

Practice Exam 1

Student Name:

Useful Formulas:

- **Magnetization** M of a multiplet with a given total angular momentum J and Landé g -factor g_J is given by

$$M = Ng_J\mu_B J B_J(x), \text{ where}$$

$$x = \frac{g_J\mu_B JB}{k_B T} \text{ and}$$

$$\mu_B = \frac{e\hbar}{2m} = 5.8 \times 10^{-5} \text{ eV/T} \text{ is the Bohr magneton.}$$

The Brillouin function is given by

$$B_J(x) = \frac{2J+1}{2J} \coth\left(\frac{(2J+1)x}{2J}\right) - \frac{1}{2J} \coth\left(\frac{x}{2J}\right).$$

It may be approximated by

$$B_J(x) \approx \frac{J+1}{3J} x \text{ for } x \ll 1.$$

- **Hydrogen atom (Z=1):**

$$R = \frac{me^4}{2\hbar^2} = 13.6 \text{ eV} \text{ Rydberg constant}$$

$$a_B = \frac{\hbar^2}{me^2} = 0.529 \text{ \AA} \text{ Bohr radius}$$

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1. (5 points) X-ray laser pulses can be used to strip atoms of electrons one by one (ionize the atom).
- (a) What is the energy required to remove the last electron from a K atom? The neutral K atom has 19 electrons. The ionization energy of the hydrogen atom is 13.6 eV.
- (b) What is the size of the Bohr radius for this last electron?
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2. (5 points) Consider an electron trapped in a 3-dimensional harmonic oscillator potential. The Hamiltonian in atomic units ($\hbar = m = e^2 = 1$) is given by

$$H = -\frac{1}{2}\nabla^2 + \frac{1}{2}r^2.$$

Let's use a trial wave function for the ground state of the form

$$\psi(\vec{r}) = \frac{1}{\sqrt{\pi\alpha^3}}e^{-r/\alpha}.$$

This gives (do **not** derive this)

$$\frac{\langle \psi|H|\psi \rangle}{\langle \psi|\psi \rangle} = \frac{1}{2\alpha^2} + \frac{3}{2}\alpha^2.$$

What is the best variational ground state energy one can get (in Hartree units)?

3. (10 points) The ground state electronic configuration of the nitrogen atom is $1s^2 2s^2 2p^3$. Treat the $1s$ and $2s$ electrons as core electrons and the $2p$ electrons as valence electrons.

- (a) What is the total spin angular momentum and total orbital angular momentum of the core? Do these core electrons contribute to the magnetic susceptibility χ of the atoms? If so, what is the sign of χ ?
- (b) According to Hund's rules, what is the lowest energy multiplet and what is its degeneracy?
- (c) What is the expression for zero-field magnetic susceptibility of 1 mole of nitrogen atoms at high temperatures T ?
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4. (5 points) A He atom is excited to the $1s^1 2p^1$ configuration. The one-electron spatial wave functions are $\phi_{1s}(\vec{r})$ and $\phi_{2p_m}(\vec{r})$.

- (a) What is the total number of 2-electron states corresponding to this configuration?
- (b) Write down the 2-electron spin triplet excited state wave functions associated with this configuration.
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5. (5 points)

- (a) Write down the wave function for the ground state of the H_2 molecule in the molecular orbital (MO) approximation. Express your answer in terms of the $1s$ hydrogen atom wave functions associated with the two protons, $a(\vec{r})$ and $b(\vec{r})$.
- (b) Draw qualitatively the ground state electronic energy, the repulsive energy between two protons, and the total energy as function of the inter-nuclear separation R .
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