Department of Chemical Sciences

Graduate Course on

MATHEMATICAL METHODS (2017)

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Course start date: August 7 (Monday)
Hours: 9:30 am – 10:30 am
Days: Monday and Wednesday
Venue: Lecture Room AG-80
Office Hours: 11 am – 1pm
(Tuesday and Friday)

Syllabus

1. **Complex numbers and analysis (6 Lectures)**
    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, Contour integration

2. **Vectors, Matrices, and Tensors (7 Lectures)**
    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 (10 Lectures)**
    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 (13 Lectures)**
   a. Ordinary differential equations (ODE) and elementary methods
      i. Classifications of equations, exact, inexact, linear, nolinear, homogenous, nonhomogenous.
      ii. Direct integration, separation of variables, integrating factors
   b. Higher order ODE and solutions
      i. Linear equations with const 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 Schrodinger equations

Text/Reference Books:

1. K. F. Riley, M. P. Hobson, S.J. Bence, *Mathematical methods for physics and gineering*,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)

Grading:

Two exams with equal weight: Part-I in October and Part-II in December
Assignments every two weeks + in-class discussion
Grade distribution (50% for each part)**:**
Assignments (10%) + in-class discussion (6 presentation + 4 participation=10%) + written exam (30%)