Chemistry 6472:
Quantum Chemistry and Molecular Spectroscopy

Instructor

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Requirements and Grading Scheme

Problem sets	30%
First test	20%
Second test	20%
Final	30%

Auditors are required to take two out of the two tests or final and demonstrate a minimal understanding of the subject. Pass/fail students are required to take both tests and the final and receive an overall passing grade.

Topics

Unit I: Overview, Mathematical Introduction

(A) Introduction to quantum mechanics:
Scope and applicability of quantum mechanics
The Schrödinger equation

(B) History of quantum mechanics

(C) Linear vector spaces:
Definitions
Inner products
Dual spaces and Dirac notation

(C) Operators:
Basic operator rules
Classes of operators: linear, hermitian, unitary, etc.
Commutators

(D) Postulates

(E) Simple problems: particle in a box (1D and 3D), free particle

Unit II: Fundamentals

(A) Harmonic oscillator
Vibrational (IR) spectroscopy, anharmonicity, group theory

(B) Heisenberg uncertainty relations

(C) Angular momentum:
Commutation rules
Spherical harmonics
Ladder operators
Rigid rotor: a model for rotational (microwave) spectroscopy

(D) The Hydrogen atom and its electronic spectrum

Unit III: Approximate Methods

(A) Variational method:
Variational theorem
Equivalence of Raleigh-Ritz procedure and diagonalization

(B) Time-independent perturbation theory

Unit IV: Advanced Fundamentals

(A) Spin and ESR spectroscopy

(B) Degenerate perturbation theory and the Stark effect in H atom

(C) Time-dependent perturbation theory and the interaction of light with matter

Unit V: Electronic Structure and Spectroscopy

(A) The molecular Hamiltonian:
Born-Oppenheimer approximation

(B) Separation into electronic, vibrational, rotational terms

(C) Introduction to Hartree-Fock theory:
Two-electron problem
Hartree products
Antisymmetry and Slater determinants
Generalization to N-electrons
Self-consistent-field

(D) Introduction to correlated methods

(E) Electronic structure of atoms

(F) Electronic structure of diatomics

(G) Electronic structure of polyatomics:
Walsh's rules

(H) Rovibronic spectroscopy and the Franck-Condon approximation

Required Textbook

1. P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 3rd ed. (Oxford University Press, Oxford, 1997).

Recommended Textbook

1. R. Shankar, *Principles of Quantum Mechanics*, 2nd ed. (Plenum, New York, 1994). Parts of chapters 1, 4-10, and 12-18 cover Units I-IV.

Supplementary Books of Possible Interest

1. G. Strang, *Linear Algebra and its Applications*, 3rd Ed., (Harcourt Brace Jovanovich, San Diego, 1988).

2. D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley, CA, 1983). Very readable introductory text.

3. H. C. Ohanian, *Principles of Quantum Mechanics* (Prentice Hall, Englewood Cliffs, NJ, 1990). Interesting introductory text.

4. I. N. Levine, *Quantum Chemistry*, 4th ed. (Prentice Hall, Englewood Cliffs, NJ, 1991). Covers most of the topics in this course at a slightly lower level.

5. E. Merzbacher, *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1998). Physics text comparable to Shankar but less verbose.

6. I. N. Levine, *Molecular Spectroscopy* (Wiley, New York, 1975). Explains the quantum mechanical details behind spectroscopy.

7. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised (Dover, 1989). Parts of chapters 1-3 cover Unit V.