Whole set of homework problems for AMO-1.

Exercise 1: Confirm the atomic units of B and of the Laser intensity are indeed given by the values shown in the lecture notes.

Exercise 2: Calculate the electron's and the proton's kinetic energy if each of their velocity is given by one atomic unit.

Exercise 3: Look for the energy separation of the hyperfine structure of the ground state of atomic hydrogen and show that its wavelength is 21 cm.

Exercise 4: confirm that 1 atomic unit in wavelength is 45.6 nm. For a Ti-Sapphire laser of wavelength 800nm, calculate its mean photon energy in eV's, its wavelength and frequency in atomic units, its period in fs and its frequency in Hertz.

 Exercise 5. You can learn a lot about hydrogen atom using Bohr model. Go over the derivation and use atomic units. Now remember to use reduced mass to go from two-body system to one-body problem. Let the total energy of the ground state of H be -13.6 eV.

>   (a)   What is the energy difference between the ground state of H and of D, in meV.
>   (b) Consider a muonic hydrogen, i.e., replace the electron by a negatively charged muon which has mass 206 in atomic units. What is the binding energy of the ground state of such a system. What is the velocity (in atomic units) and the radius of the muon with respect to the proton in the ground state? What is the wavelength for the n=2->1 transition?

Exercise 6. BJ problem 1.8 (If part a is too hard, you can skip it)

Exercise 7. BJ problem 1.9 (note that this method is used to obtain high energy gamma ray photons)

Exercise 8. BJ 2.7.

Exercise 9. BJ 2.10

Exercise 10: BJ 2.20

Exercise 11. In this exercise we want to derive eq. (2.380) and (2.381) of BJ.
   Start from the first-order coupled eqs. (2.377a,b), reduce them to two uncoupled second-order ordinary differential equations. Then solve each second-order differential equation analytically.

Problem 12: (a)Write down explicitly the wavefunctions of the two Stark states in terms of linear combination of hydrogenic wavefunctions in spherical coordinates using the formula above for m=0 and n=2.
 (b) Plot the charge density in polar coordinates for each Stark state.
 (c) Prove that each Stark state is not an eigenstate of L^2, thus parity is not a good quantum number for each Stark state.
 (d) Calculate the diagonal and off-diagonal matrix elements of the operator -eFz for an H in a static electric field along the z-axis, for two Stark states. Show that the off-diagonal term is zero. This shows that Stark states are eigenstates for a hydrogen atom in a static electric field.

 (If you are good at using computers, do this problem for m=0 and n=5, and give a good writeup. I like someone to show the density plots of the five Stark states.)

Exercise 13: Write down the $2p_{1/2}$ and $2p_{3/2}$ wavefunctions of H in the Pauli approximation explicitly. Use α and β to represent the spin-up and spin-down wavefunctions and $R_{21}(r)$ to represent the 2p radial wavefunction.

Exercise 14. The n=2 states of atomic hydrogen are degenerate in the first order approximation. Look it up and sketch the energy levels at the following successive approximations:
 (a) including spin-orbit interaction; (b) according to Dirac theory; (c) including QED effect; (d) including hyperfine interaction from the nucleus. State clearly the good quantum numbers at each level of approximation and the degrees of degeneracy. For actual splitting you may want to consult BJ or some other books

Exercise 15: To make sure that you indeed know how to do Taylor's expansion, do problem 5.4 of BJ.

Exercise 16.
 Go to the web (NIST site) to find out the ionization energies of Li, Na, K, Rb and Cs. Express the results in eV's. Find the ns-> $np_{1/2}$ and ns→$np_{3/2}$ energies where n is the principal quantum number of the outer-most shell. Express the energy difference in terms of wavelengths in nanometers.
 Find the isotopes of these alkali atoms and their nuclear spins.

Exercise 17. This exercise will guide you through the construction of the two-electron wavefunctions of a helium atom in the nonrelativistic approximation.
 (a) Assume that the electron-electron interaction can be neglected, construct explicitly the wavefunctions of the two electrons that can be labelled as $1s2p\ ^1P$ and $1s2p\ ^3P$. Consider the case that M_L=0 and M_S=0. You will write the wavefunction as the

product of the spin function and the spatial wavefunction. Show that the wavefunctions you have constructed are eigenstates of L^2, S^2. Show that under exchange of electron 1 and electron 2, the total wavefunction indeed is antisymmetric. What is the parity of each state? Find the eigenvalues of L^2, S^2, and the energy of each state.

