1. (25 points) a. Determine the expectation value, or average value of r for an excited state of the hydrogen atom where the electron is in a $2p_z$ orbital. You may leave your answer in symbolic form (in terms of numbers and physical constant(s)). The wave function for the orbital is given below.

$$\psi_{210} = \frac{1}{\sqrt{32\pi}}\left(\frac{1}{a_o}\right)^{5/2} r e^{-r/2a_o} \cos\theta$$

$\langle r \rangle =$

1b. Use your average distance from part “a” to develop an expression for the portion of the hydrogen atom’s kinetic energy that arises from the angular momentum of the electron in this excited state. You may take the reduced mass of the system to be the mass of the electron.

$<E_{rot}> =$

2. (20 points) The Hamiltonian operator that describes the energy of a three dimensional harmonic oscillator is given in spherical coordinates by,

$$\widehat{H} = \frac{-\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{k}{2}r^2 \ ,$$

where k is the vibrational force constant, μ is the reduced mass of the oscillator, and r varies over the interval from 0 to ∞ . Using the trial function, $\phi = e^{-\alpha r}$, where α is a variational parameter, estimate the ground state energy for the oscillator. The following integrals should be useful. The true ground state energy is $3\hbar\omega/2$.

$$\int_0^\infty \phi^* \widehat{H}\phi r^2\, dr = \frac{\hbar^2}{8\mu\alpha} + \frac{3k}{8\alpha^5}$$

$$\int_0^\infty \phi^* \phi r^2\, dr = \frac{1}{4\alpha^3}$$

E =

b) Does your answer conform to the variational principle?

3. (20 points) a. A standard test that chemists use for the presence of Na^+ in a mixture is a flame test. Specifically, when a small quantity of the mixture is burned, Na^+ is detected by the emission of an intense yellow light. This emission comes from the decay of an excited Na valence electron from the 3p → 3s energy state and is often referred to as the sodium "doublet" because it consists of two groups of photons with wavelengths of 589.0 and 589.6 nm. Construct an energy level diagram that explains this emission of light. Label the energy levels with the appropriate term symbols and label the spectroscopic transitions with their emission wavelengths.

b. What is the ground state term symbol of Na^+?

4. (10 points) The orbital energies for Ne and Ar determined by the Hartree-Fock self consistent field method are given in the table below.

Ne:

Orbital	ε_i (kJ/mol)
1s	-86.0
2s	-5.06
2p	-1.94

Ar:

1s	-311.35
2s	-32.35
2p	-25.12
3s	-3.36
3p	-1.65

a. Estimate the first ionization energy for each element.

b. Explain the "trend" in ionization energy you obtained in part "a." (Which element is easier to ionize and why.)

5. (15 points)

a) The radial portion of the hydrogen atom eigenfunction that describes the 3p orbital is given by

$R_{31} = \frac{4}{81\sqrt{6}}\left(\frac{1}{a_o}\right)^{3/2}\left(6x - x^2\right)e^{-x/3}$, where x = r/a_o. Determine the radial position of the node(s) in the radial distribution function for the 3p orbital.

r =

b) Given that the most probable radius for the 3p orbital is 12a_o, make a plot of its radial distribution function below. (be sure to label your axes)

6. (15 points)

a) Determine the term symbols needed to describe the excited states of the hydrogen atom with its electron in the n = 2 energy state.

n = 2 term symbols:

b) Determine the term symbols needed to describe the excited states of the hydrogen atom with its electron in the n=3 energy state.

n = 3 term symbols:

c) In the atomic emission spectrum of hydrogen, the n=3 to n=2 transition is the lowest energy transition in the Balmer series. How many unique spectroscopic transitions make up the n=3 to n=2 transition? Construct an energy level diagram to show these transitions.

of transitions: