CHEM 240 – Fall 2007

Mathematical Methods for Chemistry

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www: http://leroy.uwaterloo.ca

Textbook: The on-line course notes (which will be filled in during class) summarize the material you will be responsible for.

Lectures: Monday, Wednesday & Friday 12:30 – 1:20 PM in Phys-313

Tutorial: Wednesday 4:30 – 5:20 PM in Phys-313

Course www page: http://scienide.uwaterloo.ca/~leroy/c240/

Course Outline

Complex Numbers and Functions

– complex numbers and arithmetic, and functions of complex numbers

Topics from Calculus

– the derivative, applications of the chain rule, implicit functions, Leibnitz rule
– partial differentiation, total differentials, exact & inexact differentials
– integrals and integration

Differential Equations

– definitions, and some simple methods of solution
– boundary conditions and "eigenvalues"
– solution by series
– partial differential equations and separation of variables

Vectors, Vector Spaces and Vector Algebra

– geometric vectors, and vector arithmetic
– generalized vector spaces, and inner product vector spaces
– functions as vectors and orthogonality

Operators and Matrices

– matrix arithmetic
– determinants
– applications: solving sets of linear equations
– matrix eigenvalue problems

Some Elements of Group Theory

Grades will be based on a Final Exam (weight $\gtrsim 60\%$), two Term Tests (weight $\gtrsim 10\%$ each), and Problem Sets (weight $\lesssim 20\%$). The precise mix will only be determined at the end of the terms after the final exams are marked.

Tests will be held in the tutorial period timeslot on Wednesday October 17 and Wednesday November 21.

The Tutorial period will be mainly used to answer questions and work through sample problems (except on the days Tests are held!). Tutorials will begin on Wednesday September 12.

Lecture Notes

The lectures will be based around the skeleton notes found on the "Course Notes" link from the course www page. It is *highly* recommended that you print a single-sided (to allow yourself room for extra writing) copy of these outline notes and bring them to class. These notes will be posted as the term progresses.

Supplementary References

Mathematics for Chemistry and Physics, by G. Turrell [UW library call # QA37.3.T87 (2002)], provides a readable presentation of many of the topics covered in this course.

The Handbook of Chemistry and Physics is available both in paper format on Reserve in the Davis Centre Library (call No. QD65.H3), and electronically (http://www.hbcpnetbase.com) from any UWaterloo IP address. In addition to extensive tables of physical and chemical properties of matter, it an extensive section of "Mathematical Tables" which includes tables of derivatives and integrals of various functions, properties of series, and the properties of a number of the special functions (some of which we will discuss) which are encountered in quantum mechanics.

Handbook of Mathematical Functions, by M. Abramowitz and I.A. Stegun, is available both in paper format in the Reference section of the UW Davis Centre Library (call No. QA47.A34 1972), and electronically (http://www.knovel.com/knovel2/Toc.jsp?BookID=528) from any UWaterloo IP address. It contains extensive summaries of the properties of and tabulations of many of the special mathematical functions encountered in physics and chemistry.

Tables of Integrals, Series and Products, by I.S. Gradshteyn and I.M. Ryzhik, is available in paper format in the Reference section of the Davis Centre library (call No. QA55.R943 1994). It contains the most comprehensive tables of integrals I am aware of. We do not need this level of material for Chem-240, but you should be aware that such a collection exists.