

**Final Exam: Atomic and Molecular Physics 475**  
**April 16, 2007**

Total 105 points. Individual values follow each question. Take home exam due at 6 p.m. in my office on April 17, 2007. Some minor consultation with classmates is permissible but your work should be your own. Likewise, answers copied from books without clear explanation or evidence that you understand the steps will not receive full marks. This doesn't mean that looking at text books is cheating (in fact I would recommend it in several cases!) This is fair game but you need to explain what you are doing. Your main goal in most questions is to convince me that you understand the answer. You may use Maple if you want to work through some difficult integrations. If there are steps that you are not sure of you will be better off noting this.

1. Topic: Modern Physics

Write about one of the modern/atomic physics experiments that we discussed in class, highlighting dates, the scientists involved, the technique, any important formulas, and the new result. (10)

2. Topic: Perturbation Theory and a DC Electric Field

Consider an infinite square well containing an electron that extends from  $x = -L/2$  to  $x = L/2$ .

- (a) What are the ground state and first excited state solutions (you may state the result from a book)? (2)
- (b) Now consider adding applying a DC electric field in the  $x$  direction. How is the Hamiltonian modified? (no need for  $\vec{A}$ ) (2)
- (c) Calculate the first order correction to the ground state energy. (This is quick.) (2)
- (d) Calculate the second order correction to the ground state energy that comes from the mixing of the first excited state. (4)
- (e) Calculate the first order correction to the ground state wavefunction that comes from the mixing of the first excited state. (3)
- (f) Give the expectation value of the dipole moment for this modified ground state. (2)

3. Topic: One-electron atoms

- (a) Write the  $n = 2$ ,  $l = 1$ ,  $m = 1$  solution for the hydrogenic wavefunction (neglecting electron spin) and show that it solves 3.4 (Schrödinger's equation) with the appropriate eigenvalues. Give the value of the energy. (8)
- (b) Calculate  $\langle \frac{1}{r^2} \rangle$  for the above and show that it agrees with 3.77. (7)

4. Topic: Interaction with radiation

We spent a considerable amount of time dealing with the topic of electromagnetic radiation and its interaction with one-electron atoms. Summarise the steps that went into the development of Equation 4.100 as I did in class. When applicable please provide the names for the steps/approximations. Please explain 2 of these steps in modest detail. (15)

5. Topic: Two electron atoms (Gulp!)

I didn't discuss the helium atom in class but consider the following points if we wanted to estimate the ground state energy of helium, a system with two electrons around an (infinitely) heavy nucleus.

- (a) Write the Hamiltonian for this system. (2)
- (b) Show that if we ignore the electron-electron interaction that the equation separates so that the total electronic wavefunction is a product of the two electronic wavefunctions. Give the ground state energy of this system. (4)
- (c) Now can you estimate the interaction term in the case where the electrons have opposite spin and both have the same wavefunction. Treat it like perturbation theory where the product of the wavefunctions is the unperturbed state. The key feature is that you need to evaluate

$$\int d^3 r_1 \int d^3 r_2 |\psi_{100}(\vec{r}_1)|^2 |\psi_{100}(\vec{r}_2)|^2 \left( \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right). \quad (1)$$

This is doable but a bit tough. Instead consider an estimate using normalised functions that are step functions i.e.  $R(r) = A$ , a constant, for  $r \leq r_0$  and  $R(r) = 0$  for  $r > r_0$ . Normalisation requires that

$$1 = 4\pi \int_0^{r_0} dr r^2 A^2 \quad (2)$$

and in addition I require that the expectation value of  $r$

$$\langle r \rangle = 4\pi \int_0^{r_0} dr r^3 A^2 = \frac{3a_0}{2Z} \quad (3)$$

is related to the Bohr radius. You may now use the classical electrostatic formula for the energy of assembly of a uniformly charged sphere

$$U = \frac{3}{20\pi\epsilon_0} \frac{Q^2}{r_0} \quad (4)$$

to estimate the increase in the ground state energy over the non-interacting case. In this way you avoid the double integral. (14)

## 6. Topic: Interaction with radiation.

Suppose that you want to discuss transitions from the  $n = 3$  to  $n = 2$  levels in hydrogen.

- (a) State the explicit starting and ending states in terms of the quantum numbers that are allowed according to electric dipole transition selection rules. (you may ignore electron spin, assume that it doesn't change, so we have eigenstates of  $\mathbf{L}^2$  and  $L_z$ ). There are a fair number because of the degeneracy. (4)
- (b) Pick a specific final polarisation in terms of spherical components that gives a non-zero transition rate and calculate the dipole matrix element for one of the transitions (some are easier than others). Please use 4.118 in your calculation so that you can demonstrate calculating a Clebsch-Gordan coefficient. (6)
- (c) According to your matrix element at what angle between  $z$  and  $\vec{k}$  is the radiation maximized? What could you do experimentally to give a meaningful  $z$  direction to the atoms? (7)
- (d) Make a rough estimate of the transition rate by just using the maximum  $\vec{r}_{ba}$  and substituting it into equation 4.80b. (3)

## 7. Topic: Fine structure

- (a) What does fine structure mean? Where does it come from? By what percentage roughly do the energy levels shift? Calculate an example. (5)

- (b) Explain how changing to states that are eigenstates of total angular momentum is useful for calculating the spin-orbit coupling. Isn't that strange? Why don't you use eigenstates of spin and orbital angular momentum if you want to calculate spin-orbit coupling? Base your answer on what you learned in assignments. (5)