

Name

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(16) 1. **Short Answer:** Just answer True/False or Yes/No (no explanation required).

(a) Is the operator, ix^2 (mult. by ix^2) Hermitian?

No

(b) Is the operator $i^2 \frac{d^2}{dx^2}$ Hermitian

Yes

(c) Is the function, $Ae^{-\beta x}$, an Eigenfunction of the $\hat{p}^2$ operator?

Yes

(d) True/False: The derivative, $d\psi/dx$, must be continuous at boundaries in which the potential energy is infinite (i.e. $V \rightarrow \infty$).

False

(e) True/False: If two operators commute with a third, they will commute with each other.

False

(f) Which of following 3 operators is/are linear?

✓ $x \cdot \frac{d}{dx}$

✗ $\cosine$ (cosine of the function),

✓ $x \cdot \int$ (take the integral and multiply by x)

(g) Which (one or more) of the functions below would be acceptable as a wavefunction over the indicated interval?

✓ $e^{-x} \sin(x)$ $(0, \infty)$

✗ $e^{-|x|}$ $(-\infty, \infty)$

✗ $\frac{1}{(1-x^2)}$ $(-1, 1)$

1. Short Answer - Cont'd.

(h) True/False: The potential energy between a hydrogen nucleus and an electron is a function of "r", the distance between the nucleus and the electron, $V = -e^2/r$. Because r, and therefore, V, is a function of time, one must use the **time dependent** form of the Schrodinger Equation for the hydrogen atom.

False.

- (10) 2. An Argon Atom ($M = 40.0$ amu) has a de Broglie wavelength of 0.004 nm ($= 4.00$ pm). Calculate the energy of the Argon atom, in eV (electron volts).

$$m = 40 \text{ amu}$$

$$= 6.64 \times 10^{-26} \text{ kg}$$

$$\lambda = \frac{h}{p} \rightarrow p = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34} \text{ kg m}^2/\text{s}}{4 \times 10^{-12} \text{ m}} = 1.66 \times 10^{-22} \text{ kg m/s}$$

$$E = \frac{p^2}{2m} = \frac{(1.66 \times 10^{-22} \text{ kg m/s})^2}{2 (6.64 \times 10^{-26} \text{ kg})} = 2.07 \times 10^{-19} \text{ J (kg m}^2/\text{s}^2)$$

$$E = 2.07 \times 10^{-19} \text{ J} \times \frac{1 \text{ eV}}{1.60 \times 10^{-19} \text{ J}}$$

$$= 1.29 \text{ eV} \approx \boxed{1.3 \text{ eV}}$$

- (5) 3. Simplify the following complex expression: $\frac{(8-3i)^*}{2+i}$

Your final answer should be of the form, $a+bi$, where a and b are real constants.

$$\frac{(8-3i)^*}{2+i} \times \frac{2-i}{2-i} = \frac{(8+3i)(2-i)}{4-i^2} = \frac{16 - 8i + 6i - 3i^2}{5}$$

$$= \frac{19 - 2i}{5} = \boxed{3.8 - 0.4i}$$

- (10) 4. Consider a Helium Nucleus ($m_{\text{He}} = 4.0 \text{ amu}$) in a $12 \text{ \AA}$ box; i.e. the uncertainty in the proton's position is $12 \text{ \AA}$. Calculate the uncertainty of the Helium nucleus' velocity, in m/s.

$$\begin{aligned}
 m &= 4.0 \text{ amu} \\
 &= 6.64 \times 10^{-27} \text{ kg}
 \end{aligned}
 \quad \left\{ \begin{aligned}
 \Delta x &= 12 \text{ \AA} = 1.2 \times 10^{-9} \text{ m} \\
 \Delta p &= \frac{h/2}{\Delta x} = \frac{1.05 \times 10^{-34} \text{ kg m}^2/\text{s}}{2 (1.2 \times 10^{-9} \text{ m})} \\
 &= 4.38 \times 10^{-26} \text{ kg m/s}
 \end{aligned} \right.$$

$$\begin{aligned}
 p &= mV \rightarrow \Delta p = m \Delta V \rightarrow \Delta V = \frac{\Delta p}{m} = \frac{4.38 \times 10^{-26} \text{ kg m/s}}{6.64 \times 10^{-27} \text{ kg}} \\
 &= 6.6 \text{ m/s}
 \end{aligned}$$

(10) 5. Calculate the commutator: $\left[\frac{d}{dx}, \frac{d}{dx} - x^2 \right] \psi = \frac{d}{dx} \left(\frac{d}{dx} - x^2 \right) \psi - \left(\frac{d}{dx} - x^2 \right) \frac{d}{dx} \psi = A - B$

$$\begin{aligned}
 A &= \frac{d}{dx} \left(\frac{d}{dx} - x^2 \right) \psi = \frac{d}{dx} \left(\frac{d\psi}{dx} - x^2 \psi \right) \\
 &= \frac{d^2 \psi}{dx^2} - x^2 \frac{d\psi}{dx} - 2x \psi
 \end{aligned}$$

