CHEM 565: Quantum Chemistry I

Organizational

- Time: M/W/F 12:20–13:10
- Place: Thomas Building, Room 219
- Dates: 2018-08-20 to 2018-12-07
  - No class: Monday, September 3th, 2017 (Labor Day)
  - No class: Monday–Friday, November 18–24, 2017 (Thanksgiving Holiday)
- Teaching Assistant: Alyssa Bienvenu (bienvenu@psu.edu)

Office Hours: (tentative)

- Alyssa’s office hours: Tue/Thu 14:00-15:00 in Chemistry Building, Room 401E or 401C
- Gerald’s office hours: Mo/Fr 16:30–17:30 in Chemistry Building, Room 401A
- Other meeting times may be available (contact knizia@psu.edu).
- Short questions on homeworks or lectures can also be mailed to knizia@psu.edu.

Course Website: http://personal.psu.edu/guk15/qm1/

- Lecture slides
- Homework assignments

Textbooks

- Recommended:
  - Szabo, Ostlund – Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (1972) (for linear algebra, many-body methods, and introduction to quantitative electronic structure theory)
  - Ballentine – Quantum Mechanics, A Modern Development (for foundations of quantum mechanics)
  - Cohen-Tannoudji – Quantum Mechanics (for solvable model problems and detailed treatment of basic quantum phenomena)

Note: These are literature recommendations for further reading for interested students. Buying these books is not necessary for the course and their presence will not be assumed. But each of them is a great reference for the topics listed; for this reason I recommend interested students who wish for deeper study of a topic to investigate them in the library.
Course & Objectives

- CHEM 565 is an advanced-level introduction to theoretical quantum mechanics.
- The course aims to lay the theoretical and methodological foundations for understanding pen&paper, computational, and experimental applications of quantum theory in chemistry (at a level required for graduate studies of theoretical or physical chemistry.)
- The “language of quantum mechanics” (a peculiar form of linear algebra) and the involved mathematical structures and techniques, as well as the physical phenomena which give rise to this structure, are therefore a major topic of the course.
- By the end of the course, students should be able to:
  - Understand the nature of one-particle and $N$-particle quantum states, and their implications for the electronic structure of molecules
  - Understand and apply the core principles and equations of quantum mechanics
  - Understand and apply the core approximation techniques in quantum mechanics (variational method, perturbation theory, subspace projections)

Prerequisites

- Prior knowledge of introductory-level quantum mechanics is assumed, as typically taught in undergraduate physical chemistry courses (such as CHEM 452 at Penn State).
- A sound working knowledge of calculus and basic linear algebra (e.g., vectors, matrices, determinants, linear equation systems etc.) is assumed. Knowledge of more advanced mathematical techniques (e.g., advanced linear algebra, differential operators, differential equations, basic functional analysis) would be helpful, but is not strictly required.

Course Concept

- Monday: Lecture
- Wednesday: Lecture
- Friday: “Lab” class
  - You work on the assignments, Alyssa and I and go around and provide help and answer questions
  - Please read/try the assignments beforehand, so that you can ask targeted questions

Tentative Topics & Schedule

- Mathematical Prerequisites [4 weeks]: Advanced Linear Algebra, Probability Theory
- Principles of Quantum Mechanics [3 weeks]: State Space, Operators of Observables, Born Rule, Time-dependent and Time-independent Schrödinger Equation, Constants of Motion
and Conserved Quantities, Probability Flux, Boundary Conditions, Pure and Mixed states, Liouville-von Neumann Equation

- Simple Model Problems [4 weeks]: Free Particle, Particle-in-a-Box, Harmonic Oscillator, Spherical Potential
- Many-Particle Wave Functions [2 weeks]: Spin-Orbitals, Fermions and Bosons, Occupation Number Vectors, Fock Space, 2nd Quantization
- The Hartree-Fock Approximation [2 weeks]: Interpretation/Bonding, Uses, Breakdown

Grading

- Grading is based on homework solutions alone. There are no separate examinations. (alternatively, each homework assignment can be regarded as a small take-home exam).
- Intended grading scheme:
  - The two lowest-scoring homeworks are ignored (this is intended to take care of limited illnesses, other legitimate causes of absence, as well as “bad day”-scenarios.)
  - The remaining homework scores will be averaged; in this average, each of the remaining homeworks has equal weight (between 0% and 100% completion)
  - Based on the average score $p$, the following grades will be assigned:
    A : if $p \geq 94$
    A- : if $p \geq 90$
    B+ : if $p \geq 85$
    B : if $p \geq 80$
    B- : if $p \geq 75$
    C+ : if $p \geq 68$
    C : if $p \geq 58$
    D : if $p \geq 50$
    F : if $p < 50$