

## TCIS, Hyderabad

**Course:** Quantum Mechanics-I

**Start Date:** 02 August 2017

**Coordinates:** Monday and Wednesday between 09.30 am and 11.00 am

**Instructor:** Dr. Raghunathan Ramakrishnan ([ramakrishnan@tifrh.res.in](mailto:ramakrishnan@tifrh.res.in))

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### **Syllabus:**

#### **1. Origins of the Quantum Theory**

Classical mechanics and classical models (Hamiltonian formalism, Lagrangian formalism, adiabatic invariance, virial theorem, constants of the motion, Poisson bracket), radiation laws (cavity radiation), particle aspects of light (photoelectric effect, Compton scattering, pair-production, Bremsstrahlung, Frank-Hertz experiment), wave aspects of matter (Davisson-Germer experiment), wave-particle duality, old quantum theory with applications to simple potentials (Bohr atom, Ritz combination principle, Wilson-Sommerfeld quantization rules), specific heats (Dulong-Petit's law, Debye vs. Einstein theories), Bohr's correspondence principle, classical wave equation (1D, 2D, 3D), Stern-Gerlach experiment (angular momentum and spin)

#### **2. The Wavefunction**

The Schrodinger equation, postulates of quantum mechanics, statistical interpretation, probability, sketching wavefunctions, interpretation of wavefunction: probabilities and boundary conditions, well-behaved functions

#### **3. Foundation Topics**

Hilbert space, projection operators, uncertainty principle (energy width and lifetime of excited states), representation of operators, Dirac notation, Dirac delta function, commutation relations, dynamical variables, symmetry and conservation laws, classical limit, from position-to-momentum space and back, wavepackets (Gaussian wavepacket), Ehrenfest's theorem, probability current, bound, unbound, and continuous states

#### **4. One-dimensional Systems**

The infinite square well (aka particle-in-a-box, eigenvalue problem), series solution method, free particle, finite square well, delta-function potential, Harmonic oscillator (associated Hermite polynomials, selection rules, Wigner distribution), Ehrenfest relations, quantum mechanical virial theorem, quantum mechanical tunneling (step-barrier potential, ammonia inversion, alpha decay), periodic potential (Bloch's theorem, Kronig-Penney model), particle in a ring

#### **5. Two-dimensional Systems**

Two-dimensional square well (degenerate states), two-dimensional harmonic oscillator (isotropic oscillator, Cartesian vs polar coordinates), particle in a disk

#### **6. Three-dimensional Systems**

Three-dimensional square well, three-dimensional isotropic oscillator, spherical coordinates, central potentials (H atom), angular momentum operator (matrix representation), associated Legendre polynomials, associated Laguerre polynomials, spherical harmonics, spin (Pauli matrices), quantum numbers

#### **7. Second Quantization**

Raising and lowering operators (aka creation and annihilation operators), algebraic approach for harmonic oscillator, angular momentum algebra, spin algebra

#### **8. Time-Dependent Quantum Mechanics**

Time-dependent Schrodinger equation, time-dependent expectation values, semi-classical treatment of radiation, time-dependent potential, periodic potential, transition frequencies, transition rules,

sudden approximation (adiabatic theorem), time-dependent perturbation theory, Fermi's golden rule. two-level systems, emission and absorption of radiation.

#### **9. Approximation Methods**

Variational theory, linear and nonlinear variational methods ( $H_2^+$ , Helium, H, secular determinant), Rayleigh-Schroedinger perturbation (non-degenerate zero-order case, degenerate zero-order case, matrix eigenvalues, cubic well, quartic well, Stark effect, Van der Waals interaction), WKB method

#### **10. Many Particles**

Identical particles, indistinguishability, Pauli exclusion principle, Slater determinant, band structure of solids, quantum statistics, electron gas

#### **11. Atomic Spectra**

Term symbols, fine structure of H, Zeeman effect, hyperfine splitting in H, spin-orbit coupling, He atom, energy level diagrams, selection rules, radiation of atoms ( $2p \rightarrow 1s$  transition, lifetime and linewidth, Einstein coefficients, )

#### **12. Molecular Structure and Bonding**

Molecular hamiltonian, Born-Oppenheimer approximation, MOs as LCAOs, diatomic molecules (bond order, MO diagram), hybrid orbitals, perturbation theory for molecular orbitals, Walsh diagrams, elements of molecular spectroscopy, Hellmann-Feynman theorem

#### **13. Measurement and Interpretation**

Determinism, locality, measurement, hidden variables, EPR paradox, Bell's Theorem, cat paradox, Copenhagen interpretation

#### **Required Texts**

1. *Introduction to Quantum Mechanics*, Edition-2, D.J. Griffiths, Pearson (2016, Indian Edition).
2. *Quantum Mechanics: Concepts and Applications*, Edition-2, N. Zettili, Wiley (2016, Indian Edition)

#### **Reference Texts**

1. *Quantum Chemistry*, D.A. McQuarrie, Viva (2016, Indian Edition).
2. *Quantum Mechanics*, D. McIntyre, C.A. Manogue, J. Tate, Pearson (2016, Indian Edition).
3. *Quantum Physics*, S. Gasiorowicz, John Wiley (1996), Recent Indian edition available along with web-content.
4. *Quantum Mechanics*, Edition-2, B.H. Bransden, C.J. Joachain, Pearson (2008, Indian Edition).

#### **Evaluation Method:**

Assignments with participation in discussion classes (20 %), two in-class exams (40 %), final exam (40 %)