(b) Construct the same wavefunctions using the Slater determinants. Prove that the resulting wavefunctions are identical to the one derived from (a).

Exercise 18. Use eq. (6) and the variationally obtained effective charge, calculate the total energy of the two-electron Hamiltonian. Compare this energy with the ground state of the one-electron Hamiltonian, i.e., after one electron has been removed. The difference of these two energies gives the binding energy. Do the calculation for He and H⁻. Compare your answers to the experimental data.

Exercise 19. This exercise is related to the calculation of binding energies of a spherical model potential.

The model potential for describing the bound orbitals for oxygen atom can be written in the form V(r)=-Z(r)/r where the effective charge has the form
$$Z(r) = 1 + 7\exp(-ar) + br\exp(-cr)$$
with a=1.41881, b=-6.22735 and c=2.5114.

Calculate the orbital energies of 1s, 2s, 2p of the oxygen atom. Also calculate the energies of the excited states 3s and 3p. Compare your results that you can find from the experiment.
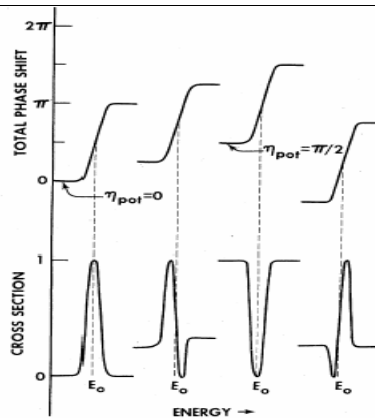
Exercise 20. The Hund's rule.
In this exercise, we will consider two electrons on the same shell. Consider $2p^2$ configuraton. Without the Pauli exclusion principle, the total L=0,1,2 and S=0,1 are allowed. Write down the two-electron wavefunctions for the possible L and S, and demand that the total wavefunction be antisymmetric under exchange of the two electrons, show that the allowed L and S satisfy L+S=even. Thus only ^{1}S, ^{3}P and ^{1}D are allowed for the $2p^2$ configuration.

Evaluate the expectation values of the electron-electron interaction <LS|1/r_{12}|LS> for ^{1}S, ^{3}P and ^{1}D, respectively and work out the angular integrals analytically using the formula given in the handout on angular momentum algebra. The remaining radial integral is positive definite so you can see the Hund's rule works.

Exercise 21.
In the elastic scattering region one can write the elastic phase shift near the resonance region as $\delta = \delta_{pot} + \delta_{res}$ where the first term is a constant and the second term is the standard rapidly changing phase shift near the resonance. Show that the elastic cross section near the resonance can be expressed in the form of the Fano

profile, and find the expression of the q-parameter for the four cases shown in the figure. Assume s-wave scattering.

Exercise 22. Doubly excited states of He

Let us write the helium Hamiltonian as $H=H_0+H_1$ where the first term consists of one-electron hydrogenic operators only and the second term is the $1/r_{12}$ interaction. Thus the zeroth order wavefunctions 2s3p ^1P and 2p3s ^1P states are degenerate. According to the +/- designation of Fano, the two states should be given by (2s3p + 2p3s) ^1P and (2s3p- 2p3s) ^1P, respectively. Write down explicitly the wavefunctions of these two states in terms of radial hydrogen wavefunctions and coupled angular momentum functions. You can omit the spin part for this purpose.

1. Use 1st order perturbation theory to evaluate the matrix element of H_1 for each of these two states.

2. Work out all the angular integrals analytically (similar to problem 20) to reduce them to summation of terms involving only radial integrals -- the so-called Slater integrals.

3. You can write a simple 2D integration program to calculate these Slater integrals. Note that the 2s, 2p, 3s and 3p are just hydrogenic orbitals. (If you are not good at programming, ask the results of these integrals from your fellow classmates, but give them credits.)

4. Use the results from (2) and (3) to calculate the binding energies of these two states. Compare them with the values given in the table on the third page of Lecture note-13. (Look at the n=3 of the (N,K)=(2,0) and (2,1) groups.) Express the difference of your calculations in eV's.

