Chemistry 410A **Exam 1** **Spring 2016**

NAME:

Instructions:

1. Keep this exam closed until instructed to begin.
2. **Please write your name on this page but not on any other page.**
3. Please silence any noisy electronic devices you have.
4. Attached sheet(s) provide potentially useful constants and equations. You may detach these from the exam.
5. To receive full credit for your work, please
   (a) put your name on your exam;
   (b) show all your work, using only the exam papers, including the back of this sheet if necessary;
   (c) specify the correct units, if any, for your final answers;
   (d) use an appropriate number of significant digits for final numerical answers;
   (e) **stop writing and close your exam immediately when time is called.**

Other notes:

- **Problem 1 (covering all of page 3) of the exam is worth 40 points.** Partial credit for these problems is not necessarily available.
- **Your 2 best scores of the 3 remaining problems will count towards the other 60 points.** Partial credit is available for these problems, so try each problem and do not erase any of your work.

1. **40 points.**

(a) The highest measured energy for a photon is (at this writing) 16 TeV, where 1 TeV $= 1.602 \cdot 10^{-6}$ J. Calculate the wavelength in meters for this photon.

(b) Calculate the transition energy from the (2,2,2) to the (3,3,3) state of an electron in a cube-shaped box if the energy of the (1,1,1) state is $1.0 \cdot 10^{-17}$ J.

(c) If a hydrogen atom begins in the $n = 4$ state, what is the value of the quantum number n of the final state in the transition that *emits the highest frequency* photon?

(d) A particle is placed in a box of length a and has an uncertainty in momentum $\delta p = 1.0 \cdot 10^{-24}$ in SI units.

i. What are the SI units for δp?

ii. We then divide the length of the box in half. What does the uncertainty principle predict is the new value of δp?

2. (a) Normalize the function

$$\psi(x) = \begin{cases} A(1+x) & 0 \le x < 3 \\ 0 & x < 0 \text{ and } 3 \le x \end{cases}$$

(b) Calculate the probability density of the particle between $x = 0$ and $x = 1$.

3. For each of the following particle-in-a-1D-box systems, write **A** or **B** to indicate which case has the *greater number of nodes* in the wavefunction, or write **both** if A and B have an equal number of nodes:

(a) (A) the $n = 2$ state of an electron
(B) the $n = 4$ state of an electron in the same box.

(b) (A) the $n = 2$ state of an electron
(B) a proton at the same energy in the same box.

(c) (A) the $n = 2$ state of an electron
(B) the $n = 2$ state of a proton in the same box.

(d) (A) the $n = 2$ state of an electron in a box of length a
(B) an electron at the same energy in a box of length $2a$

(e) (A) the $n = 2$ state of an electron in a box of length a
(B) the $n = 2$ state of an electron in a box of length $2a$

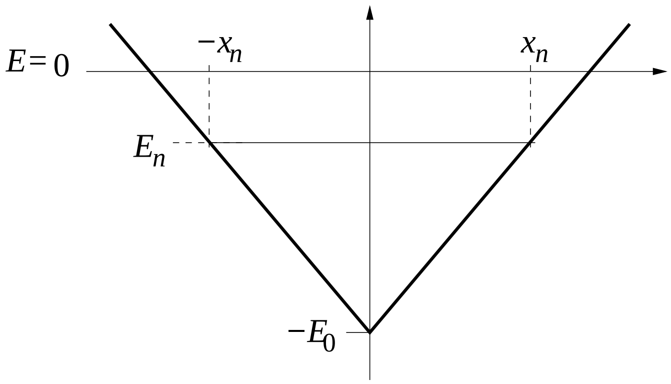
(f) (A) the $n = 2$ state of an electron in a box of length a
(B) the $n = 8$ state of an electron in a box of length $2a$

4. Imagine that Bohr had decided to quantize the *radial* motion of the electron instead of the angular motion, letting the electron travel only along a straight line (let's call it the x axis) through the nucleus. To simplify the problem, we'll use a different potential energy function, graphed below:

$$U(x) = c\,|x| - E_0.$$

If we apply classical mechanics the way Bohr did, this potential energy predicts that the electron will oscillate back and forth between two points x_n and $-x_n$, where the speed at any *positive* value of x is

$$v(x) = \sqrt{-\frac{2c}{m}(x - x_n)}.$$



(a) If the electron is again treated as a de Broglie wave, will this atom radiate electromagnetic radiation? Give a brief (1 sentence) justification for your answer.

