CHEM 565: Quantum Chemistry I

Organizational

- Time: M/W/F 12:20–13:10
- Place: Thomas Building, Room 121
- Dates: 2017-08-21 to 2017-12-08
  - No class: Monday, September 4th, 2017 (Labor Day)
  - No class: Monday–Friday, November 19–25, 2017 (Thanksgiving Holiday)

Office Hours: M/W/F 14:30–15:30 in Chemistry Building, Room 401A.

- Other meeting times may be available (primarily M/W/T/F after 15:30).
  Please contact knizia@psu.edu for scheduling an appointment.

- 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: (i.e., literature recommendations for further reading for interested students)
  - 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)

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.)
• 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).

Course Concept
• Monday: Lecture
• Wednesday: Lecture
• Friday: “Lab” class
  – You work on the assignments, I 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
• 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 \( p < 50\% \)