CH 4412 - Quantum Mechanics and Spectroscopy

Instructor: Prof. John F. Stanton (NPB 2336, johnstanton@ufl.edu)

Office Hours: W, Th 10-12

Teaching Assistants: Rohit Rana and Josie Kilburn

Office Hours (tentative): M 10-11 (Kilburn), F 2-3 (Rana) Zoom Links (for office hours): Stanton, Kilburn, Rana

Textbook: None (see discussion on piazza: Resources→Course Information)

Course Schedule

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Week	Dates	Material
	F	Fundamental Quantum Mechanics
I	$\mathrm{Jan}\ 6^{\dagger}$	Overview and Perspective
II	Jan 13,15	Boot Camp and Historical Background
III	Jan $20,22^{\dagger \ddagger}$	The Dawn of Quantum Mechanics
IV	Jan 27,29	The Postulates
V	Feb $1,3^{\dagger \ddagger}$	Solvable Problems I
VI	Feb $8*,10$	Solvable Problems II
VII	Feb $15,17^{\dagger\ddagger}$	Solvable Problems III
	\mathbf{A}_{1}	pplications of Quantum Mechanics
VIII	Feb 22,24	Application of Approximate Methods to Simple Problems
IX	Mar $1,3^{\dagger \ddagger}$	The Hydrogen and Helium Atoms
X	Mar 15,17	Hartree-Fock Theory and Orbitals
XI	Mar $22^*, 24^{\dagger \ddagger}$	What is a Molecule? The Born-Oppenheimer Model
XII	$Mar\ 29,31$	Diatomic Molecules I
XIII	Apr $6.8^{\dagger\ddagger}$	Diatomic Molecules II
XIV	Apr $13^*,15$	Polyatomic Molecules
XV	Apr 20 [‡]	Wrapping Up

^{† -} Homework assignments will be passed out.

Class Website

The class website is hosted on piazza, from which you have obtained this syllabus. In addition to posting notes, homework and exam solutions, and so on, piazza is also an extremely useful resource for asking questions outside of class and/or office hours. This system has been quite effective and popular since I started to use it a several years ago, and <u>you</u> are encouraged to answer the questions of your classmates if you are able. The TAs and I will also answer questions in a time frame ranging from "right away" to a few days, but all of you are encouraged to help each other and post answers if you think that they are correct. Both the TAs and I will monitor the goings on, and will intercede with corrections when and if warranted.

^{‡ -} Homework assignments will be collected.

^{* -} Hour examination will be administered.

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 a new age at the beginning of the 20th century, all the while emphasizing those areas particularly relevant to chemistry. 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 some connections 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.

Homework

Homework problems will be assigned every other Thursday 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 Thursday will not be accepted. If you anticipate that it will be impossible to arrive by that time, there are three 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 Thursday afternoon; 3) make arrangements with a TA to send it to them electronically sometime before the deadline. 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. For the most part, homework assignments will be most pertinent to lecture material from the two weeks prior to the week that the assignment is due in class. As an example, the problems assigned on the Thursday of Week V will be due in class on the Thursday of Week VII, and will mostly cover material from Weeks V and VI. Solution sets will be posted on piazza, usually on the evening after the homework is due.

Examinations

There will be three open-book, open-note examinations administered during the usual class time, as well as a final examination that will be held April 28 from 5:30-7:30 PM. 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 generally do so only for very good reasons (medical and family emergencies, 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 median will receive an A or B; those scoring below generally receive a C, D or F. However, who score above 850 are guaranteed an A, while those scoring above 750 are guaranteed 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 failing grade.

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 seem always to be a few students in 4412 that suffer from it. If you make an effort, you are certain to pass the class, but you do need to make an effort.

Disabilities

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, or this link) 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 this link 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 here. 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 here. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals. Summaries of course evaluation results are available to students here.