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

$$A - B = \frac{d^2 \psi}{dx^2} - x^2 \frac{d\psi}{dx} - 2x \psi - \left(\frac{d^2 \psi}{dx^2} - x^2 \frac{d\psi}{dx} \right) = -2x \psi$$

$$\therefore \left[\frac{d}{dx}, \frac{d}{dx} - x^2 \right] = \boxed{-2x}$$

$$\hat{K} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad \left(\psi = A e^{i k x - i \omega t} \right)$$

$$m = 32 \text{ amu} \times 1.66 \times 10^{-27} \text{ kg} = 5.31 \times 10^{-26} \text{ kg}$$

(12) 6. A suitable wavefunction for a free particle [$V(x)=0$, $-\infty < x < +\infty$] is given by:

$$\psi = A e^{i k x - i \omega t}, \text{ where } k = 4.0 \times 10^{10} \text{ m}^{-1}.$$

(9) (a) Consider an O_2 ($M = 32 \text{ amu}$) molecule moving freely in one dimension. Show that the above wave function is an eigenfunction of the Kinetic Energy Operator, and determine the average kinetic energy of the O_2 molecule (in J)

$$\frac{d\psi}{dx} = i k \psi \rightarrow \frac{d^2\psi}{dx^2} = (i k)^2 \psi = -k^2 \psi$$

$$\hat{K}\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m} (-k^2) \psi = \frac{\hbar^2 k^2}{2m} \psi$$

$$KE = \frac{\hbar^2 k^2}{2m} = \frac{(1.05 \times 10^{-34} \text{ J}\cdot\text{s})^2 (4.0 \times 10^{10} \text{ m}^{-1})^2}{2 (5.31 \times 10^{-26} \text{ kg})} = 1.66 \times 10^{-22} \text{ J}$$

$$\frac{J^2 s^2}{kg m^2} = \frac{J^2}{kg m^2}$$

$$= 1.66 \times 10^{-22} \frac{J^2}{kg m^2} = \boxed{1.66 \times 10^{-22} \text{ J}}$$

I showed the unit analysis. However, it's probably easier to be sure to use MKS, which yields energy in Joules

(3) (b) Explain why the above complex function is a valid wavefunction for a free particle, whereas the real function, $\psi = A \cos(kx - \omega t)$, is not a valid wavefunction for a free particle. A sentence or two (if correct) should be sufficient

If the particle is in free space, one expects $\psi\psi = \text{const}$ (for all x)

$\psi\psi = A^2 \cos^2(kx - \omega t)$ is not constant.

$$m = m_e = 9.11 \times 10^{-31} \text{ kg}$$

Note: The following 3 questions are all based upon a one-dimensional Particle in a Box (PIB).
However they are NOT related. i.e. a result of one of the questions is not needed in another question

- (11) 7. Consider an electron in a one dimensional box of length, a . When the electron drops from the $n=8$ level to the $n=5$ level, it emits a photon with the wavelength, $2600 \text{ \AA}$ ($1 \text{ \AA} = 1 \times 10^{-10} \text{ m}$). Calculate a (the length of the box), in nm.

$$\lambda = 2600 \text{ \AA} \times \frac{10^{-10} \text{ m}}{1 \text{ \AA}} = 2.6 \times 10^{-7} \text{ m}$$

$$E_{ph} = h\nu = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(3 \times 10^8 \text{ m/s})}{2.6 \times 10^{-7} \text{ m}} = 7.65 \times 10^{-19} \text{ J}$$

$$E_{ph} = \Delta E = E_8 - E_5 = \frac{8^2 h^2}{8ma^2} - \frac{5^2 h^2}{8ma^2} = \frac{39 h^2}{8ma^2}$$

$$\begin{aligned} \therefore a^2 &= \frac{39 h^2}{8m E_{ph}} = \frac{39 (6.63 \times 10^{-34} \text{ J}\cdot\text{s})^2}{8 (9.11 \times 10^{-31} \text{ kg}) (7.65 \times 10^{-19} \text{ J})} \\ &= 3.07 \times 10^{-18} \text{ m}^2 \\ &= 3.07 \times 10^{-18} \text{ m}^2 \end{aligned}$$

$\left(\frac{\text{J}\cdot\text{s}^2}{\text{kg}\cdot\text{J}} = \frac{\frac{\text{kg}\cdot\text{m}^2}{\text{s}^2} (\text{s}^2)}{\text{kg}} \right)$

$$\therefore a = \sqrt{3.07 \times 10^{-18} \text{ m}^2} = 1.75 \times 10^{-9} \text{ m}$$

$$\times \frac{1 \text{ nm}}{10^{-9} \text{ m}} = \boxed{1.75 \text{ nm}}$$

Again, you might find it easier to use MKS
 & assume the unit works out - rather than a
 complete unit analysis

(10) 8. Consider a particle in a box, defined by the potential

$$V(x) = 0 \quad -2b \leq x \leq +2b$$

$$V(x) \rightarrow \infty \quad x < -2b, x > +2b$$

An approximate wavefunction is:

$$\psi = C \cos\left(\frac{\pi}{4b}x\right) \quad -2b \leq x \leq +2b$$

$$\psi = 0 \quad x < -2b, x > +2b$$

C is the normalization constant

Calculate the normalization constant, C, as a function of b

Hint: The needed integral is on the information sheet.

