Chemistry 713: Quantum Chemistry

Last update: for Fall 2014
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Syllabus

Lecture Meetings: Tue, Thu 3:30-4:45 pm, P-147
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: Ira N. Levine, Quantum Chemistry, preferably 7th ed., but you may be able to find earlier editions around.

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. A complete undergraduate, calculus-based p-chem course (the equivalent of our CHEM 410A and 410B) is expected. 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:

- 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: 15% each (drop lowest score)
- computational project: 20%
- presentation: 20%
- final: 25%

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 2014**
- exam 1: Tue Sep 23
- exam 2: Tue Oct 21
- exam 3: Tue Nov 18
- final exam: Thu Dec 11 1:00pm-3:00pm

**Computational Project and Paper Presentation**

I may modify these instructions, 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.