\,e^{-\frac{x^2}{L^2}}$$

a) Use Schrodinger equation setting $E = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = \cancel{E}^{\,0}\,\psi(x) \quad \text{—— (1)}$$

$$\frac{d\psi}{dx} = -A\,2\frac{x^2}{L^2}e^{-\frac{x^2}{L^2}} + A\,e^{-\frac{x^2}{L^2}}$$

$$\frac{d^2\psi}{dx^2} = -4A\frac{x}{L^2}e^{-\frac{x^2}{L^2}} + 4A\frac{x^3}{L^4}e^{-\frac{x^2}{L^2}} - 2A\frac{x}{L^2}e^{-\frac{x^2}{L^2}}$$

$$= -6A\frac{x}{L^2}e^{-\frac{x^2}{L^2}} + 4A\frac{x^3}{L^4}e^{-\frac{x^2}{L^2}}$$

$$= \underbrace{A\,x\,e^{-\frac{x^2}{L^2}}}_{\psi(x)}\left(4\frac{x^2}{L^4} - \frac{6}{L^2}\right) \quad \text{—— (2)}$$

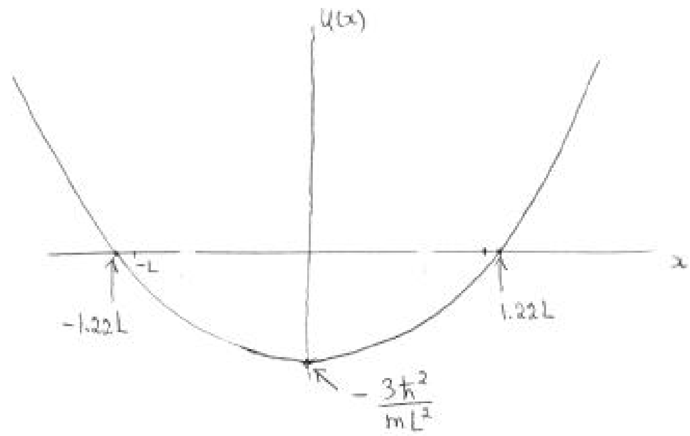
(2) into (1) $\Rightarrow$ $$-\frac{\hbar^2}{2m}\left(4\frac{x^2}{L^4} - \frac{6}{L^2}\right)\psi(x) + U(x)\,\psi(x) = 0$$

$$\Rightarrow U(x) = \frac{\hbar^2}{2m}\left(4\frac{x^2}{L^4} - \frac{6}{L^2}\right)$$

or $$\boxed{U(x) = \frac{\hbar^2}{2mL^2}\left(\frac{4}{L^2}x^2 - 6\right)}$$

b) When $x = 0$ $\quad U(0) = -\dfrac{3\hbar^2}{mL^2}$

when $U(x) = 0 \Rightarrow \dfrac{4}{L^2}x^2 - 6 = 0 \Rightarrow x = \pm\sqrt{\dfrac{6}{4}}\,L = \pm 1.22\,L$



5.12

$\lambda = 694.3$ nm . Energy of an electron in a box is quantized and given by $E_n = \dfrac{n^2\pi^2\hbar^2}{2m_e L^2}$ $\quad n = 1, 2, 3, \ldots$

$$\Delta E_{n=2\to n=1} = \frac{4\pi^2\hbar^2}{2m_e L^2} - \frac{\pi^2\hbar^2}{2m_e L^2} = \frac{3}{2}\frac{\pi^2\hbar^2}{m_e L^2}$$

where L is the width of the box

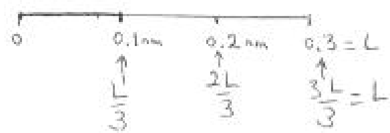
$$\Delta E = hf = \frac{hc}{\lambda} = \frac{3}{2}\frac{\pi^2\hbar^2}{m_e L^2}$$

$$\Rightarrow L = \sqrt{\frac{3}{2}\frac{\pi^2\hbar^2\lambda}{m_e\, hc}} = \boxed{7.9\times 10^{-10}\ \text{m}}$$