(b) Assume that the energy must still satisfy the equation $E = -b/n^2$ and solve for x_n in terms of b, c, m, n, and E_0.

Fundamental Constants

Avogadro's number	$\mathcal{N}_A$	$6.0221367 \cdot 10^{23}$ mol^{-1}
Bohr radius	$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$	$5.29177249 \cdot 10^{-11}$ m
Boltzmann constant	k_B	$1.380658 \cdot 10^{-23}$ J K^{-1}
electron rest mass	m_e	$9.1093897 \cdot 10^{-31}$ kg
fundamental charge	e	$1.6021773 \cdot 10^{-19}$ C
permittivity factor	$4\pi\epsilon_0$	$1.113 \cdot 10^{-10}$ C^2 J^{-1} m^{-1}
gas constant	R	8.314510 J K^{-1} mol^{-1}
	R	0.08314510 L bar K^{-1} mol^{-1}
	R	0.08206 L atm K^{-1} mol^{-1}
hartree	$E_\mathrm{h} = \frac{m_e e^4}{(4\pi\epsilon_0)^2\hbar^2}$	$4.35980 \cdot 10^{-18}$ J
Planck's constant	h	$6.6260755 \cdot 10^{-34}$ J s
	$\hbar$	$1.05457266 \cdot 10^{-34}$ J s
proton rest mass	m_p	$1.6726231 \cdot 10^{-27}$ kg
neutron rest mass	m_n	$1.6749286 \cdot 10^{-27}$ kg
speed of light	c	$2.99792458 \cdot 10^8$ m s^{-1}

Unit Conversions

	K	cm^{-1}	kJ mol^{-1}	kcal mol^{-1}	erg	kJ
kHz =	$4.799 \cdot 10^{-8}$	$3.336 \cdot 10^{-8}$	$3.990 \cdot 10^{-10}$	$9.537 \cdot 10^{-11}$	$6.626 \cdot 10^{-24}$	$6.626 \cdot 10^{-34}$
MHz =	$4.799 \cdot 10^{-5}$	$3.336 \cdot 10^{-5}$	$3.990 \cdot 10^{-7}$	$9.537 \cdot 10^{-8}$	$6.626 \cdot 10^{-21}$	$6.626 \cdot 10^{-31}$
GHz =	$4.799 \cdot 10^{-2}$	$3.336 \cdot 10^{-2}$	$3.990 \cdot 10^{-4}$	$9.537 \cdot 10^{-5}$	$6.626 \cdot 10^{-18}$	$6.626 \cdot 10^{-28}$
K =	1	0.6950	$8.314 \cdot 10^{-3}$	$1.987 \cdot 10^{-3}$	$1.381 \cdot 10^{-16}$	$1.381 \cdot 10^{-26}$
cm^{-1} =	1.4388	1	$1.196 \cdot 10^{-2}$	$2.859 \cdot 10^{-3}$	$1.986 \cdot 10^{-16}$	$1.986 \cdot 10^{-26}$
kJ mol^{-1} =	$1.203 \cdot 10^{2}$	83.59	1	0.2390	$1.661 \cdot 10^{-14}$	$1.661 \cdot 10^{-24}$
kcal mol^{-1} =	$5.032 \cdot 10^{2}$	$3.498 \cdot 10^{2}$	4.184	1	$6.948 \cdot 10^{-14}$	$6.948 \cdot 10^{-24}$
eV =	$1.160 \cdot 10^{4}$	$8.066 \cdot 10^{3}$	96.49	23.06	$1.602 \cdot 10^{-12}$	$1.602 \cdot 10^{-22}$
hartree =	$3.158 \cdot 10^{5}$	$2.195 \cdot 10^{5}$	$2.625 \cdot 10^{3}$	$6.275 \cdot 10^{2}$	$4.360 \cdot 10^{-11}$	$4.360 \cdot 10^{-21}$
erg =	$7.243 \cdot 10^{15}$	$5.034 \cdot 10^{15}$	$6.022 \cdot 10^{13}$	$1.439 \cdot 10^{13}$	1	10^{-10}
J =	$7.243 \cdot 10^{22}$	$5.034 \cdot 10^{22}$	$6.022 \cdot 10^{20}$	$1.439 \cdot 10^{20}$	10^{7}	10^{-3}
dm^3 bar =	$7.243 \cdot 10^{24}$	$5.034 \cdot 10^{24}$	$6.022 \cdot 10^{22}$	$1.439 \cdot 10^{22}$	$1.000 \cdot 10^{9}$	0.1000
kJ =	$7.243 \cdot 10^{25}$	$5.034 \cdot 10^{25}$	$6.022 \cdot 10^{23}$	$1.439 \cdot 10^{23}$	10^{10}	1

