Chemistry 6491: Quantum Mechanics

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: Fundamentals of Quantum Mechanics

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

(B) Linear vector spaces:
Definitions (S 1.1; S&O 1.1.1)
Inner and outer products (S 1.2; S&O 1.1.2-1.1.3)
Dual spaces and Dirac notation (S 1.3; S&O 1.1.4)

(C) Operators:
Basic operator rules (S 1.5-1.6)

Classes of operators: linear, hermitian, unitary, etc. (S 1.6; S&O 1.1.2)
Diagonalization and eigenvalue equations (S 1.8; S&O 1.1.6)
Change of basis (S 1.7; S pp 43-54; S&O 1.1.5)
The Propagator (S pp 43-54)
Functions of matrices (S 1.9; S&O 1.1.7)
Commutators; Campbell-Baker-Hausdorff theorem (notes)
Connection between functions and Dirac notation (S 1.10; S&O 1.2)

(D) Postulates of QM (S Chapt 4)

(E) Review of simple problems in 1D (S 5.1-5.2)

(F) The classical limit: Ehrenfest's theorem (S Chapt 6)

(G) Second quantization; example of harmonic oscillator (S Chapt 7)
Application of Harmonic Oscillator to IR spectroscopy (handouts)

(H) Introduction to path integrals (S Chapt 8)

(I) Angular momentum:
Commutation rules
Spherical harmonics
Ladder operators

Unit II: Approximate Methods

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

(B) Time-independent perturbation theory

Unit III: Advanced Fundamentals

(A) Spin

(B) Addition of angular momenta

(C) Degenerate perturbation theory

(D) Time-dependent perturbation theory

(E) Interaction of light with matter

Unit IV: Electronic Structure Theory

(A) The molecular Hamiltonian:
Details of the Born-Oppenheimer approximation

(B) Electronic structure of atoms

(C) Electronic structure of diatomics

(D) Electronic structure of polyatomics

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

(F) Introduction to correlated methods:
Configuration Interaction (CI)
Many-body perturbation theory (MBPT)
Coupled-cluster theory

(G) A survey of quantum chemical methods

Textbooks

1. R. Shankar, *Principles of Quantum Mechanics*, 2nd ed. (Plenum, New York, 1994). Intermediate-level physics book covering the pure quantum part, some lecture material drawn directly from here.

Recommended Supplementary Books

1. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised (Dover, 1989).

2. I. N. Levine, *Quantum Chemistry*, 5th ed. (Prentice Hall, Englewood Cliffs, NJ, 2000). Covers most of the topics in this course at a slightly lower level.

3. G. Strang, *Linear Algebra and its Applications*, 3rd Ed., (Harcourt Brace Jovanovich, San Diego, 1988). Good intro to linear algebra.

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

5. E. Merzbacher, *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1998). Advanced physics text.