Chemistry 713: Quantum Chemistry

Last update: for Fall 2017
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Tentative course calendar (course_calendar.php)

Syllabus

Lecture Meetings: Tue, Thu 5:00-6:15 pm, SSW-2512
Office Hours: Mon/Wed 9:30-10:30 am, CSL-310. These office hours are shared with an undergraduate class, so please be patient if you come by and I'm with other students.
Textbook: *Physical Chemistry: Quantum Chemistry and Molecular Interactions*, Andrew Cooksy. This book is intended for an undergraduate physical chemistry course, but has enough advanced topics and additional material that I think it will be suitable for our class, while providing a lot more support in case you haven't had to think about quantum for a while. The bookstore will have this, but you **do not need** the online homework subscription, so if you can find a used copy, that will be fine.

General Idea

This course is intended to benefit chemistry graduate students in all areas, as well as students in other departments with interests in the fundamentals of molecular structure and interactions. As a prerequisite, the complete undergraduate, calculus-based p-chem course (the equivalent of our CHEM 410A and 410B) is expected (as well as the year of calculus and calculus-based physics that are prerequisite to p-chem). You're welcome to contact me if you want to ask about the course content or what would be suitable preparation for the course. The emphasis should be on the principles of quantum mechanics common to all applications of chemistry, so students are encouraged to bring issues from their own research (or of other interest) to the attention of the instructor for discussion (the sooner the better).

Student learning objectives:

At the conclusion of the course, the student should be able to:

- Apply existing exact solutions to the quantum mechanics of ideal systems (such as the particle in a box, harmonic oscillator, and one-electron atom) to real systems.
- Qualitatively solve the Schrödinger equation, predicting the general features of the energies and wavefunctions based on the potential energy function of any system.
- Write (but not necessarily solve) the Schrödinger equation for any chemical system, and judiciously apply available approximations and numerical tools.
- Set up and carry out computations to solve for the properties of a molecule based on its wavefunction.
- Successfully interpret the results of a typical electronic structure calculation.

Course material

Chemical quantum mechanics, which is where to begin if you want chemistry to ever really make any sense.

General Plan:

Quantum Physics
- The Schrödinger equation, operators, and wavefunctions
- Solutions to idealized potentials: the box, the ring, the harmonic oscillator
- Quantized angular momentum

Quantum Chemistry
- One-electron atoms
- Many-electron atoms and practical quantum mechanics
- Little molecules
- Bigger molecules

Computational Chemistry
- Your Application Here

I don't intend to stray from the book's general sequence too much, but I may cover two or three chapters as a group, because I don't think some things separate as nicely as the book would like. I hope to add one or two things and will definitely skip a lot of things as we go along.

Prerequisite Math

You should be comfortable with algebra and the simple derivatives and integrals (especially of the functions ax^n, e^{ax}, and $\sin(ax)$ or $\cos(ax)$). We will cover some matrix algebra, but you don't need to have seen it before.

Grading criteria

Grading Scheme

- homework: 5%
- three exams: 25% each (drop lowest score)
- computational project: 20%
- presentation: 25%
- final: there will be no final exam for the course, to give you more time to work on projects and presentations.

The grading scale is fairly lenient:
A 80-100%
B 65-80%
C 50-65%
It is quantum mechanics, after all.

Exam Dates for Fall 2017

- exam 1: Tue Sep 26
- exam 2: Tue Oct 31
- exam 3: Tue Dec 12

Computational Project and Paper Presentation

I may modify these intrsuctions, but here is the handout (projects_handout.pdf) describing these projects from Spring 2010. Comments are welcome.

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.

Academic Honesty

Students are expected never to represent someone else's work as their own or assist others in doing so. Violations of this rule will be documented and may result in automatic failure and disciplinary review by the University. Please see the SDSU academic honesty page (http://go.sdsu.edu/student_affairs/srr/cheating-plagiarism.aspx) for further information.