$$1 = \int_{-2b}^{2b} \psi^2 dx = \int_{-2b}^{2b} C^2 \cos^2\left(\frac{\pi x}{4b}\right) dx = C^2 \int_{-2b}^{2b} \cos^2 \alpha x dx$$

$\alpha = \frac{\pi}{4b}$

$$= C^2 \left[\frac{1}{2}x + \frac{1}{4\alpha} \sin 2\alpha x \right]_{-2b}^{2b}$$

$$= C^2 \left\{ \left[\frac{1}{2}(2b) + \frac{1}{4\alpha} \sin(2\alpha \cdot 2b) \right] - \left[\frac{1}{2}(-2b) + \frac{1}{4\alpha} \sin(-2\alpha \cdot 2b) \right] \right\}$$

$$= C^2 [b - (-b)] = C^2 (2b) = 1$$

$$C^2 = \frac{1}{2b}$$

$$C = \sqrt{\frac{1}{2b}}$$

$$2\alpha \cdot 2b = 2 \frac{\pi}{4b} 2b$$

$$= \pi$$

$$\sin \pi = \sin -\pi$$

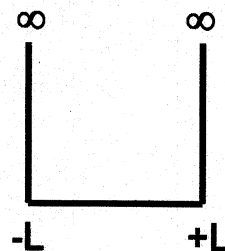
$$= 0$$

(16) 9. Consider a particle in a box defined by the potential:

$$\begin{aligned} V(x) &= 0 & -L \leq x \leq +L \\ V(x) &\rightarrow \infty & x < -L, x > +L \end{aligned}$$

An approximate **normalized** wavefunction for the ground state of the particle is:

$$\begin{aligned} \psi &= B(L^2 - x^2) & B = \sqrt{\frac{15}{16L^5}} & -L \leq x \leq +L \\ \psi &= 0 & x < -L \text{ and } x > +L \end{aligned}$$



(8) (a) Calculate the probability that the particle will be in the region between $x = 0$ and $x = +L/2$

$$\begin{aligned} P(0 \leq x \leq L/2) &= \int_0^{L/2} \psi^2 dx = \int_0^{L/2} B^2 (L^2 - x^2)^2 dx \\ &= B^2 \int_0^{L/2} (L^4 - 2L^2 x^2 + x^4) dx = B^2 \left[L^4 x - 2L^2 \frac{x^3}{3} + \frac{x^5}{5} \right]_0^{L/2} \\ &= B^2 \left[L^4 \left(\frac{L}{2} \right) - \frac{2L^2}{3} \left(\frac{L}{2} \right)^3 + \frac{1}{5} \left(\frac{L}{2} \right)^5 \right] - 0 \\ &= B^2 \left[\frac{L^5}{2} - \frac{L^5}{12} + \frac{L^5}{160} \right] \\ &= \left(\frac{15}{16L^5} \right) (0.4229 L^5) \\ &= 0.396 \approx \boxed{0.40} \end{aligned}$$

Part b on next page

$$\hat{K} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$$

9 (Cont'd.)

(8) (b) Calculate the average (i.e. expectation) value of the kinetic energy as a function of $\hbar$, m and L .

$$\psi = B(L^2 - x^2) \rightarrow \frac{d^2\psi}{dx^2} = -2Bx \rightarrow \frac{d^2\psi}{dx^2} = -2B$$

$$\langle K \rangle = \int \psi \left(\frac{-\hbar^2}{2m} \right) \frac{d^2\psi}{dx^2} dx = -\frac{\hbar^2}{2m} \int B(L^2 - x^2)(-2B) dx$$

$$= -\frac{\hbar^2}{2m} (-2B^2) \int_{-L}^L (L^2 - x^2) dx$$

$$= \frac{\hbar^2}{2m} B^2 \left[L^2 x - \frac{x^3}{3} \right]_{-L}^L$$

$$= \frac{\hbar^2}{2m} B^2 \left[\left(L^2 L - \frac{L^3}{3} \right) - \left(-L^2 L - \frac{L^3}{3} \right) \right]$$

$$= \frac{\hbar^2}{2m} B^2 \left[2L^3 - \frac{2}{3} L^3 \right] = \frac{\hbar^2}{2m} B^2 \left(\frac{4}{3} L^3 \right)$$

$$= \frac{\hbar^2}{2m} \left(\frac{15}{16L^5} \right) \left(\frac{4}{3} L^3 \right) = \frac{60}{96} \frac{\hbar^2}{m L^2} = \frac{5}{8} \frac{\hbar^2}{m L^2}$$

$$= \frac{5}{8} \frac{1}{(2\pi)^2} \frac{\hbar^2}{m L^2} = \frac{5}{32\pi^2} \frac{\hbar^2}{m L^2}$$

$$= 0.0158 \frac{\hbar^2}{m L^2}$$