5. Look up on the web for the binding energy of the ground state of He.

6. Calculate the photon energy (in eV) needed to excite the He atom from the ground state to these two states. Compare your results with what you can read from Fig.4 on

page 2 of note-13. (You can get even more precise values by going to the original paper indicated there.)

7. Calculate the energies of the ejected electron when these two doubly excited states autoionize.

Exercise 23.

(1)   Enumerate the possible L and S of the 2s2p3p configuration.
Find the possible L and S for the $2p^2 3p$ configuration.

(2)   Go to the web to look for the mean term energy ($<E>$=weighted averaged of E_J) of the ground state configuration of C, N, O atoms and confirm that the terms do satisfy the Hund's rule.

(3) Go to the web to find out the mean energy levels of the $2\ell 2\ell' 2\ell''$ intrashell states of O IV. The convention for atoms is that the neutral oxygen is written as O I. Thus O IV is O^{3+}. Intrashell states mean that the principal quantum numbers of the open shell orbitals are identical. Thus the possible configurations in this case is $2s^2 2p$, $2s2p^2$ and $2p^3$. Find out all the possible L and S for each configuration(you can even just look them up) and the mean energies of all these states according to the configurations. Check if the Hund's rules are satisfied for the $2p^3$.

Follow the example of Fig. 5 of Morishita and Lin, J. Phys. B31, L209 (1998) and order the energy levels you found in the similar way. The energy pattern in this new ordering show the rotational level structure of a symmetric top. (Will be further discussed briefly in the class.)

(4) In the class we talked about the Lande interval rule, and we have said " It is empirically shown that if the shell is more than half-filled then the fine structure level is inverted." Check this statement by looking at the fine-structure energy levels of $1s^2 2s2p\ ^3P_J$ of Be. Check the same for the term $1s^2 2s^2 2p^5\ ^2P$ of Ne II.

Exercsie 24. Z-Scaling along the isoelectronic sequence.

(a) Write down the Schrodinger equation for atomic hydrogen, and for He^+. From the equation for He^+, do a change of variable by using a new $r'=Zr$ for Z=2, show that the resulting equation is the same as the Schrodinger equation for atomic hydrogen except that the new energy $E'=E/Z^2$, where E' is the hydrogenic energy and E is the energy for He^+. Thus shows the Z^2 scaling of the eigen-energies with Z.

(b)   From this exercise, what is the relation between the expectation values,
$<\phi | \dfrac{1}{r} | \phi >$, of H and of He^+.

(c) Now use eq. (5,16) and (5.17) for the spin-orbit interaction expression, show that the spin-orbit interaction term shall scale like Z^4 for hydrogenic systems.

(d) Convince yourself then that the Slater integral shall scale like Z for the two-electron helium-like ions.

(e) Extend the method to scaling with respect to the reduced mass for hydrogenic systems: How the expectation value of 1/r scales with the reduced mass?

Exercsie 25. Selection rules for autoionization.

 (a) The 2s2p $^1P^o$ doubly excited state of He is about 60 eV from the ground state. When this state autoionizes, what is the energy of the ejected electron, in eV?

 (b) Note that electron-electron interaction is responsible for the autoionization. This is a scalar operator, such that the L, S and parity, before and after the autoionization should be identical.   Based on this, what is the orbital angular momentum of this ejected electron? How about its spin?

 (c) It is well-known that the $2p^2$ $^3P^e$ state cannot autoionize, why? Try to follow the argument used in (b).

Exercsie 26. Multitudes of coupling schemes.

 (a) The LS coupling is not always the best coupling scheme. Consider the configuration $1s^2 2s^2 2p^5 3p$ of Ne. The first nine electrons are rather tight, but the excited 3p electron tends to stay further out. The better coupling scheme is that $1s^2 2s^2 2p^5$ first couple to ^2P_j with j=3/2 and j=1/2. Then the j of the core couples with the orbital angular momentum of the outer electron to form a new quantum number, say K. Finally the K couples with the spin of the outermost electron to form the total J of the atom. Go to the NIST website for the energy levels listed there, sketch the energy levels for all the possible J. List all the states that have identical J together.

 (b) Now if you think LS coupling should be better, identify all the L and S that couple to the same J, and group these states together.

 (c) You can also use jj coupling and group all the states that have the same final J.

