

CH 4412 - Quantum Mechanics and Spectroscopy

Instructor: Prof. John F. Stanton (NPB 2336)

Office Hours: T 5:30-7:30, Th 12:30-2:30 PM

Teaching Assistants: Nitai Sahoo

Office Hours: TBA

Textbook: None

Course Schedule

Week	Dates	Material
Fundamental Quantum Mechanics		
I	Aug 24 [†]	Boot Camp
II	Aug 29,31	Boot Camp and Historical Background
III	Sep 5,7 ^{†‡}	Early Twentieth Century Developments
IV	Sep 12,14	Solvable Problems I
V	Sep 19,21 ^{†‡} ,6*	Solvable Problems II
VI	Sep 26,28	Solvable Problems III
VII	Oct 3,5 ^{†‡}	Solvable Problems IV
Applications of Quantum Mechanics		
VIII	Oct 10,12	Application of Approximate Methods to Simple Problems
IX	Oct 17 ^{†‡} ,19*	The Hydrogen and Helium Atoms
X	Oct 24,26	Hartree-Fock Theory and Orbitals
XI	Oct 31 ^{†‡} ,Nov 2	What is a Molecule? The Born-Oppenheimer Model
XII	Nov 7,9	Diatomic Molecules I
XIII	Nov 14 ^{†‡} ,16*	Diatomic Molecules II
XIV	Nov 21	Polyatomic Molecules
XV	Nov 28,30 [†]	Wrapping Up

† - Homework assignments will be passed out.

‡ - Homework assignments will be collected.

* - Hour examination will be administered.

There may also be one or two extra lectures held, tentatively, on Saturday mornings after the weather gets nicer. We have done this before, and the students who came (which was about half of the class) enjoyed, and got quite a bit out of them. There will be no material from these lectures that will “be on” an exam, but there definitely will be new things to learn and perhaps different perspectives on the material to be obtained by attending the lectures. These will be scheduled via Piazza, which will be the central website for the course. Try to keep Saturday mornings open on your schedule, unless they are already blocked. It is *not* vital that you attend, but you might find them interesting.

Scope of Material

CHM 4412 covers the subject of quantum mechanics from a chemist's point of view. The course will begin with a "review" of concepts from mathematics (trigonometry and calculus, primarily) that are seen again and again in this course, followed by a historical overview of the subject, covering physics from the time of Newton to the dawn of the new age at the beginning of the 20th century. This is followed by an outline of the framework of quantum mechanics and its application to model systems for which the Schrödinger equation can be solved exactly. In chemistry, however, *all* systems of interest involve mathematically intractable Schrödinger equations and approximations are the name of the game. The rest of the course deals with the fundamental principles that underlie atoms and molecules: the existence of discrete energy levels, their qualitative interpretation, and the ability of electromagnetic radiation (photons) to induce transitions between these levels and the connection between quantum mechanics and thermodynamics. I will warn you now that this course (particularly the early part of it) involves some rather serious and involved mathematics. If you were overwhelmed with the math encountered in CHM 4411, you might find yourself significantly more overwhelmed by this course. It's tough, but worth it for those who expend the effort.

Advanced Warning: You should not take this class unless you are ready to do a fair amount of work. While I previously thought "senioritis" was a disease that afflicted only high school students, there were six students in a recent class who were graduating seniors. Four of them failed, largely because of a profound lack of effort.

Homework

Homework problems will be assigned every other Tuesday throughout the semester and are due *at the beginning of class* two weeks later. *Assignments turned in later than 3:05 PM on the specified Tuesday will not be accepted.* If you anticipate that it will not be possible to arrive by that time, there are two options: 1) get a friend to turn it in for you; 2) slide your homework under my office door sometime BEFORE 3:00 PM on Tuesday afternoon. Please show all work on the sheets provided in the homework packet. If there is not enough room underneath the problem statement to write down your calculations and/or reasoning along with the solution, you should attach extra pages to the assignment packet, order them properly and then *restaple it* before submission. For those of you who want challenging and sometimes algebraically brutal problems, I will not disappoint.

Examinations

There will be three open-book, open-note examinations administered during the usual class time, as well as a final examination. *I expect you to be responsible and avoid scheduling conflicts that interfere with exams.* Take note of the exam dates *now* and plan things such as medical school interviews accordingly. I rarely give make-up exams, and do so only for very good reasons (medical emergencies, death of a relative, religious holidays *etc.*).

Grading Policy

The basis for grades in CHM 4412 will be performance on the hour exams, the final exam and the homework assignments. Only the five highest of seven homework scores will be counted. The distribution of points is given below.

Homework	200
Hour Exam I	200
Hour Exam II	200
Hour Exam III	200
Final Exam	200
Total	1000

In general, the basis for grade assignment is the class score distribution; those of you scoring above roughly the 40th percentile will receive an A or B; those scoring below receive a C, D or F. However, those scoring above 850 are guaranteed an A, while those scoring above 700 will receive at least a B grade. While I generally do not give a lot of A's, it works both ways: only truly determined students who dedicate themselves to not trying or working hard will get a D or an F.

Disabilities

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter, which must be presented to the instructor when requesting accommodations. Students with disabilities should follow this procedure as early as possible in the semester.

Counseling

The University of Florida provides counseling services for students, staff, and faculty. See <http://www.counsel.ufl.edu> or call (352) 392-1575 during regular service hours (8am - 5pm). For other hours or on weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352) 392-1171.

Honor Code

This class will operate under the policies of the student honor code, which can be found at: <http://www.registrar.ufl.edu/catalog/policies/students.html>. The students, instructor, and TAs are honor-bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

Evaluations

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.ua.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.ua.ufl.edu/public-results/>.