C455A - Homework 7 -- Due Tues. Nov 14 at **5PM in the Professor's MAILBOX**
***Staple your work together*. PUT CHEM 455 on the top page. etc. etc.**

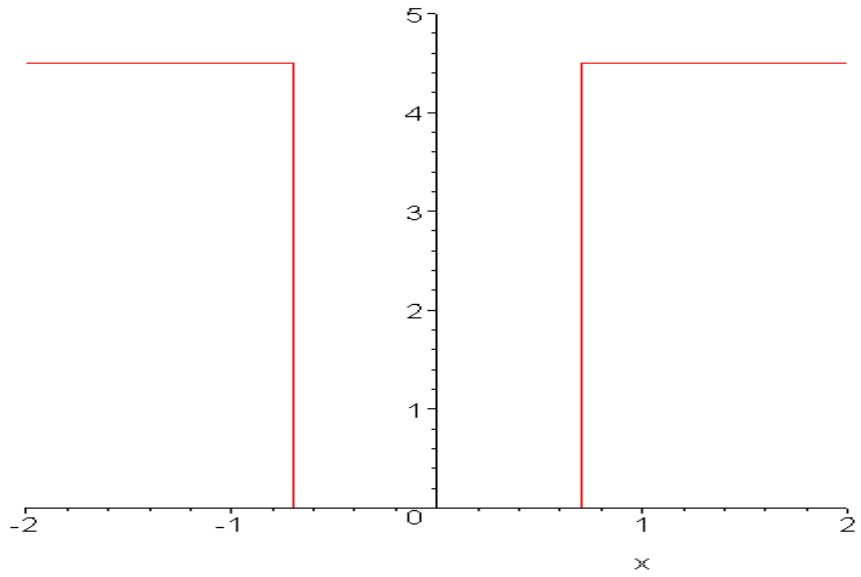
Text Problems

10.2 Symmetric and antisymmetric spin functions
10.3 Eigenfunctions of $S_{z\text{-total}}$ (note in Engel's notation for this chapter $S_z=S_{z1}+S_{z2}$)
10.7 Pauli Spin Matrices (OPTIONAL but recommended for serious students)
10.8 Prove the Variational Theorem (you *know* you want to!) (Hint: when I assign a problem that seems like 'math' there is always a reason. This won't be an exam question, but it is another abstract example where the concept of expanding an arbitrary wave-function in terms of eigenfunctions is used, and produces a valuable result!)

Additional Problems
1) If UV radiation of wavelength 58.4 nm were directed at a sample of atomic hydrogen gas (i.e. H, *not* H_2), what speed would the emitted electrons have? What would the wavelength of an electron with this speed be?

2) What are the dipole selection rules for electron transitions between states in the hydrogen atom? Give a *physical interpretation* for the selection rule involving Δl.

3) Let $\psi_n(x)$ denote the n^{th} eigenfunction of the Hamiltonian for an electron placed in the potential below:



a) SKETCH the wavefunctions for the n=1, n=2, n=3 (ground, first and second excited states)
b) The transition dipole moment for transitions between states $\psi_n(x)$ *and* $\psi_m(x)$ for this potential can be evaluated as:

$\mu_{nm} = \int_{-\infty}^{\infty} \psi^*_n(x)\mu_x\psi_m(x)dx$ where the transition dipole moment operator for this potential is $\mu_x=ex$ (e being the electronic charge)

Show that transitions from levels separated by |n-m| = 2, 4, 6… are *forbidden* ($u_{nm}=0$).
Hint: this problem shouldn't require much complicated integration!

4) Why can't the time independent Schrödinger Equation for be solved exactly for He (or any other multielectron atom)? *Write out the Hamilitonian, assign a physical interpretation to each term and comment on which term(s) in the Hamiltonian are problematic?*

5) Practice your spin orbitals
a) Write out *all* of the allowed wave-functions for the first excited state of the He atom including electron spin. Which are triplet states and which are singlet states?
b) List 5 "particles" (fundamental or composite) that are Fermions. List 5 that are Bosons. (use resources other than your lecture notes and textbook!). What do you notice as far as a trend goes for the 'fundamental' particles?

6) Is the average energy of the wavefunction $\psi(x)=x(a-x)$ going to be larger or smaller than the actual average ground state energy of a particle in a box of width *"a"*?

7) Suppose one were to use a trial function of the form:
$\phi(r) = c_1 e^{-\alpha r} + c_2 e^{-\beta r^2}$
to carry out a variational calculation *for the ground (1s) state of the hydrogen atom*. Determine (*no calculation allowed!)* what the values of the variational parameters alpha, beta, c1, and c2 are. ***Explain*.**

8) Download the Variational theorem Excel spreadsheet from the course discussion board and read the instruction sheet. For credit, find the best possible trial function with at least two terms, print out plots of your best trial function, *and at least one other trial function*, note the trial energies, compare the two, and COMMENT. **Extra credit**: *improve the numerical accuracy of the worksheet so that you can obtain the correct E_true=0.125002 with two trial terms*. Note: Even if you work on this in a group you should download and print out your own Excel sheet and solution.