

Please show your work, and your thinking, in the space provided. Be brief, but complete. Long, wandering answers typically demonstrate a lack of understanding...

$$\hbar = 1.054 \times 10^{-34} \text{ J s}$$

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$m_e = 9.109 \times 10^{-31} \text{ kg}$$

$$c = 2.998 \times 10^8 \text{ m s}^{-1}$$

$$k = 1.381 \times 10^{-23} \text{ J K}^{-1}$$

$$e = 1.602 \times 10^{-19} \text{ C}$$

$$4\pi\epsilon_0 = 1.113 \times 10^{-10} \text{ J}^{-1} \text{ C}^2 \text{ m}^{-1}$$

$$N_0 = 6.022 \times 10^{23} \text{ mol}^{-1}$$

$$\pi = 3.14159$$

$$H_{\text{translational}} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$$

$$p_{\text{translational}} = \frac{\hbar}{i} \frac{d}{dx}$$

Particle in a 1D box

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{n^2 \hbar^2}{8mL^2} \quad n = 1, 2, 3, \dots$$

1D Harmonic oscillator

$$\psi_v = N_v H_v(y) e^{-\frac{1}{2}y^2} \quad y = \frac{x}{\alpha} \quad \alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}$$

$$N_v = \left(\frac{1}{2^v v! \pi^{1/2} \alpha}\right)^{1/2} \quad H_v(y) = \text{Hermite Polyn}$$

$$E_v = \left(v + \frac{1}{2}\right) \hbar\omega \quad v = 0, 1, 2, 3, \dots$$

1. Consider the wavefunction: $\psi = k\hbar e^{ikx}$

a) (20 points) Show that it is an eigenfunction of H

$$H\psi = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} k\hbar e^{ikx} = \frac{-\hbar^2}{2m} k\hbar \frac{d^2}{dx^2} e^{ikx} = \frac{-\hbar^2}{2m} k\hbar (ik) \frac{d}{dx} e^{ikx} = \frac{-\hbar^2}{2m} k\hbar (ik)^2 e^{ikx}$$

$$H\psi = \frac{\hbar^2 k^2}{2m} k\hbar e^{ikx} = \frac{\hbar^2 k^2}{2m} \psi$$

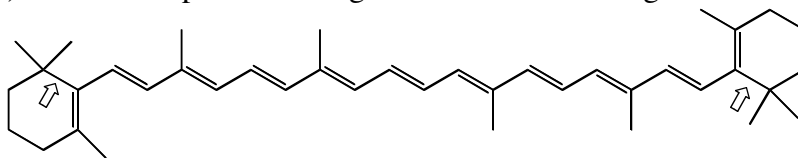
b) (10 points) What can you conclude about the *motion* of an electron described by this wavefunction? Your conclusions should be both quantitative and qualitative.

We can use the operator for momentum to find out about motion

$$p_{\text{translational}}\psi = \frac{\hbar}{i} \frac{d}{dx} k\hbar e^{ikx} = \frac{\hbar}{i} (ik) k\hbar e^{ikx} = \hbar k (k\hbar e^{ikx}) = \hbar k \psi$$

From this we can see that the momentum is positive. The particle is *moving forward* (towards positive x) with momentum $\hbar k$

2. (20 points) The chromophore which gives carrots their orange color is beta-carotene.



The color of tomatoes is due to a similar molecule, in which the rings have undergone scission where indicated. What color are tomatoes (*explain* briefly)?

Of course, we know that tomatoes are red. The transition is at lower energy and so the box must be bigger. How could that be?

Looking at the structure above, there are clearly steric issues surrounding the bond linking the long chain to the ring – the ring cannot be purely coplanar with the connector. Thus, the “box” does not contain the double bond within the ring (or it contains it “less”). Cleavage where indicated relieves the steric strain induced by the two methyl groups, so that the (previously ring) double bond can now fully conjugate into the system (on both ends).

3. (25 points) An electron is confined to a one dimensional box of length L . What should the length of the box be in order for the electron's zero point energy to be equal to its rest mass energy of $m_e c^2$?

Use the equation for the energy of the particle in a box:

$$m_e c^2 = E_1 = \frac{1^2 h^2}{8mL^2}$$

$$L^2 = \frac{h^2}{8m_e m_e c^2}$$

$$L = \frac{h}{\sqrt{8}m_e c} = \frac{6.626 \times 10^{-34} \text{ J s}}{\sqrt{8}(9.109 \times 10^{-31} \text{ kg})(2.998 \times 10^8 \text{ m s}^{-1})} \left(\frac{1 \text{ kg m}^2}{\text{J s}^2} \right) = 8.58 \times 10^{-13} \text{ m} = 0.86 \text{ pm}$$

4. a) (15 points) The potentials below left show the scenario described for the simple one-dimensional particle in a box. Draw on top of the potentials, the functions for the $n=1$ (top) wavefunction and the $n=2$ (lower) wavefunction.

This is simple. As we saw in class, The lowest energy wavefunction is a sine wave with no nodes. The second is a sine wave with one node.

- b) (10 points) The potentials below right show a slightly modified potential in which one “wall of the box” is not at infinitely high potential. Draw the same wavefunctions for $n=1$ and $n=2$, but illustrating how the wavefunction will change in this new potential. Think about what you expect from the limits of classical behavior.

The primary point here is that whereas the particle will not go where there is an infinitely large potential, lowering that potential should increase the probability of finding the particle in the high potential area. Thus the wavefunction must be non-zero in this region.

