

EXAM 1: INFORMATION

Potentially Useful Formulas

De Broglie Wavelength: $\lambda = \frac{h}{p}$ **Uncertainty Principle:** $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

An Hermitian operator satisfies the relation: $\int \psi_j^* \hat{A} \psi_i d\tau = \int \psi_i (\hat{A} \psi_j)^* d\tau$

One Dimensional Schrödinger Equation: $H = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \psi = E \psi$

One Dimensional PIB Energies: $E_n = \frac{n^2 h^2}{8ma^2} \quad n = 1, 2, 3, \dots$

Momentum Operators: $\hat{p} = \frac{\hbar}{i} \frac{d}{dx} \quad \hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$

Kinetic Energy: $KE = \frac{1}{2} mv^2 = \frac{p^2}{2m}$

Integrals (you will not need most of them)

$$\int \sin^2(\alpha x) dx = \frac{1}{2} x - \frac{1}{4\alpha} \sin(2\alpha x)$$

$$\int \cos^2(\alpha x) dx = \frac{1}{2} x + \frac{1}{4\alpha} \sin(2\alpha x)$$

$$\int \sin(\alpha x) \cos(\alpha x) dx = \frac{1}{2\alpha} \sin^2(\alpha x)$$

Constants and Conversions:

$$h = 6.63 \times 10^{-34} \text{ J}\cdot\text{s} = 6.63 \times 10^{-34} \text{ kg}\cdot\text{m}^2/\text{s}$$

$$\hbar = h/2\pi = 1.05 \times 10^{-34} \text{ J}\cdot\text{s} = 1.05 \times 10^{-34} \text{ kg}\cdot\text{m}^2/\text{s}$$

$$1 \text{ J} = 1 \text{ kg}\cdot\text{m}^2/\text{s}^2$$

$$c = 3.00 \times 10^8 \text{ m/s} = 3.00 \times 10^{10} \text{ cm/s} \quad k \cdot N_A = R$$

$$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$$

$$k = 1.38 \times 10^{-23} \text{ J/K}$$

$$1 \text{ atm.} = 1.013 \times 10^5 \text{ Pa}$$

$$R = 8.31 \text{ J/mol}\cdot\text{K}$$

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

$$R = 8.31 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$$

$$1 \text{ \AA} = 10^{-10} \text{ m}$$

$$m_e = 9.11 \times 10^{-31} \text{ kg (electron mass)}$$

$$m_p = 1.67 \times 10^{-27} \text{ kg (proton mass)}$$

$$1 \text{ amu} = 1.66 \times 10^{-27} \text{ kg}$$

Name _____

(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?(b) Is the operator $i^2 \frac{d^2}{dx^2}$ Hermitian(c) Is the function, $Ae^{-\beta x}$, an Eigenfunction of the $\hat{p}^2$ operator?(d) True/False: The derivative, $d\psi/dx$, must be continuous at boundaries in which the potential energy is infinite (i.e. $V \rightarrow \infty$).

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

(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?

$$e^{-x} \sin(x) \quad (0, \infty)$$

$$e^{-|x|} \quad (-\infty, \infty)$$

$$\frac{1}{(1-x^2)} \quad (-1, 1)$$

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.

- (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).

- (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.

- (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.

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

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

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

(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)

(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

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.

(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

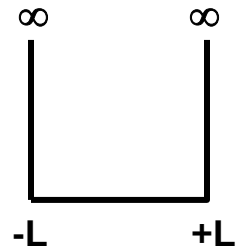
Hint: The needed integral is on the information sheet.

(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 $x = +L/2$

Part b on next page

9 (Cont'd.)

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