

CHM 521: Mathematics for Chemistry

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Lectures: TThF 0800 WL 222

Office Hours: M W 1500 - 1600 SL 302

Course description: Linear Algebra, Differential Equations, Group Theory

Course Details

1. **Vectors, Matrices and Linear Algebra:** Vectors and Scalars, Vector operations, Gradient, Divergence, Curl, Greens Theorem and Stokes Theorem, Matrices, Hermitian and Unitary Matrices, Eigenvalues, Eigenvectors, Matrix Diagonalization, Basis vectors, Curvilinear Coordinates. (10 lectures)
2. **Differential Equations:** Ordinary differential equations, general solution, particular solution, second order differential equations with constant coefficients, integrating factor method for solving DEs, power series method, Sturm-Liouville Problem, basis functions, Fourier Transforms, Delta Functions, distribution functions, statistics, mean, standard deviation, error estimates, Taylor series, approximate methods. (18 lectures)
3. **Group Theory:** Group, subgroup, symmetry elements, symmetry point groups, group representations, great orthogonality theorem, wavefunctions as bases for irreducible representations, symmetry adapted linear combinations. (12 lectures)

Prerequisites: Basic knowledge of mathematical concepts of integration, differentiation, and some exposure to linear algebra, complex analysis and probability theory will be assumed. In this course, we will not have time to go into details of many of the topics discussed, so you will have to learn some of the topics on your own.

Books: There is no prescribed book for this course. I prefer to make my notes after reading different books. There are many excellent books in Engineering Mathematics and you will be well-served by reading one or more of them. Most of what I will cover will be found in one of the books below.

1. G.B. Arfken and H.J. Weber *Mathematical Methods for Physicists*
2. E. Kreyszig *Advanced Engineering Mathematics*
3. D.A. McQuarrie *Mathematical Methods for Scientists and Engineers*
4. C.L. Perrin *Mathematics for Chemists*
5. F.A. Cotton *Chemical Applications of Group Theory*
6. R.L. Carter *Molecular Symmetry and Group Theory*

Internet Resources and Mathematical Software: There are many online resources, but there is no guarantee that they provide the correct information. You are encouraged to search on the internet. Some resources that might be useful are given below.

1. <http://www.wolfram.com/mathematica> : This is the homepage of the software and programming language Mathematica. It has many good mathematical tips too. You will have to learn this program and you will use it to solve all your assignments.
2. <http://www.mathworks.com/MATLAB>: Another mathematical software and an associated programming language.

Grading System

1. Homework Assignments: (25 points total) : This is the most important part of the entire course. If you do all the assignments sincerely and understand the problems asked, you will not have a problem doing well in the course. You will be given a total of 5 assignments. You will have about one week to complete each assignment. You are encouraged to speak to each other and work together on assignments, but each person has to submit their own assignments. If you do not understand anything in the assignment, you can discuss with me. Late assignments will be penalized at the rate of 20% per day.
2. Mid Semester 1 : (15 points): In-class 1 hour exam.
3. Mid Semester 2 : (15 points): This will be a week long take-home exam. You have to attempt this on your own, without help from anyone else.
4. Final Exam : (45 points): In class 3 hour exam.

Letter Grades: Letter grades will be awarded based on the total points out of 100. The grades will be given based on average(A) and standard deviations(σ) from average. Passing points will not be less than $A - 2\sigma$.

Warnings: Any misdemeanours in the Exams or HW assignments will result in the student obtaining zero for the exam. A second misdemeanour will result in an F grade for the course.