

TCIS Hyderabad

Course : Quantum Mechanics - I
Credits : 4
Coordinates : Monday & Wednesday 11.00 - 12.30 hrs.
Contact Hours : 48 hrs.
Instructor/s : Subodh R Shenoy & Raghunathan Ramakrishnan

Syllabus

- **The need for QM:** Movies on Davisson & Germer electron diffraction; Young's 2-slit with photons. Ideas from de Broglie, Bohr, Heisenberg, Schroedinger, Born. 'First' quantized momentum & position, and commutator. Heuristic argument for Schroedinger's equation, starting from free particle.
- **Quantum Concepts:** Wave-functions and bra-ket notation; ortho-normality; completeness, unitary transforms; local continuity for probability density; special role of hermitian operators; uncertainty principle; symmetry operators, common eigenfunctions, degeneracies; Pauli exchange and fermions/bosons; Slater determinants.
- **Bound States:** Non-bound wave-functions e.g. 1D square barrier. Bound states of 1 D & 3D square well; 1D circle and 3D spherical-well; Angular momentum algebra and eigenfunctions. 1D simple harmonic oscillator (SHO), minimum uncertainty product in ground state; 1D SHO re-visited: operator approach. Hydrogen atom, Rung-Lenz degeneracy. Hund's Rules, L.S coupling; spectroscopic level notation; Periodic Table, and filling of atomic levels.
- **Molecules and bonding:** Born-Oppenheimer approx; Heitler-London valence bonds versus Mulliken molecular orbitals; bonding/ anti-bonding states; qualitative ideas of σ , π bond-overlaps; sp^3 hybridization. [Handout: Shape, Structure Molecules by C A Coulson.]
- **Approximation Methods:** Variational methods (e.g. attractive delta function and Gaussian trial). Time-independent perturbation theory for single/ degenerate energy levels (e.g. Zeeman/ Stark effects). Selection rules for electric dipole matrix elements. [Handout: Time-dependent perturbations and decay rates]

Text / References Books

- D. Griffiths, Introduction to Quantum Mechanics (Pearson Education)
- R. Shankar, Principles of QM, (Springer, Prism Books)
- E. Fermi, Lecture Notes on QM (U of Chicago Press)
- C.A. Coulson, The Shape and Structure of Molecules (Oxford Chemistry Series)
- JP Lowe and KE Petersen, Quantum Chemistry (Elsevier)