

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) show all your work, using only the exam papers, including the back of this sheet if necessary;
 - (b) specify the correct units, if any, for your final answers;
 - (c) use an appropriate number of significant digits for final numerical answers;
 - (d) **stop writing and close your exam immediately when time is called.**

Other notes:

- **The first page portion 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) What are the quantum numbers for the wavefunction in a three-dimensional that has one node along x , three nodes along y , and no nodes along z ?
- (b) For the $4d$ subshell of an atom:
- what is the value of l ?
 - what are all the possible values of m_l ?
 - what are all the possible values of m_s ?
 - how many orbitals are there?
- (c) In the Hamiltonian for Be:
- how many electron kinetic energy terms appear?
 - how many electron-electron repulsion terms appear?
- (d) For $2s$ electrons in the ground state atoms Be, B^+ , and Li^- :
- which has the greatest amount of shielding?
 - which has the lowest energy $2s$ electrons (having the highest ionization energy)?

2. Find all the states (n_x, n_y, n_z) with energy $7\pi^2\hbar^2/(ma^2)$ for a particle of mass m in a three-dimensional box with sides of length a , $b = a$, and $c = 2a$.

3. Identify the n , l , and m_l quantum numbers of the electron and the atomic number Z of the one-electron atom being analyzed by the integral below, and state in words the property being evaluated. To receive credit for the numerical values, the supporting math or brief explanation must be given.

$$-\frac{128\hbar^2}{3\pi a_0^5} \int_0^\infty \int_0^\pi \int_0^{2\pi} r \left(1 - \frac{r}{a_0}\right) e^{-2r/a_0} \sin\theta e^{-i\phi} \left\{ \nabla^2 \left[r \left(1 - \frac{r}{a_0}\right) e^{-2r/a_0} \sin\theta e^{i\phi} \right] \right\} r^2 dr \sin\theta d\theta d\phi$$

4. Find an equation for the r value of the maximum radial probability density in any orbital where $l = n - 1$, as a function of Z and n .

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

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

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

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

Laplacian: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

Angular and radial terms in the one-electron wavefunctions.

l	m_l	$Y_l^{m_l}(\theta, \phi)$	n	l	$R_{nl}(r)$
0	0	$\sqrt{\frac{1}{4\pi}}$	1	0	$2 \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
1	0	$\sqrt{\frac{3}{4\pi}} \cos \theta$	2	0	$\frac{1}{\sqrt{2}} \left(\frac{Z}{a_0}\right)^{3/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/(2a_0)}$
1	± 1	$\sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$	2	1	$\frac{1}{\sqrt{24}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) e^{-Zr/(2a_0)}$
2	0	$\sqrt{\frac{5}{6\pi}} (3 \cos^2 \theta - 1)$	3	0	$\frac{2}{\sqrt{27}} \left(\frac{Z}{a_0}\right)^{3/2} \left(1 - \frac{2Zr}{3a_0} + \frac{2Z^2 r^2}{27a_0^2}\right) e^{-Zr/(3a_0)}$
2	± 1	$\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi}$	3	1	$\frac{4\sqrt{2}}{27\sqrt{3}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) \left(1 - \frac{Zr}{6a_0}\right) e^{-Zr/(3a_0)}$
2	± 2	$\sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}$	3	2	$\frac{2\sqrt{2}}{81\sqrt{15}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/(3a_0)}$
3	0	$\sqrt{\frac{7}{16\pi}} \cos \theta (5 \cos^2 \theta - 3)$	4	0	$\frac{1}{4} \left(\frac{Z}{a_0}\right)^{3/2} \left(1 - \frac{3Zr}{4a_0} + \frac{Z^2 r^2}{8a_0^2} - \frac{Z^3 r^3}{192a_0^3}\right) e^{-Zr/(4a_0)}$
3	± 1	$\sqrt{\frac{21}{64\pi}} \sin \theta (5 \cos^2 \theta - 1) e^{\pm i\phi}$	4	1	$\frac{1}{16\sqrt{3}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) \left(1 - \frac{Zr}{4a_0} + \frac{Z^2 r^2}{80a_0^2}\right) e^{-Zr/(4a_0)}$
3	± 2	$\sqrt{\frac{105}{32\pi}} \sin^2 \theta \cos \theta e^{\pm 2i\phi}$	4	2	$\frac{1}{64\sqrt{5}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 \left(1 - \frac{Zr}{12a_0}\right) e^{-Zr/(4a_0)}$
3	± 3	$\sqrt{\frac{35}{64\pi}} \sin^3 \theta e^{\pm 3i\phi}$	4	3	$\frac{1}{768\sqrt{35}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^3 e^{-Zr/(4a_0)}$

Integrals

$\int x^n dx = \frac{1}{n+1} x^{n+1} + C$	$\int adx = a(x + C)$
$\int \frac{1}{x} dx = \ln x + C$	$\int e^x dx = e^x + C$
$\int \ln x dx = x \ln x - x + C$	$\int \frac{dx}{x(a+bx)} = -\frac{1}{a} \ln\left(\frac{a+bx}{x}\right) + C$
$\int \sin x dx = -\cos x + C$	$\int \cos x dx = \sin x + C$
$\int \sin^2(ax) dx = \frac{x}{2} - \frac{\sin(2ax)}{4a} + C$	$\int \cos^2(ax) dx = \frac{x}{2} + \frac{\sin(2ax)}{4a} + C$
$\int [f(x) + g(x)] dx = \int f(x) dx + \int g(x) dx$	$\int_a^b dx = x _a^b = b - a$
$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$	$\int_0^\infty e^{-ax^2} dx = \frac{1}{2} \left(\frac{\pi}{a}\right)^{1/2}$
$\int_0^\infty x e^{-ax^2} dx = \frac{1}{2a}$	$\int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4} \left(\frac{\pi}{a^3}\right)^{1/2}$
$\int_0^\infty x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}}$	$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{[1 \cdot 3 \cdot 5 \dots (2n-1)] \sqrt{\pi}}{2^{n+1} a^{n+1/2}}$

Fundamental Constants

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

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}
$\text{dm}^3 \text{ bar}$ =	$7.243 \cdot 10^{24}$	$5.034 \cdot 10^{24}$	$6.022 \cdot 10^{22}$	$1.439 \cdot 10^{22}$	$1.000 \cdot 10^9$	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 =	$1.66054 \cdot 10^{-27} \text{ kg}$
energy	1 J =	$1 \text{ kg m}^2 \text{ s}^{-2} = 10^7 \text{ erg}$
force	1 N =	$1 \text{ kg m s}^{-2} = 10^5 \text{ dyn}$
electrostatic charge	1 C =	$1 \text{ A s} = 2.9979 \cdot 10^9 \text{ esu}$
	1 D =	$3.3357 \cdot 10^{-30} \text{ C m} = 1 \cdot 10^{-18} \text{ esu cm}$
magnetic field strength	1 T =	$1 \text{ kg s}^{-2} \text{ A}^{-1} = 10^4 \text{ gauss}$
pressure	1 Pa =	$1 \text{ N m}^{-2} = 1 \text{ kg m}^{-1} \text{ s}^{-2}$
	1 bar =	$10^5 \text{ Pa} = 0.98692 \text{ atm}$