CHEM 2430: Quantum Chemistry

Fall 2018

At a Glance

Lectures MW 10am-11:15am in 228 Eberly

Office Hours TBD - please take poll by Weds. 8/29

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Recommended Texts There is no *required* text for this course, but you may find one or more of the following references useful:

Quantum Chemistry
Donald A. McQuarrie
2nd edition (2008)

Quantum Chemistry
Ira N. Levine
6th edition (2008) or 7th edition (2013)

Elements of Quantum Mechanics
Michael D. Fayer
(2011)

Modern Quantum Mechanics
J. J. Sakurai and Jim Napolitano
2nd edition (2011)

Introduction to Quantum Mechanics
David J. Griffiths
2nd edition (2005 or 2016 (revised))

A summary of these books, including a listing of the chapters/sections most relevant to the course material, is available on CourseWeb. For reference, last year's students generally found McQuarrie and Levine most helpful.

All of these texts are on reserve in the chemistry library; you may also be able to borrow copies of Levine from past students.

Course Goals

Overview Chem 2430 is a first year graduate course in quantum chemistry. My goal in this course is to help students develop a firm conceptual and mathematical grounding in quantum mechanics and its applications in chemistry and the physical sciences.

Key Concepts By the end of the course, students will understand and be able to apply:

- The properties of operators, eigenfunctions and eigenvalues, and their relationship to experimental observables
- Boundary conditions and their relationship to the behavior of allowed wavefunctions
- The connection between the time-dependent and time-independent Schroedinger equations, and the time-evolution of quantum mechanical systems
- Matrix mechanics, and the application of ideas from linear algebra and differential equations to quantum mechanical problems
- Rotational motion, angular momentum, and electron spin, and their consequences on the electronic structure of atoms and molecules

- Approximation methods necessary for complex potentials and multi-electron systems, such as the variational method, perturbation theory, the Born-Oppenheimer approximation, Huckel theory, and the Hartree-Fock method

Core Topics We will explore the key concepts in the context of several classic problems of quantum mechanics, including:

- Particles in bound potentials, including one- and three-dimensional infinite square wells and harmonic oscillators
- Particles in unbound potentials, including free particles and non-infinite wells
- Particles undergoing rotational motion in two and three dimensions
- Atomic systems, including the hydrogen and helium atoms
- Simple molecular systems

Special Topics As time permits, we may also explore some or all of the following topics:

- Time-dependent perturbation theory, Fermi's golden rule, and their application to energy level transitions in spectroscopy and light-matter interactions
- Quantum mechanical foundations for popular electronic structure methods used in computational packages like Gaussian
- Electrons in periodic potentials, the Bloch theorem, and applications to the band structure of electronic materials
- Other topics related to student interests

If you have a request for a specific topic that you would like to see covered in the last third of the course, please feel free to send me an email or come to office hours to discuss.

Course Structure

Grading This course will be graded using standards-based grading. Your grade will be based on your performance in three key areas:

[1] Mastery of course content objectives and big ideas, as demonstrated on midterms and the final exam;
[2] Ability to correctly and clearly present your work, as demonstrated on regular professional problems; and
[3] Ongoing effort to improve your skills as a quantum chemist, as demonstrated on weekly problem sets.

A list of the content objectives for the course is provided as a separate handout. These are the things that I expect you to be able to *do* by the end of this course. The content objectives are grouped into six "Big Ideas;" your grade in this class will be determined to a large extent by how many of these big ideas you can demonstrate that you have mastered (by demonstrating mastery of the objectives within that group) by the end of the semester.

You will have the chance to demonstrate your mastery of the content objectives on several exams over the course of the semester. Each exam item will target one or more content objectives, each of which will be assessed according to the following rubric:

- **E (Excellent):** the work demonstrates excellence in all respects, is clearly communicated, and contains no notable mistakes.
- **M (Mastered):** the work generally demonstrates mastery of the targeted content objective(s), but may not be clearly communicated or may contain minor mistakes.
- **P (Progressing):** the solution contains some relevant work, but contains a fundamental error or misunderstanding; or, work that demonstrates promise but is incomplete.

- **X (No Evidence):** the work does not demonstrate progress toward mastery or is not presented clearly enough to assess student's knowledge.

This rubric will also be used for professional problems and weekly problem sets (see below), although these items will be graded as a whole (e.g. one score for the entire piece of work) rather than divided up by content objective. A handout with examples of the level of work necessary to achieve each of these scores will be provided separately.

Your course grade will be determined by the number of assignments and big ideas in which you demonstrate sufficient progress, as outlined in the following table:

	Big Ideas Mastered	**Professional Problems**	**Problem Sets**
A	6 of 6	6 E's	10 P's or higher
A-	5 of 6	6 E's or M's	10 P's or higher
B+	5 of 6	5 E's or M's	9 P's or higher
B	4 of 6	4 E's or M's	8 P's or higher
B-	3 of 6	3 E's or M's	8 P's or higher
C	2 of 6	2 E's or M's	7 P's or higher
F	fewer than 2 of 6	fewer than 2 E's or M's	fewer than 7 P's or higher

You will receive the highest grade for which you meet ALL of the listed requirements. These requirements may be reduced (e.g. if we do not have time to cover all of the listed content areas) but will in no case be increased.