$$= 7.9\ \text{Å}$$

5.16

$L = 0.30 \text{ nm}$



a) In the ground state

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$$

$$P = \int_0^{L/3} |\psi_1|^2 \, dx = \frac{2}{L} \int_0^{L/3} \sin^2\left(\frac{\pi}{L}x\right) dx$$

use $\sin^2\alpha = \frac{1}{2}(1 - \cos 2\alpha)$

$$P = \frac{1}{L} \int_0^{L/3} \left[1 - \cos\frac{2\pi}{L}x\right] dx = \frac{1}{L}\left[x\Big|_0^{L/3} - \left(\frac{L}{2\pi}\right) \sin\frac{2\pi}{L}x \Big|_0^{L/3} \right]$$

$$= \frac{1}{L}\left[\frac{L}{3} - \frac{L}{2\pi}\left(\sin\frac{2\pi}{3} - 0\right)\right] = \frac{1}{3} - 0.1378 = 0.195$$

$$= \boxed{19.5\%}$$

b) In the 100^{th} state

$$\psi_{100} = \sqrt{\frac{2}{L}} \sin\left(\frac{100\pi}{L}x\right)$$

$$P = \frac{2}{L} \int_0^{L/3} \sin^2\left(\frac{100\pi}{L}x\right) dx$$

$$= \frac{1}{L} \int_0^{L/3} \left[1 - \cos\frac{100\pi}{L}x\right] dx = \frac{1}{L}\left[\frac{L}{3} - \frac{L}{100\pi} \sin\frac{100\pi}{L}x \Big|_0^{L/3}\right]$$

$$= \frac{1}{L}\left[\frac{L}{3} - \frac{L}{100\pi}\left(\sin\frac{100\pi}{3} - 0\right)\right] = \frac{1}{3} - 3.1\times 10^{-3}$$

$$= 0.33 = \boxed{33\%}$$

c) Yes, when n becomes large the probability becomes equal to the classical value of 1/3.

#5.26

For the quantum oscillator $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$

but $E = \frac{1}{2} k A^2$ for a classical oscillator

$$\Rightarrow \frac{1}{2} k A^2 = \left(n+\frac{1}{2}\right)\hbar\omega = \frac{1}{2}(2n+1)\hbar\omega$$

$$\Rightarrow A = \sqrt{\frac{(2n+1)\hbar\omega}{k}}$$

but $k = \omega^2 m \Rightarrow \boxed{A = \sqrt{\frac{(2n+1)\hbar}{\omega m}}}$

#5.30

$$\psi(x) = \begin{cases} 0 & x<0 \\ C e^{-x}(1-e^{-x}) & x>0 \end{cases}$$

a) $\int_{-\infty}^{+\infty} |\psi_{(x)}|^2 dx = 1 \Rightarrow C^2 \int_0^{+\infty} e^{-2x}(1-e^{-x})^2 dx = 1$

$$C^2 \int_0^{+\infty} e^{-2x}(1-2e^{-x}+e^{-2x})\,dx = C^2 \int_0^{\infty} (e^{-2x} - 2e^{-3x} + e^{-4x})\,dx$$

$$= C^2 \left[-\frac{1}{2} e^{-2x}\Big|_0^{+\infty} + \frac{2}{3} e^{-3x}\Big|_0^{+\infty} - \frac{1}{4} e^{-4x}\Big|_0^{+\infty} \right]$$

$$= C^2\left(\frac{1}{2} - \frac{2}{3} + \frac{1}{4}\right) = C^2\left(\frac{1}{12}\right) = 1 \Rightarrow \boxed{C = \sqrt{12}}\ (nm^{-1})$$

b) The electron is most likely to be where the probability is highest.

