TIFR, Hyderabad

Course: Quantum Mechanics for Chemists
Credits: 4
Preferred time slots: 8:30 - 10:00 AM
No. of classes: 30 (45 Hrs)
Start Date: July 2026
Instructor(s): Raghunathan Ramakrishnan

Syllabus:

1. **Origins and foundations of quantum mechanics:** Historical origins of quantum theory; failure of classical physics for microscopic radiation and matter; blackbody radiation, photoelectric effect, Bohr quantization, and wave-particle duality. Schrödinger equation, wavefunctions, probability interpretation, normalization, expectation values, operators, eigenvalue equations, Hermitian operators, commutators, uncertainty principle, Dirac notation, and matrix representation of operators.
2. **Exactly solvable model systems:** Particle in a 1D box, finite barriers and tunneling, boundary conditions, quantization, nodes, orthogonality, and degeneracy. Harmonic oscillator as a model for molecular vibration, vibrational energy levels, and ladder-operator treatment. Rigid rotor as a model for molecular rotation, rotational energy levels, spherical harmonics, and rotational quantization. Hydrogen atom, central Coulomb potential, separation of variables, quantum numbers, radial and angular wavefunctions, orbital shapes, degeneracy, and selection rules.
3. **Angular momentum and spin:** Orbital angular momentum, angular momentum operators, commutation relations, simultaneous eigenfunctions of L^2 and Lz, spherical harmonics, ladder operators, and angular momentum algebra. Spin as intrinsic angular momentum, spin-1/2 systems, Pauli matrices, spin measurements, singlet and triplet spin functions, addition of angular momentum, coupled and uncoupled bases, and basic Clebsch–Gordan coefficients.
4. **Approximation methods:** Variational principle, trial wavefunctions, variational parameters, helium effective nuclear charge calculation, linear variation method, basis functions, secular determinants, and matrix eigenvalue problems. Nondegenerate perturbation theory, first- and second-order energy corrections, wavefunction corrections, degenerate perturbation theory, level splitting, time-dependent perturbation theory, transition amplitudes, transition probabilities, Fermi's golden rule, and selection rules.
5. **Many-electron atoms and antisymmetry:** Helium atom, electron-electron repulsion, orbital approximation, exchange, and electron correlation. Indistinguishable particles, symmetric and antisymmetric wavefunctions, Pauli principle, spin-space symmetry, spin multiplicity, Slater determinants, many-electron wavefunctions, determinant algebra, many-electron atoms, atomic term symbols, Hund's rules, and atomic spectra.
6. **Hartree–Fock and many-electron machinery:** Independent-particle models, Slater determinants as many-electron trial wavefunctions, variational basis of Hartree–Fock theory, self-consistent field method, optimized orbitals, orbital energies, Koopmans' theorem, Fock operator, Roothaan equations, basis-set representation, overlap matrix, density matrix, open-shell systems, and configuration interaction.
7. **Molecular quantum mechanics and chemical bonding:** Born–Oppenheimer approximation, molecular Hamiltonian, separation of electronic and nuclear motion,

potential energy surfaces, nuclear motion on electronic surfaces, molecular electronic transitions, and transition dipole moments. Quantum treatment of H2+, H2, and simple diatomic molecules; LCAO-MO theory, bonding and antibonding orbitals, overlap, Coulomb and resonance integrals, valence-bond and molecular-orbital descriptions, exchange, electron pairing, and qualitative chemical bonding.

8. **Molecular orbital and electronic structure theory:** Localized and delocalized molecular orbitals, hybridization, nonlinear molecules, symmetry, Hückel theory, semiempirical molecular orbital methods, secular equations, molecular orbital diagrams, conjugated molecules, and qualitative reactivity from MO coefficients. Hartree–Fock theory and an introductory overview of electron correlation, configuration interaction, Møller–Plesset perturbation theory, coupled cluster theory, and density functional theory.
9. **Spectroscopic applications:** Rotational, vibrational, and electronic transitions; transition dipole moments, selection rules, spin-orbit effects, Zeeman splitting, Franck–Condon principle, molecular electronic spectra, and the qualitative connection between quantum mechanics, molecular structure, and molecular spectroscopy.

Pre-requisite courses (the courses which have to be taken before opting for this course): None. Prior exposure to elementary quantum models such as particle in a box, harmonic oscillator, rigid rotor, and hydrogen atom is desirable.

Primary Text:

1. Frank Pilar, Elementary Quantum Chemistry, Dover.

Reference Books:

1. Donald A. McQuarrie, Quantum Chemistry, University Science Books.
2. Ira N. Levine, Quantum Chemistry, Pearson.
3. Attila Szabo and Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover.
4. Nouredine Zettili, Quantum Mechanics: Concepts and Applications, Wiley.

Evaluation Method: Assignment-based class tests (40 marks), mid-term (30 marks), finals (30 marks)

Course Outcome (CO):

Sr. No.	On completing the course, the student will be able to:
CO 1	Use the postulates, operator formalism, and Dirac notation of quantum mechanics.
CO 2	Solve and interpret standard quantum model systems relevant to atoms and molecules.
CO 3	Apply variational and perturbation methods to chemical and spectroscopic problems.
CO 4	Understand angular momentum, spin, antisymmetry, and many-electron wavefunctions.
CO 5	Explain the quantum-mechanical basis of molecular bonding, molecular orbitals, and spectroscopy.
CO 6	Develop the foundation needed for advanced quantum chemistry or a physics-style QM-II course.