CHM 3411 - Physical Chemistry 2
Second Hour Exam
March 20, 2015

There are five problems on the exam. Do all of the problems. Show your work.

$N_A = 6.022 \times 10^{23}$	$m_e = 9.109 \times 10^{-31}$ kg	1 eV = 1.602×10^{-19} J
$c = 2.998 \times 10^{8}$ m/s	$k = 1.381 \times 10^{-23}$ J/K	1 cm^{-1} = 1.986×10^{-23} J
$h = 6.626 \times 10^{-34}$ J·s	1 kg = 6.022×10^{26} amu	

1. (30 points) Consider the following radial wavefunction as a possible solution to the TISE for the hydrogen atom.

$$R(r) = N\, r \exp(-2r/a_0) \qquad (1.1)$$

where a_0 is the Bohr radius and N is a normalization constant.

a) Find the value for N that makes R(r) a normalized radial wavefunction.

b) How many radial nodes are there for the above wavefunction? Where are they located?

c) What is the value for r_{mp}, the most probable distance between an electron and the nucleus, for an electron whose radial wavefunction is given by eq 1.1? Give your final answer n terms of a_0.

2. (12 points) Without using any summation symbols write the hamiltonian operator for a lithium atom (Z = 3, 3 electrons).

3. (12 points) Consider the following spin wavefunction for a three electron atom

$$\psi_{spin} = (1/2)^{1/2} [\alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3)] \qquad (2.1)$$

a) Is ψ_{spin} an eigenfunction of the operator P_{12} (the operator that exchanges electrons 1 and 2)? If your answer is yes, give the corresponding eigenvalue.

b) Is ψ_{spin} an eigenfunction of the operator P_{13} (the operator that exchanges electrons 1 and 3)? If your answer is yes, give the corresponding eigenvalue.

Note that you need to show sufficient work to justify your answer to receive full credit.

4. (14 points) For each of the following transitions indicate whether the transition is allowed or forbidden. For forbidden transitions list all of the reasons why the transition is forbidden. You only need to use the selection rules that apply for the information given in the problem.

a) $^3D \rightarrow {}^3S$ (in an atom)

b) $^1\Sigma_g^- \rightarrow {}^1\Sigma_u^-$ (in a homonuclear diatomic molecule)

c) $^1\Delta \rightarrow {}^3\Sigma^+$ (in a heteronuclear diatomic molecule)

5. (32 points) For each of the following atoms or molecules find the lowest energy electron configuration and requested electronic states. For cases where there are several electronic states rank them in order from lowest energy to highest energy. For diatomic molecules also indicate the bond order. The ordering of molecular orbitals for heteronuclear diatomic molecules is given.

a) Fe (lowest energy electron configuration and ground state term symbol only)

b) Fe^{3+} (lowest energy electron configuration and ground state term symbol only)

c) NO (lowest energy electron configuration, all term symbols for that configuration, ordering of these states in terms of energy, and bond order)

d) NO^{-} (lowest energy electron configuration, all term symbols for that configuration, ordering of these states in terms of energy, and bond order)