 Convince yourself that the number of states for a given total J is the same, independent of what scheme you start with.

     Refer to Note-17 for the equations given below

Exercsie 27. Prove eq. (2.15). Consider the x-component only and use the hint given above that equation.

Exercsie 28. You can use eq. (2.20) to calculate the spontaneous transition rate.
 (a) Show that the 2p state of atomic hydrogen indeed has a lifetime of 1.6 ns.
 (b) What is the lifetime of the 2p state of He$^+$. Use scaling argument.
 (c) If a beam of 1000 hydrogen atoms are travelling at one-tenth the speed of light. At t=0, all of them are excited to the 2p state, for example, like in a beam-foil experiment. How many atoms can be found in the ground state after the beam has travelled 1 cm, 10 cm?

Exercsie 29. (a) One millions atoms of hydrogen initially are in the 5p states. Consider all the possible initial radiative decay paths (by electric dipole transitions) from this state.
   (b) Since all the excited states eventually will decay to the ground state, find out the different photon energies that you can get if the initial state is a 5p state.

Comments: If you can calculate the transitions rates for all the states you have considered you should be able to find out how many photons for each energy if you know initially how many atoms you have. Transition rates of atomic hydrogen have been tabulated in the classic book by Bethe and Salpeter, " Quantum Mechanics of one- and two-electron atoms. "

Exercsie 30. Calculate the **relative** spontaneous emission rates of $2p_{3/2}$ and $2p_{1/2}$ rates of atomic hydrogen to $1s_{1/2}$.

Note that the good quantum numbers here are the J's. Use the wavefunctions for $2p_{3/2}$ and $2p_{1/2}$ from Problem 13 earlier. Since I ask for the relative rates only, there is no need to calculate any radial integrals.

Exercsie 31. Relative intensities of the emission lines for hydrogen atoms in a magnetic field.

(a) For simplicity, we will neglect the spin-orbit interaction and consider the transitions from 3d to 2p only. First you note that the 2p state will be splitted into three states, and the 3d will be splitted into five states. Sketch the levels of 3d and 2p in a weak magnetic field.
(b) In a magnetic field, how many different emission lines will you observe?
(c) Calculate the relative intensities of these lines.
Hint: Use Wigner-Eckhart theorem. There are no integrals to calculate.

Exercsie 32. Radiative lifetimes along the Rydberg series.
Consider the $np \rightarrow 1s$ transitions in atomic hydrogen. What would be roughly the lifetime of the 20p state? How about 25p state? Use scaling method given in the hint below. The lifetime of the 2p state is 1.6ns.

Hint: From eq. (2.20), the major difference comes from the radial integrals. Since the 1s wavefunction is localized in a small volume, we need to figure out how the excited state wavefunctions behave at small r. For a given ℓ, from the hydrogen wavefunction, you can see it behaves like $1/n^{3/2}$ approximately. Look up the hydrogenic wavefunctions for $n\ell$ states and write down the normalized wavefunction for small r to convince yourself that it indeed scales like $1/n^{3/2}$.

Exercsie 33. This exercise is to identify the dominant radiative transitions between two states. Consider E1, M1, E2, M2 only. Also consider if two-photon transitions could be important. Note that if J is given then J is consider to be the only good quantum number. If only L is given, then L is considered to be a good quantum number.

(1) For atomic hydrogen:
(a) 2s-> 1s (b) $2s_{1/2} \rightarrow 1s_{1/2}$ (c) $3d \rightarrow 1s$ (d) The transition between the two hyperfine levels of the ground state of hydrogen

(2) For helium

    (a) $1s2s\,^1S \rightarrow 1s^2\,^1S$

    (b) $1s2s\,^3S_1 \rightarrow 1s^2\,^1S_0$

    (c) $1s2p\,^3P_{0,1,2} \rightarrow 1s^2\,^1S_0$ there are three cases here.

(3) The intercombination lines in O I (go to NIST data center for the energy levels)

    (a) $2s^2 2p^4\,^1D_2 \rightarrow 2s^2 2p^4\,^3P_{0,1,2}$ (b) $2s^2 2p^4\,^1S_0 \rightarrow 2s^2 2p^4\,^3P_{0,1,2}$

    Identify the type of transition and the energy of each transition.