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To be an acceptable wave function for particle in the box:

$\psi$  and its partial derivatives must be continuous.

$\int \psi^* \psi$  must exist (i. e.  $\psi$  must be quadratically integrable).

$\int \psi^* \psi$  is the probability density so it must be single valued.

$\psi$  cannot be infinite over a finite region of space.

$\psi$  must satisfy the boundary conditions ( $\psi(0) = \psi(a) = 0$ ).

- a) is not acceptable, since  $\psi(0) \neq 0$
- b) is not acceptable, since  $\psi(a) \neq 0$
- c) is acceptable for the part of  $\psi$  in the box and can be normalized.  $\psi$  outside the box must be zero.
- d) is not acceptable, since  $\psi(0) \neq 0$  and  $\psi$  at  $x = 0$  is not continuous

5-1

$$\left| \frac{F}{A} \right|^2 = \frac{1}{1 + \frac{(k^2 + \kappa^2)^2}{4(\kappa k)^2} \sinh^2 \kappa a}$$

$$\sinh \kappa a = \frac{e^{\kappa a} - e^{-\kappa a}}{2} \quad \text{and} \quad \kappa = \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$$

$$\Rightarrow \sinh \kappa a \approx \frac{e^{\kappa a}}{2} \quad (\text{if } \kappa a \gg 1 \text{ e. g. when the barrier is very wide or } E \ll V_0)$$

$$\left| \frac{F}{A} \right|^2 = \frac{1}{1 + \frac{(k^2 + \kappa^2)^2}{16(\kappa k)^2} e^{2\kappa a}} = \left( 1 + \frac{(k^2 + \kappa^2)^2}{16(\kappa k)^2} e^{2\kappa a} \right)^{-1}$$

$$\Rightarrow \left| \frac{F}{A} \right|^2 \propto e^{-2\kappa a}$$

5-5

$$C = C - C = C - C = C - C = C$$

$$\text{length of the box} = 3 \times 154 + 4 \times 135 = 1002 \text{ pm}$$

Because there are 8 pi electrons, they occupy the first four energy levels. So exciting one pi electron means going from 4<sup>th</sup> to 5<sup>th</sup> level.

$$E = \frac{n^2 \hbar^2}{8ma^2} \Rightarrow E_5 - E_4 = \frac{(5^2 - 4^2) \times \hbar^2}{8 \times 9.11 \times 10^{-31} \times (1002 \times 10^{-12})^2} = 1.23 \times 10^{48} \times \hbar^2$$

$$\lambda = \frac{c}{\nu} = \frac{c}{\frac{E}{h}} = \frac{2.998 \times 10^8}{1.23 \times 10^{48} \times 6.626 \times 10^{-34}} = 368 \times 10^{-9} \text{ m}$$

6-5

$$\text{a) } \Delta E = \left( \frac{dE}{dp_x} \right) \Delta p_x = \frac{2p_x}{2m} \Delta p_x = \frac{p_x}{m} \Delta p_x = v_x \Delta p_x$$

$$\text{b) } \Delta E \Delta t = v_x \Delta p_x \Delta t = \frac{\Delta x}{\Delta t} \Delta p_x \Delta t = \Delta x \Delta p_x \Rightarrow \Delta E \Delta t \geq \frac{\hbar}{2}$$

$$\text{c) } \Delta E \Delta t \geq \frac{\hbar}{2} \Rightarrow \Delta E \geq \frac{\hbar}{2\Delta t} = \frac{h}{4\pi\Delta t} = h\Delta\nu$$

$$\Delta\nu = \frac{1}{4\pi\Delta t} = \frac{1}{4\pi(1.0 \times 10^{-9})} = 8.0 \times 10^7 \text{ s}^{-1}$$

$$\Delta\nu(\text{cm}^{-1}) = \frac{\Delta\nu(\text{s}^{-1})}{c} = \frac{8.0 \times 10^7 \text{ s}^{-1}}{2.998 \times 10^{10} \frac{\text{cm}}{\text{s}}} = 0.00265 \text{ cm}^{-1}$$

$$\Delta\nu = \frac{1}{4\pi\Delta t} = \frac{1}{4\pi(1.0 \times 10^{-11})} = 8.0 \times 10^9 \text{ s}^{-1}$$

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6-7

$$\begin{aligned} \left[ x^2 - \frac{d^2}{dx^2}, x - \frac{d}{dx} \right] f(x) &= \left( x^2 - \frac{d^2}{dx^2} \right) \left( x - \frac{d}{dx} \right) f(x) - \left( x - \frac{d}{dx} \right) \left( x^2 - \frac{d^2}{dx^2} \right) f(x) \\ &= \left( x^2 - \frac{d^2}{dx^2} \right) \left( x f(x) - \frac{d f(x)}{dx} \right) - \left( x - \frac{d}{dx} \right) \left( x^2 f(x) - \frac{d^2 f(x)}{dx^2} \right) \\ &= \left( x^3 f(x) - x^2 \frac{d f(x)}{dx} - \frac{d^2}{dx^2} (x f(x)) + \frac{d^3 f(x)}{dx^3} \right) \\ &\quad - \left( x^3 f(x) - x \frac{d^2 f(x)}{dx^2} - \frac{d}{dx} (x^2 f(x)) + \frac{d^3 f(x)}{dx^3} \right) \\ &= -x^2 \frac{d f(x)}{dx} - \frac{d^2}{dx^2} (x f(x)) + x \frac{d^2 f(x)}{dx^2} + \frac{d}{dx} (x^2 f(x)) \end{aligned}$$

For clarity, we evaluate the second and fourth terms below:

$$-\frac{d^2}{dx^2} (x f(x)) = -\frac{d}{dx} \left( f(x) + x \frac{d f(x)}{dx} \right) = -\frac{d f(x)}{dx} - \frac{d f(x)}{dx} - x \frac{d^2 f(x)}{dx^2} = -2 \frac{d f(x)}{dx} - x \frac{d^2 f(x)}{dx^2}$$

$$\frac{d}{dx}(x^2 f(x)) = 2xf(x) + x^2 \frac{df(x)}{dx}$$

So:

$$= -x^2 \frac{df(x)}{dx} - 2 \frac{df(x)}{dx} - x \frac{d^2 f(x)}{dx} + x \frac{d^2 f(x)}{dx^2} + 2xf(x) + x^2 \frac{df(x)}{dx} = -2 \frac{df(x)}{dx} + 2xf(x)$$