PHYS 850: Atomic and Molecular Structure Lecture: MWF 10:30, CW 023

Fall 2006

Instructor:

Dr. Brett Esry CW 329 esry@phys.ksu.edu http://www.phys.ksu.edu/personal/esry

Textbook:

 $Physics \ of \ Atoms \ and \ Molecules, \ Second \ Edition, \ Bransden \ and \ Joachain$

Supplements:

• Theoretical Atomic Physics, Friedrich

• Handbook of Atomic, Molecular, and Optical Physics, Editor: Drake

• Your favorite quantum mechanics texts ...

Grading:

Course philosophy and goals:

My primary goal for this course is to educate you about the atomic and molecular structure that you need to know for your research. Given the diversity within our AMO group and within this class, however, not everything we cover will relate directly to each and every person's research. Moreover, we will not be able to cover everything any of you will need to know about atomic and molecular structure. A secondary goal of this course is thus to give you enough knowledge to be able to learn the rest on your own.

Another secondary goal of this course is to give you a broader education in atomic and molecular physics. In the course of your career, you will talk to many people outside of your immediate area of expertise and you will listen to many talks similarly outside your expertise. A broader education will let you participate more intelligently in these exchanges. In addition, few of us continue doing just one type of AMO physics throughout our career. A broader education provides opportunities and helps you to recognize them. It also makes it easier to switch directions ... maybe for a postdoc position.

To achieve any of these goals, though, requires active participation from you, and that means homework. I will assign regular homework, but will strive to keep their time demands in check as I know most of you have research to do. You will be most time efficient if you discuss the problems with your classmates. You should, however, write up the assignment on your own. Some assignments will require computer work.

Guidelines for homework:

- Discuss your homework with classmates as much as you like, but write your homework solutions on your own!
- As a scientist in training, you need to learn to communicate scientific information in an effective, efficient manner. You should consider homework assignments as practice in this art. It is your responsibility to present your

homework solutions in a readable, logical manner — not mine to decipher and interpret them.

- In keeping with the above two points, I will require that you cite any work or results that you take from sources other than our text book.
- In an incorrect solution, I will reward statements in homework and on exams that show you know it is incorrect and why. I will also reward any effort above and beyond what is explicitly asked for in a problem.

Students with disabilities:

If you have any condition such as a physical or learning disability that will make it difficult to carry out the work as I have outlined it or that will require academic accomodations, please notify me and contact the Disabled Students Office (Holton 202) in the first two weeks of the course.

Plagiarism:

Plagiarism and cheating are serious offenses and may be punished by failure on the exam, paper, or project; failure in the course; and/or expulsion from the University. For more information refer to the "Academic Dishonesty" policy in the K-State Undergraduate Catalog and the Undergraduate Honor System Policy on the Provost's web page at http://www.ksu.edu/honor/.

Tentative Course Topics:

I have reviewed Prof. Thumm's QM-1 and 2 course topics and will assume you know that material. We will start with a *very* quick review of some of the topics important for this course, however. We will not necessarily cover the topics in the order they are presented below ...

Chaps. 1–3

These should largely be review. We will cover the variational principle and one-electron atoms in parabolic coordinates.

Chap. 4 Interaction of one-electron atoms with electromagnetic radiation

Should also be review, but we'll make sure it's all clear since atomic and molecular structure is traditionally revealed through spectroscopy — usually laser spectroscopy.

Chap. 5 One-electron atoms: fine structure and hyperfine structure

Review to get the basic ideas of the physics behind these effects.

Chap. 6 Interaction of one-electron atoms with external electric and magnetic fields

Review of Stark and Zeeman effects.

Chap. 7 Two-electron atoms

Examine various approximations and doubly excited states. Chap. 8 Many-electron atoms

Hartree-Fock method, LS coupling, alkali atoms and quantum defects, model potentials, density functional theory.

Chap. 9 Interaction of many-electron atoms with electromagnetic radiation and with static electric and magnetic fields

Selection rules, Stark and Zeeman effects.

Chap. 10 Molecular structure

Born-Oppenheimer approximation, electronic structure of diatomics, rotation and vibration of diatomics, electronic structure of polyatomics.

Chap. 11 Molecular spectra

Diatomics: ro-vibrational spectra, electronic spectra, dipole selection rules, Stark effect.