CHM 3411, Dr. Chatfield, February 19, 2018

Exam 1

Questions 1-6 are worth 14 points each, and question 7 is worth 16 points. You may use a calculator (non-graphing), but nothing else. If you need extra room, use the back of exam pages and direct the grader where to look. You may also use scratch paper, but ***put all final answers on the exam itself and attach any scratch paper with work the grader should read.***. ***Read all problems carefully***. Set up problems methodically, show your work, and be neat. Partial credit will be given when it is possible for me to follow your work. If you are having trouble with a problem, go on to the next and come back.

GOOD LUCK!

Constants:

$h = 6.626 \times 10^{-34}\, Js$ $\quad \hbar = \frac{h}{2\pi}$ $\quad m_e = 9.11 \times 10^{-31}\, kg$ $\quad c = 3.00 \times 10^{8}\, m\, s^{-1}$

$k_B = 1.38 \times 10^{-23}\, J\, K^{-1}$ $\quad N_A = 6.022 \times 10^{23}\, mol^{-1}$ $\quad amu = 1.66 \times 10^{-27}\, kg$

Equations (others are given directly in exam questions):

$\lambda = \frac{h}{p}$ $\quad \Delta x \Delta p \geq \frac{\hbar}{2\pi}$ $\quad \lambda \nu = c$ $\quad \tilde{\nu} = \frac{1}{\lambda}$ $\quad \Delta E = h\nu = \hbar\omega$ $\quad d\tau = r^2 sin\theta dr d\theta d\phi$

$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x)$ $\quad \hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + \hat{V}(x)$ $\quad E = \left(v + \frac{1}{2}\right)\hbar\omega$ $\quad E = l(l+1)\frac{\hbar^2}{2I}$ $\quad |l_z| = m_l \hbar$

$|l^2| = l(l+1)\hbar^2$ $\quad \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$

E

1.This question concerns a harmonic oscillator with frequency $\omega = 9.00 \times 10^{12}\, s^{-1}$.

(a) Determine the zero point energy (in Joules).

$ZPE = \frac{1}{2}\hbar\omega = \boxed{4.75 \times 10^{-22}\, J}$

$(v = 0, 1, 2 \ldots;\ v_{min} = 0;\ ZPE = (v_{min} + \frac{1}{2})\hbar\omega = \frac{1}{2}\hbar\omega)$

(b) Suppose the harmonic oscillator is originally in the v = 3 state and makes a transition to the v=2 state, emitting a photon. Determine the wavelength of the photon.

$\Delta E = E_{photon}$

$h\nu = \frac{hc}{\lambda}$

$\frac{7}{2}\hbar\omega - \frac{5}{2}\hbar\omega = \hbar\omega$

$(3 + \frac{1}{2})\hbar\omega$

$\hbar\omega = \frac{hc}{\lambda}$

$\lambda = \frac{hc}{\hbar\omega} = \frac{2\pi c}{\omega}$

$3.00 \times 10^{8}\, m\, s^{-1}$

$\boxed{\lambda = 2.09 \times 10^{-4}\, m}$

E

2. Consider the following unnormalized wavefunction:

$$\psi(x) = Nx(L-x) \qquad 0 \le x \le L$$
$$\psi(x) = 0 \qquad \text{otherwise } (x < 0 \text{ or } x > L)$$

(a) Determine the value of N, the normalization constant.

$$1 = \int_0^L \psi^* \psi \, dx = N^2 \int_0^L x^2 (L-x)^2 dx$$

$$\tfrac{1}{2} L x^4$$

$$\frac{1}{N^2} = \int_0^L (L^2 x^2 - 2Lx^3 + x^4)\, dx = \frac{1}{3} L^2 x^3 - \frac{2}{4} L x^4 + \frac{1}{5} x^5 \Big|_0^L$$

$$= \left(\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right) L^5 = \frac{10-15+6}{30} L^5 = \frac{L^5}{30}$$

$$\boxed{N = \sqrt{\frac{30}{L^5}}}$$

(b) You want to determine the probability of finding the particle between x=0 and x=0.3L. Write an explicit equation (include all limits and write out all functions), but do not evaluate it.