To ensure that you have ample opportunities to meet the requirements for the grade you are targeting, most content areas will appear on at least two exams (midterms or the final) over the course of the semester.

You will each also have three 'free passes' that can each be used for either of the following:

[1] a two-day extension on a problem set (except for those due immediately before an exam);
[2] a chance to revise a professional problem on which you were not satisfied with your initial grade.

Revisions on professional problems must be turned in within one week after the graded work handed back in order to be eligible for regrade consideration. Additional opportunities may be offered to revise selected exam problems, but if offered, these revisions will not require use of one of your free passes.

Problem Sets Problem sets will be assigned approximately weekly and will be due *by the start of class* one week after they are assigned. These problem sets will consist primarily of practice problems, on which you will be assessed on completion and effort only. Additionally, 6 times over the course of the semester, you will be assigned an extended *professional problem* on which you will be assessed on the accuracy and clarity of your presented work. A detailed description of expectations for your work on both types of problems will be provided as a printed handout and is available on CourseWeb.

These assignments are a key chance for you to practice and develop your skills as a quantum chemist, and you should accordingly plan to dedicate sufficient time (typically 10-12 hours/week for last year's students) to work through these problems and prepare your solutions. You are allowed - and in fact highly encouraged! - to discuss the problem sets with other students in the class; however, each student must write up and turn in their own answers independently.

To facilitate efficient marking and return of submitted work, we will use Gradescope for submission of problem sets and professional problems. If you are officially registered for this class, you should receive an invitation to Gradescope within the next 24 hours; if you are auditing and are not officially registered, please contact the instructor for access. Unless you are using one of your free passes for late submission, problem sets and professional problems must be submitted through Gradescope *by the start of class* on the due date. If you are unable to submit your work online due to technical problems, you should email a copy of your completed work to the instructor before the start of class, or, if absolutely necessary, may bring a hard copy to turn in in class.

Exams Exams will be based on the material from the lectures and the problem sets. Midterms will be given during the normal class meeting times (see schedule, below); the final exam will be a take-home exam to allow you the maximum time possible to demonstrate mastery in as many content areas as necessary. More details on exam format and expectations will be provided as the exam dates approach.

A Note About Lectures Course meetings will consist of lectures interspersed with in-class activities, including both short problems for practice and discussion, and more extended guided problem solving and derivations.

While class participation will not be factored directly into your final grade, you should plan to attend class consistently and participate fully in these in-class activities, as they will both provide key opportunities for you to develop your own understanding of the material, and will be used as jumping-off points for exercises on the exams and problem sets.

Schedule

Important Dates Class will meet regularly on Mondays and Wednesdays at 10:00 am, with the following exceptions:

Sept. 3	No class - Labor Day
Sept. 26	Midterm 1 (tentative)
Oct. 15	No class - fall break
Oct. 16	Class meets on Tuesday (fall break make-up)
Oct. 24	Midterm 2 (tentative)
Nov. 21	No class - Thanksgiving
Nov. 28	Midterm 3 (tentative)
Dec. 12	Final Exam

Please note that exam dates are *tentative* and are subject to change; finalized exam dates will be announced as soon as they are scheduled, and in all cases no later than one week before the exam.

Other Policies

Office Hours If you are unable to attend regularly scheduled office hours, please send me an email to set up an individual meeting. Please note that these meetings are *by appointment only*, and must be scheduled at least 24 hours in advance.

Email I will make an effort to respond to all course-related emails within 24 hours on weekdays and 48 hours on weekends.

If you have a more immediate question, especially about the problem sets, you are encouraged to discuss it with your fellow students, either in person or via the course discussion forums on CourseWeb/Blackboard.

Classroom Environment I strongly believe in the importance of the diversity of views, experiences, and identities of those in our scientific community. It is my goal that students from all backgrounds and perspectives be welcomed and well-served by this course. If there are aspects of the design, instruction, and/or your experiences within this course that you feel are acting as barriers to your full participation or achievement, please notify me as soon as possible so that we may take steps to address them.

Classroom Recording To ensure the free and open discussion of ideas, students may not record classroom lectures, discussion and/or activities without the advance written permission of the instructor, and any such recording properly approved in advance can be used solely for the student's own private use. If you have (or think you may have) a disability such that you need to record or tape classroom activities, you should contact your instructor and the Office of Disability Resources and Services (see below) to request an appropriate accommodation.

Academic Integrity Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity (http://www.cfo.pitt.edu/policies/policy/02/02-03-02.html). Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity. This may include, but is not limited to, the confiscation of the examination of any individual suspected of violating University Policy. Furthermore, no student may bring any unauthorized materials to an exam, including dictionaries and programmable calculators.

Disabilities If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and the Office of Disability Resources and Services (http://www.drs.pitt.edu/), 140 William Pitt Union, (412) 648-7890, drsrecep@pitt.edu, (412) 228-5347 for P3 ASL users, as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course.

Absences & Make-Up Policy If you must miss a required class activity or exam for any reason, please contact me as soon as possible so that we can make alternate arrangements.

While some exceptions may apply, make-up work (including both problem sets and exams) will generally only be offered in the case of conflicts with religious observances, documented illnesses, and personal or family emergencies.