

# Chemistry 6491: Quantum Mechanics

## Instructor

Instructors: Prof. C. David Sherrill  
Email: sherrill@gatech.edu  
Phone: 404-894-4037  
Office: MS&E 2100N  
Office Hours: MW 2-3

## Requirements and Grading Scheme

Problem sets	25%
Math recitation	5%
First test	20%
Second test	20%
Final	30%

Auditors are required to attend a minimum of 1/2 of the lectures. Pass/fail students are required to take both tests and the final and receive an overall passing grade.

## Topics

In the list below, “S” denotes the primary textbook by Shankar. “S&O” denotes the optional supplementary book by Szabo & Ostlund (which covers more electronic structure theory, a topic we might touch on at the end if there is time, but it also has some good review of linear algebra in Chapter 1).

### 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) Angular momentum (S Chapt 12):
  - Spherical harmonics (S 12.5)
  - Ladder operators (S 12.5)
  - Rigid rotator and Rotational spectroscopy
  - Central force problems (S 12.6)
  - Hydrogen atom (S Chapt 13)

## Unit II: Approximate Methods

- (A) Variational method:
  - Variational theorem (S 16.1)
  - Equivalence of Raleigh-Ritz procedure and diagonalization
- (B) Time-independent perturbation theory (S 17.1-17.2)

## Unit III: Advanced Fundamentals

- (A) Spin (S Chapt 14)
- (B) Addition of angular momenta (S Chapt 15)
- (C) Interaction of light with matter

## 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.

## Other Books that may be Helpful

1. D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley, CA, 1983). Very readable introductory text.
2. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised (Dover, 1989). Short review of linear algebra and Dirac notation, and thorough introduction to Hartree–Fock theory.
3. 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.
4. G. Strang, *Linear Algebra and its Applications*, 3rd Ed., (Harcourt Brace Jovanovich, San Diego, 1988). Good intro to linear algebra.
5. E. Merzbacher, *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1998). Advanced physics text.