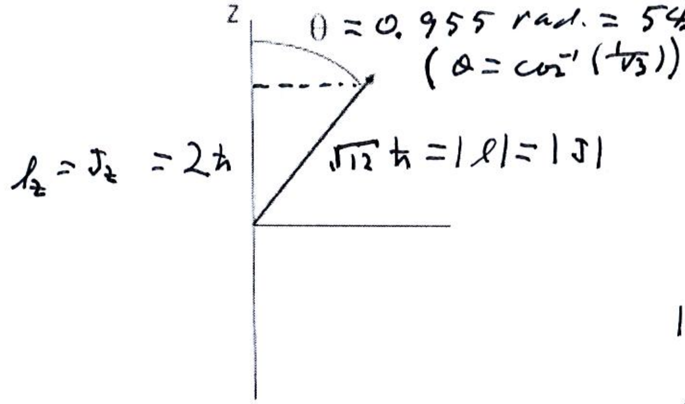
$$P = \int_0^{0.3} \psi^* \psi \, dx = \frac{30}{L^5} \int_0^{0.3L} x^2 (L-x)^2 dx$$

M

3. Consider the l=3, m_l = 2 state of a particle on the surface of a sphere.

(a). Below is a vector diagram for the angular momentum. Calculate and label on the diagram:

1. The magnitude of the angular momentum.
2. The value of the z-component of the angular momentum.
3. The value of the angle θ. If you cannot determine the numerical value, an algebraic expression is sufficient.

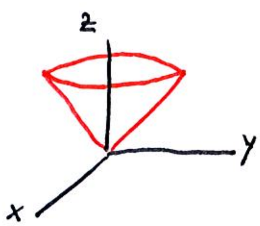


$$|\ell^2| = \ell(\ell+1)\hbar^2 \Rightarrow |\ell| = [\overset{3}{\ell}(\ell+1)]^{1/2}\hbar = \sqrt{12}\,\hbar$$

$$|\ell_z| = \overset{2}{m_\ell}\,\hbar = 2\hbar$$

$$\cos\theta = \frac{2\hbar}{\sqrt{12}\,\hbar} = \frac{1}{\sqrt{3}} \qquad \theta = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 0.955 \text{ rad.} = 54.7^\circ$$

(b) Draw a cone diagram for this same state.



(c) The cone model is a better model. Explain why.

One cannot simultaneously specify J_z and J_x or J_z and J_y because J_x, J_y and J_z are complementary variables ($[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$ etc.). However, $J_x^2 + J_y^2 = J^2 - J_z^2$.

D

4. Suppose that the wavefunction is the following superposition of momentum eigenfunctions:

$$\psi(x) = 0.63e^{2ikx} + 0.45e^{4ikx} + 0.32e^{5ikx} + 0.55e^{7ikx}$$

(a) What values of the momentum can result from an individual measurement? Give the values in terms of k.

Note: e^{inx} is a momentum eigenfunction for any n b/c

$$\hat{p}_x e^{inx} = \frac{\hbar}{i}\frac{d}{dx} e^{inx} = \frac{\hbar}{i}\cdot in\, e^{inx} = \underbrace{n\hbar}_{\text{eigenvalue}}\, e^{inx}$$

The values allowed for a measurement are the eigenvalues corresponding to the eigenfunctions that compose the wavefunction

$\boxed{\therefore \text{ allowed values} = 2k\hbar,\ 4k\hbar,\ 5k\hbar,\ 7k\hbar}$

(b) For each value you listed for (a), determine the probability than an individual measurement will yield that value.

$$\psi(x) = c_1\phi_1 + c_2\phi_2 + c_3\phi_3 + c_4\phi_4 \quad \text{where} \begin{Bmatrix} \phi_1 = e^{2ikx} & \phi_2 = e^{4ikx} \text{ etc} \\ w_1 = 2k\hbar & w_2 = 4k\hbar \end{Bmatrix}$$

$$P(w_i) = |c_i|^2 \Rightarrow$$

$$\boxed{\begin{array}{ll} P(2k\hbar) = 0.63^2 = 0.40 & P(5k\hbar) = 0.32^2 = 0.10 \\ P(4k\hbar) = 0.45^2 = 0.20 & P(6k\hbar) = 0.55^2 = 0.30 \end{array}}$$

