

CSI 783 Computational Quantum Mechanics - Syllabus

Course Description

This course deals with the theoretical and computational aspects of quantum mechanics, from both the chemistry and physics point of view. The aim is to present state-of-the-art computational methods for physical problems in computational physics and chemistry, and to give direct experience of using numerical computations to model real systems. Students will learn how to run quantum codes efficiently and how to interpret output data correctly, and will be able to perform calculations of practical importance. To this end, this course will provide a formal understanding of quantum mechanics, from atoms, to molecules to extended systems. The integration of theory and computation of quantum mechanics will be of great value to students interested in theoretical and computational physics and chemistry, as well as materials science and engineering. This course is cross-linked with computational quantum physics (PHY 736).

Instructor

Prof. Howard Sheng

Office: Rm 370, Research I

Email: hsheng@gmu.edu

Phone: 703-993-8576

Lectures

Tuesdays 4:30 - 7:10 PM, Rm 301, Research I Building

Objectives

- Provide a formal understanding of quantum mechanics. Get familiar with theoretical underpinnings of computational methods.
- Familiarize the students with computational quantum mechanics. Understand the scope, possibilities and limitations of various quantum computational methods.

- Be able to solve physical problems using quantum computational methods, both in course work and in his/her future research.
- Keep abreast with the current research and development of quantum computational methods. Where to go, and what to expect.

Textbook

Teaching materials will be collected from different textbooks. The recommended textbook will be:

- Quantum Chemistry by J. Lowe and K. Peterson, Academic Press 2005 (third edition)

Additional reference books:

- Quantum Chemistry by Levine, Prentice Hall 1998 (fifth edition).
- Introduction to Computational Chemistry by F. Jensen, New York: John Wiley and Sons, 1999.
- Ab initio Molecular Orbital Theory by W.J. Hehre, et al., New York: John Wiley and Sons, 1986. (focusing on calculations performed with Gaussian.)
- Electronic Structure: Basic Theory and Practical Methods, by R.M. Martin, Cambridge, UK: Cambridge University Press, 2004. (Electronic structure calculations from the physics standpoint, focusing on DFT)
- Atomic and electronic structure of solids by E. Kaxiras, Cambridge Univ. Press, 2003.

Other referenced text (book chapters, scientific papers, monographs) will be distributed in teaching handouts.

Prerequisite

There are not specific prerequisite, just permission of the instructor. Students are expected to relatively quickly become comfortable with advanced concepts from mathematics and physics.

Homeworks and Final Project

Each student will be responsible to cover the material in the textbook or lecture notes, do the assigned homework exercises, and develop a certain number of short computational projects. There will be a mid-term exam. Each student is required to complete a final project. A formal written report and oral presentation are required. Project topics will be available to students as class progresses.

Software

Gaussian03, CPMD, VASP

Other quantum codes may be considered: NWCHEM, ABINIT, WIEN2K, PWSCF

Computers

Students will have access to wk*.cos.gmu.edu workstations running Scientific Linux. User accounts will be created for computational projects in this course.

Office hours

I do not plan to hold regular office hours, but will have an open-door policy. Students are welcome to drop by my office any time. If you would like to make an appointment with me at a specific time, send emails to: hsheng@gmu.edu

Evaluation

- 30% acquired through the final project
- 30% mid-term exam
- 20% homework exercises (written)
- 20% homework (computational)

Ethics

In this course, I expect students to be honest and truthful. Ethical violations include cheating on exams, plagiarism, unauthorized collaboration, alteration of graded assignments, forgery, falsification, lying, facilitating academic dishonesty, and unfair competition. More will be discussed on the first day of class.

Tentative Class Schedule

- Week1: Introduction to Quantum Mechanics
- Week2: Solving the Schrodinger Equation
- Week3: The Hydrogen-like Atom
- Week4: Many-electron Atoms
- Week5: The Variation Method and Perturbation Theory

- Week6: The Hatree-Fock Method and Matrix Manipulations
- Week7: Molecular-Orbital Theory
- Week8: Gaussian Basis Sets
- Week9: Electronic Classroom Tutorial
- Week10: Ab initio calculations and Density Functional Theory
- Week11: DFT - Solution of Kohn-Sham Equations and Exchange-Correlation Functionals
- Week12: The Planewave Pseudopotential Method
- Week13: Ab initio Molecular Dynamics and Applications
- Week14: Student Project Presentation