Chemistry 3730: Quantum Principles and Spectroscopy
Fall 2002

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Office hours

Office hours will be held from **4:00 to 5:00 p.m. on Mondays**, from **8:00 to 9:00 a.m. on Wednesdays**, and from **8:30 to 9:15 a.m. on Thursdays**. I will try to guard office hours vigorously against other demands on my time, but if for some reason I can't attend a scheduled office hour, I will send an email to the class mailing list and indicate when else I will be available for student consultations.

If you can't meet me during office hours, you are **strongly encouraged** to phone or email me to make an appointment. I guarantee nothing if you just drop in without an appointment.

Course prerequisites

Chemistry 2720, Mathematics 2560 and Physics 2000 are prerequisites for this course. If you lack any of these prerequisites, you should talk to me as soon as possible (if you haven't already done so).

Textbook

The textbook for this course is *Introduction to Quantum Mechanics in Chemistry* by Ratner and Schatz. We will cover chapters 2–11 and 13–15 (time permitting). You should read chapter 1, which is review of material covered in the prerequisite courses, on your own time. This material is essential background for everything that will follow.

Grading scheme

Type	Number	Weight	Dates and times
Tests	3	20% each	Sept. 30, Oct. 28 and Nov. 25, 1:00 p.m.
Final exam	1	40% (or more*)	Dec. 16, 9:00 a.m.

*If you miss a test during the term with reasonable cause (e.g. illness), the weight of the missed test will be transferred to the final examination.

If you miss the final examination, the policy enunciated in the 2002/2003 University Calendar (Academic Regulations, section 4, subsection f, paragraph 10) will govern the procedure to be followed.

Computer-assisted instruction

Most of the interesting problems in quantum chemistry are either difficult or impossible to solve by hand. Accordingly, we will use two computer programs to help us out. The first, Maple, is a symbolic algebra system. It will help you perform integrals, solve equations, and so on. Later in the course, we will use HyperChem to help us study the quantum mechanics of atoms and molecules. These software systems will be used in assignments and quizzes and in the final examination.

Both of these systems are powerful, but they have their quirks. Therefore, in addition to studying from your class notes, you will have to practice using Maple and HyperChem. To help you do this, you will spend two to three hours every Monday afternoon in the computer lab. You should also spend some time practicing using these systems on your own time. You could, for instance, try working through some of the old test problems posted on the course web site.

Maple and HyperChem should be accessible from most of the computer labs on campus. The HyperChem license server is sometimes a little difficult. If you try HyperChem on one computer and it won't start up, just move to another computer.

About the tests

All the tests, including the final examination, will be held in the computer lab. Many of the questions will be answered using Maple or HyperChem, but there will be some questions which probe your general knowledge of quantum chemistry as well.

You will be permitted to bring one U.S. letter-sized ($8\frac{1}{2} \times 11$-inch) piece of paper to the tests containing any information you want. (Note that you can use both sides of the page.) The tests will contain *some* hints to help you solve some of the problems, but you must know how to use the software and how to carry out basic procedures. You will be allowed to use Maple's and HyperChem's help systems, so it makes sense to spend some time playing around with these in preparation for the tests. To summarize, you will have access to Maple, to HyperChem, to their help systems, and to one additional piece of paper containing any information of your choosing. **No other written or printed information, and no other electronic aids will be allowed.**

There are some things that will be given to you (if needed) so that you **don't** have to put them on your formula sheet:

- numeric data (Planck's constant, etc.)
- wavefunctions and energies for specific systems (particle in a box, harmonic oscillator, etc.)