(c). Calculate the expectation value of the momentum, <p$_x$>. Remember that the momentum eigenfunctions are orthonormal.

$$\langle p_x \rangle = \int \psi^* \frac{\hbar}{i}\frac{d}{dx}\psi\, dx = \int \left(0.63e^{-2ikx} + 0.45e^{-4ikx} + \dots\right)\frac{\hbar}{i}\frac{d}{dx}\left(0.63e^{2ikx} + 0.45e^{4ikx} + \dots\right)dx$$

$$= \sum_i \sum_j c_i^* c_j w_j \underbrace{\int \phi_i^* \phi_j\, dx}_{\substack{=1 \ i=j \\ =0 \ i\neq j}} = \sum_j |c_j|^2 w_j$$

$$= 0.63^2(2k\hbar) + 0.45^2(4k\hbar) + 0.32^2(5k\hbar) + 0.55^2(6k\hbar)$$

$$\boxed{\langle p_x \rangle = 3.93k\hbar}$$

6. Answer the following multiple choice questions by circling the correct answer(s).

M

(a). Circle all of the following statements that are true.

(A) Quantum mechanical operators commute with each other.

(B) Quantum mechanical operators are normalizable.

(C) Quantum mechanical operators have real eigenvalues.

(D) Quantum mechanical operators have real eigenfunctions.

E

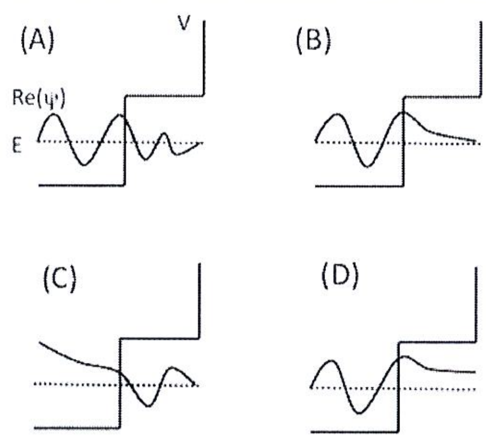
(b). When the wavefunction $\psi(x) = Nx^3$ is normalized over the interval 0 to 5, what is the value of the normalization constant *N*?

(A) $N = \left(\int_0^5 x^3 dx\right)^{-\frac{1}{2}}$ (B) $N = \int_0^5 x^6 dx$

(C) $N = \int_0^5 x^3 dx$ (D) $N = \left(\int_0^5 x^6 dx\right)^{-\frac{1}{2}}$

M

(c). Circle the correct figure. The height of E is the total energy, V is the potential energy (a step function that goes to infinity at the right), the dotted line is the baseline for the wavefunction, and the real part of the wavefunction is shown. These are labeled in (A) only but pertain to all figures.



decays in tunneling region ✓
(E < V)
decays to zero b/c $V \to \infty$

E

(d). Which of the following statements demonstrate the quantization of energy? Circle all that apply.

(A) Blackbody radiation (B) Heat capacity of crystalline solids

(C)) Photoelectric effect (D) Electron diffraction

7. Short answer: answer the following questions succinctly.

E

(a) Explain the concept of quantum mechanical tunneling, giving two examples. Your audience is an intelligent non-scientist.

Tunneling occurs when a particle enters a region that is classically forbidden, i.e., $E_{tot} < V$.

Examples: Scanning tunneling microscope
Electron transfer in enzymes (often)

M

(b) Explain the meaning of the classical correspondence principle, giving an example.

The results of quantum mechanics approach those of classical mechanics as the quantum number(s) get very large.

Example: Particle in box as $n \to \infty$

Classical: Probility density is same throughout box

QM: Probability density is peaked around middle of box for $n=1$ but becomes more and more "spread out" as n increases.

$n=1$ $n=2$ $n=3$ ... $n=$ large