

Course of Study

1. Birth of Quantum Mechanics

Failures of Classical Mechanics in Black Body Radiation, Photoelectric Effects, Heat capacity of Solids, and Atomic Spectra; Quantum Mechanics - the Saviour; Birth of Quantum Chemistry.

2. Principles and Postulates of Quantum Mechanics

State Functions; Operators; Eigenfunctions; Expectation Values; Time Evolution of Expectation Values; Ehrenfest Theorem; Hermitian Property; Schmidt Orthogonalization; Dirac Notation; Dirac Delta Function; Commutation of Operators; Heisenberg's Uncertainty Principle; Parity Operator.

3. Exactly Solvable Models

• Translational Motions

Particle in a 1D box; Bohr's Correspondence Principle; Free Particle; Particle in a 3D box; Degeneracies; Particle in a Rectangular Well; Tunneling Through Barrier; Scanning Tunneling Microscopy.

• Vibrational Motions

Harmonic Oscillators; Creation-Annihilation Operators; Hermite Polynomials; Vibrational Spectroscopy

• Angular Motions

Angular Momentum Operators; Ladder Operators; Spherical Harmonics.

• Rotational Motions

Particle in a ring; Particle on a sphere; Rigid Rotor;

• Hydrogen Atom

Solution of H-atom; Bound-state H-atom Wave Functions; Radial Distribution Functions; H-like Orbitals; Zeeman Effect; H-atom with Electron Spin; Spin-Orbit Interaction; Atomic Spectra with Spin-Orbit Interaction in Magnetic Field.

4. Approximate Methods

Variational Theorem; He atom with Variational Method; Perturbation Theory; 1st and 2nd Order Perturbation Correction to He atom; Time Dependent Perturbation Theory; SCF Method; Koopmann Theorem; Slater Determinants; Valence bond and Molecular Orbital Theories.

5. Molecular Spectroscopy

Interaction of light with matter; Rotational Spectroscopy by Rigid-Rotor and Non-Rigid Rotor Approximation; Vibrational Spectroscopy with Harmonic Oscillators and with Anharmonicity; Fundamentals, Overtones, and Fermi Resonance; Hot Bands; Rovibrational Spectra and P-Q-R Branches; Raman Effect; Rotational and Vibrational Raman Spectroscopy; Franck-Condon Factors; Electronic Transitions and Symmetry; Rovibronic Spectra and Fortrat Diagrams. Photo-electron Spectroscopy.

Books:

- Quantum Chemistry by I. N. Levine.
- Molecular Quantum Mechanics by P. W. Atkins and R. S. Friedman.
- Quantum Chemistry by D. A. McQuarrie.
- Modern Spectroscopy by J. M. Hollas.
- Fundamental of Molecular Spectroscopy by C. N. Banwell and E. M. McCash