distance	1 Å =	10^{-10} m	
mass	1 amu =	$1.66054 \cdot 10^{-27}$ kg	
energy	1 J =	1 kg m^2 s^{-2}	= 10^7 erg
force	1 N =	1 kg m s^{-2}	= 10^5 dyn
electrostatic charge	1 C =	1 A s	= $2.9979 \cdot 10^9$ esu
	1 D =	$3.3357 \cdot 10^{-30}$ C m	= $1 \cdot 10^{-18}$ esu cm
magnetic field strength	1 T =	1 kg s^{-2} A^{-1}	= 10^4 gauss
pressure	1 Pa =	1 N m^{-2}	= 1 kg m^{-1} s^{-2}
	1 bar =	10^5 Pa	= 0.98692 atm

$$\text{Balmer:} \qquad E_{\text{photon}} = (2.180 \cdot 10^{-18}\,\text{J}) \left(\frac{1}{n''^2} - \frac{1}{n'^2} \right)$$

$$\text{Bohr atom:} \qquad r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{Z m_e e^2} = \frac{n^2}{Z} a_0 \qquad v_n = \frac{Ze^2}{4\pi\epsilon_0 n\hbar}$$

$$E_n = -\frac{Z^2 m_e e^4}{(4\pi\epsilon_0)^2 2n^2\hbar^2} = -\frac{Z^2}{2n^2} E_{\text{h}} \qquad L_n = m_e r_n v_n = n\hbar$$

$$\text{momentum operator:} \qquad \hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$$

$$\text{kinetic energy operator:} \qquad \hat{K} = -\frac{\hbar^2}{2m}\nabla^2$$

$$\text{particle in a 1-D box:} \qquad \psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$\text{particle in a 3-D box:} \qquad \psi(x,y,z) = \left(\frac{8}{abc}\right)^{1/2} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi x}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

$$\text{Laplacian:} \qquad \nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\text{1-electron Hamiltonian:} \qquad \hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{(4\pi\epsilon_0) r}$$

$$\begin{aligned}
\int x^n dx &= \tfrac{1}{n+1}x^{n+1} + C & \int a\,dx &= a(x+C) \\
\int \tfrac{1}{x} dx &= \ln x + C & \int e^x dx &= e^x + C \\
\int \ln x\,dx &= x\ln x - x + C & \int \tfrac{dx}{x(a+bx)} &= -\tfrac{1}{a}\ln\left(\tfrac{a+bx}{x}\right) + C \\
\int \sin x\,dx &= -\cos x + C & \int \cos x\,dx &= \sin x + C \\
\int \sin^2(ax)dx &= \tfrac{x}{2} - \tfrac{\sin(2ax)}{4a} + C & \int \cos^2(ax)dx &= \tfrac{x}{2} + \tfrac{\sin(2ax)}{4a} + C \\
\int [f(x) + g(x)]dx &= \int f(x)dx + \int g(x)dx & \int_a^b dx &= x|_a^b = b - a \\
\int_0^\infty x^n e^{-ax} dx &= \tfrac{n!}{a^{n+1}} & \int_0^\infty e^{-ax^2} dx &= \tfrac{1}{2}\left(\tfrac{\pi}{a}\right)^{1/2} \\
\int_0^\infty x e^{-ax^2} dx &= \tfrac{1}{2a} & \int_0^\infty x^2 e^{-ax^2} dx &= \tfrac{1}{4}\left(\tfrac{\pi}{a^3}\right)^{1/2} \\
\int_0^\infty x^{2n+1} e^{-ax^2} dx &= \tfrac{n!}{2a^{n+1}} & \int_0^\infty x^{2n} e^{-ax^2} dx &= \tfrac{[1\cdot3\cdot5\ldots(2n-1)]\sqrt{\pi}}{2^{n+1}a^{n+(1/2)}} \\
\int_0^s x^n\ e^{-ax}\ dx &= \tfrac{n!}{a^{n+1}} - e^{-as}\ \sum_{i=0}^n \tfrac{n! s^{n-i}}{a^{i+1}(n-i)!}
\end{aligned}$$