That is where the wavefunction is largest $\Rightarrow \frac{d\psi}{dx} = 0$

$$\frac{d\psi}{dx} = c\left[-e^{-x}(1-e^{-x}) + e^{-x}\cdot e^{-x}\right] = 0$$

$$\Rightarrow -e^{-x} + 2e^{-2x} = 0$$

$$\Rightarrow e^{-x}\cdot\underbrace{(2e^{-x}-1)}_{=0} = 0 \Rightarrow e^{-x} = \frac{1}{2} \Rightarrow -x = -\ln 2$$

$$\Rightarrow \boxed{x = +0.693\,\text{nm}}$$

c) $\langle x \rangle = \int_{-\infty}^{+\infty} x\,|\psi|^2\,dx = c^2\int_0^{+\infty} x\,e^{-2x}(1-e^{-x})^2\,dx$

average value of the position

$$= c^2\int_0^{+\infty} x\,(e^{-2x} - 2e^{-3x} + e^{-4x})\,dx$$

use the fact that $\int_0^{+\infty} x\,e^{-\alpha x}\,dx = \frac{1}{\alpha^2}$ and $c^2 = 12$

$$\langle x \rangle = 12\left[\int_0^{+\infty} x\,e^{-2x}\,dx - 2\int_0^{+\infty} x\,e^{-3x}\,dx + \int_0^{+\infty} x\,e^{-4x}\,dx\right]$$

$$= 12\left[\frac{1}{4} - 2\,\frac{1}{9} + \frac{1}{16}\right] = \boxed{1.083\ \text{nm}}$$

$\langle x \rangle$ is greater than the most probable location of the electron because the values x larger than $\langle x \rangle$ are weighted more in the calculation of $\langle x \rangle$.

#5.32

$\psi(x) = C\,e^{-\frac{|x|}{x_0}}$ where x_0 = Constant and $C = \frac{1}{\sqrt{x_0}}$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\,|\psi|^2\,dx = \int_{-\infty}^{+\infty} \underbrace{x}_{\text{odd}}\,\underbrace{e^{-\frac{2|x|}{x_0}}}_{\text{even}}\,dx = 0$$

You can try it with mathematica!

$$\langle x^2 \rangle = \frac{1}{x_0}\int_{-\infty}^{+\infty} x^2\, e^{-\frac{2|x|}{x_0}}\,dx = \frac{2}{x_0}\underbrace{\int_0^{+\infty} x^2 e^{-\frac{2x}{x_0}}\,dx}$$

integration by parts: $\int u\,dv = uv - \int v\,du$

let $u = x^2 \Rightarrow du = 2x\,dx$

$dv = e^{-\frac{2x}{x_0}}dx \Rightarrow v = -\frac{x_0}{2}e^{-\frac{2x}{x_0}}$

$$\Rightarrow \int_0^{+\infty} x^2 e^{-\frac{2x}{x_0}}\,dx = \underbrace{-x^2\frac{x_0}{2}e^{-\frac{2x}{x_0}}\Big|_0^{+\infty}}_{\to 0} + \cancel{2}\frac{x_0}{\cancel{2}}\underbrace{\int_0^{+\infty} x\, e^{-\frac{2x}{x_0}}\,dx}_{\text{integrate by parts}}$$

$u = x \Rightarrow du = dx$

$dv = e^{-\frac{2x}{x_0}}dx \Rightarrow v = -\frac{x_0}{2}e^{-\frac{2x}{x_0}}$

$$\int_0^{+\infty} x\, e^{-\frac{2x}{x_0}}\,dx = \underbrace{-x\frac{x_0}{2}e^{-\frac{2x}{x_0}}\Big|_0^{+\infty}}_{\to 0} + \frac{x_0}{2}\underbrace{\int_0^{\infty} e^{-\frac{2x}{x_0}}\,dx}_{= -\frac{x_0}{2}(0-1) = \frac{x_0}{2}}$$

$$\Rightarrow \langle x^2\rangle = \frac{2}{x_0}\times x_0 \times \frac{x_0^2}{4} = \frac{x_0^2}{2}$$

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \sqrt{\frac{x_0^2}{2}} = \boxed{\frac{x_0}{\sqrt{2}}}$$

$$P = \int_{-\Delta x}^{+\Delta x} |\psi|^2\,dx = \frac{2}{x_0}\int_0^{+\Delta x} e^{-\frac{2x}{x_0}}\,dx = \frac{2}{x_0}\left(-\frac{x_0}{2}\right)e^{-\frac{2x}{x_0}}\Big|_0^{\frac{x_0}{\sqrt{2}}}$$

$$= -\left(e^{-\frac{2}{\sqrt{2}}} - 1\right) = 1 - e^{-\sqrt{2}} = 1 - 0.24 = 0.76$$

$$= \boxed{76\%}$$

End