

CHM 322/642: Principles of Quantum Chemistry (4)

Prerequisites: MTH 101, PHY 101, CHM 101, MTH 102, PHY 102, MTH 201, PHY 201 or their equivalent **Not allowed for Physics majors**

Review of basic concepts of quantum theory: wave-particle duality and de Broglie wavelengths, uncertainty principle, superposition and state of a quantum system.

Mathematical background: Operators in quantum mechanics and their properties, eigenvalues and eigenfunctions, commutation relations, unitary transformations and change of basis. Matrix representation of operators.

Postulates of quantum mechanics: States and wavefunctions, observables and the measurement hypothesis, Born interpretation of wavefunction, time evolution of states and the Schrodinger equation, stationary states, compatible observables and the generalized uncertainty principle.

One-dimensional problems: Particle in a well and transmission through a barrier. Probability currents and the equation of continuity. Two and three-dimensional potential wells and degeneracy. Applications to conjugated molecules and other one-dimensional systems. Linear harmonic oscillator – ladder operator method, parity of harmonic oscillator eigenfunctions. Rigid rotor problem, angular momentum, angular momentum eigenvalues and eigenfunctions.

The hydrogen atom: Atomic orbitals – radial and angular wavefunctions and distributions, electron-spin and spin operators. Virial theorem and application to hydrogen atom and other problems. Hydrogen-like atoms.

Atoms in external fields: Zeeman and Stark effect.

Approximation methods: Time-independent perturbation theory – Anharmonic oscillator, He atom, H^{2+} molecular ion. Variational theorem - He atom, H^{2+} molecule and the LCAO approach.

Suggested Books:

- Levine, I., *Quantum Chemistry*, Ed. 6th, Pearson Press, **2009**.
- McQuarrie, D. A., *Quantum Chemistry*, Ed. 2nd, University Science Books, **2008**.
- Zettili, N., *Quantum Mechanics*, Ed. 2nd, John Wiley, **2009**.
- Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, Oxford University Press, **2008**.