

Department of Chemical Sciences

Graduate Course on

Mathematical Methods

Course Content

1. Complex numbers and analysis

- a. Argand's diagram, complex algebra
- b. de Moivre's theorem and applications
- c. Functions of complex variables
 - i. Analytic functions, multi-valued functions, singularities and zeros
 - ii. Complex integration and series expansions
 - iii. Residue theorem and applications

2. Vectors, Matrices, and Tensors

- a. Vectors
 - i. Vector algebra, differentiation and integration
 - ii. Vector operators, gradient, divergence, curl
 - iii. Line, surface, and volume integrals
 - iv. Integral (Green's, Divergence, and Stokes) theorems and applications
- b. Matrix representations and operators
 - i. Notation, algebra and matrix operations, Special square matrices
 - ii. Change of basis, eigenvalues and eigenvectors
 - iii. Applications
- c. Tensors (Cartesian)
 - i. Notation and algebra, quotient law, Kronecker delta, Levi civita symbols

3. Orthogonal functions and Integral Transforms

- a. Orthogonal functions
 - i. Even, odd, orthogonal, and orthonormal functions
 - ii. Fourier series, expansion in terms of orthonormal functions
 - iii. Gram-Schmidt orthogonalization, Schwarz inequality
 - iv. Hermite, Legendre, and Laguerre polynomials and associate properties
- b. Fourier transforms
 - i. Definitions, Properties
 - ii. Convolutions/deconvolutions
 - iii. Correlations functions, energy spectra
 - iv. Parseval's theorem
- c. Laplace transforms
 - i. Definitions and properties
 - ii. Transforms of derivatives and integrals

4. Differential Equations

- a. Ordinary differential equations (ODE) and elementary methods
 - i. Classifications of equations, exact, inexact, linear, nonlinear, homogenous, nonhomogenous

- ii. Direct integration, separation of variables, integrating factors
- b. Higher order ODE and solutions
 - i. Linear equations with constant coefficients,
 - ii. Linear equations with variable coefficients,
 - iii. Solutions using Laplace transforms
 - iv. Solutions using Greens functions
- c. Series solutions of ODE
 - i. Solutions about ordinary and singular points
 - ii. Wronskian and derivative methods
 - iii. Fuch's theorem
- d. Eigenfunction methods
 - i. Operators: Adjoint, Hermitian and properties
 - ii. Sturm-Liouville equations
 - iii. Superposition of eigenfunctions
- e. Partial differential equations
 - i. Diffusion, Wave, Laplace, Poisson, and Schrödinger equations

Text/Reference Books:

1. K. F. Riley, M. P. Hobson, S.J. Bence, *Mathematical methods for physics and engineering*, 3rd edition, Cambridge University Press (2002)
2. M. L. Boas, *Mathematical methods in physical sciences*, 3rd editions, Wiley-India (2006)
3. J. M. Anderson, *Mathematics for quantum chemistry*, Dover Publications (2005)
4. W. W. Bell, *Special functions for Scientists and Engineers*, Dover Publications (1996)

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Venue: Lecture room AG-80

Days: Tuesdays and Thursdays

Time: 9:30 hr to 11:30 hr

The first lecture starts on August 13, 2015.