CHEMISTRY 540: QUANTUM MECHANICS

Fall Semester 2021
Instructor: Prof. Nancy Makri
Lectures: Tues. & Thur. 9:30-10:50 a.m. online

Course Outline

1. Introduction
The two-slit experiment.
The particle-wave nature of matter.
The Schrödinger equation.

2. General structure and formalism of quantum mechanics
Postulates of quantum mechanics.
Dirac notation.
Operators and commutator algebra.
Position and momentum operators.
Orthonormality, completeness and basis sets. Dirac's delta function.
Symmetries and conservation laws.
Discrete vs. continuous spectra.
Matrix formulation of quantum mechanics. Solution of the eigenvalue problem.

3. Exactly solvable time-independent problems
Free particle and the momentum representation.
Potential barriers. Particle in a box. Particle on a ring.
The harmonic oscillator; raising and lowering operators.
Probability density and quantum-classical correspondence.
Separable multidimensional problems; degeneracy.
Introduction to normal mode transformations.
Tunneling; two-level systems and inversion splitting.
Hückel theory.

4. Angular momentum
Angular momentum operators; eigenvalues and eigenfunctions (spherical harmonics).
Orbital angular momentum. The hydrogen atom.
Spin. Exchange symmetry for identical particles; bosons and fermions. Spin-orbitals.

5. Time-independent approximation methods
Perturbation theory (non-degenerate and degenerate). Projection operators and Green's functions.
The variational principle. Linear variations and basis set expansions.
The Born-Oppenheimer approximation. Potential functions.

6. Introduction to time-dependent quantum mechanics
The time-dependent Schrödinger equation. Stationary states.
Evolution of non-stationary states.
The Heisenberg equation of motion.