PH3082 - Mathematics for Chemistry / Physics

Credits: 20.0  Semester: 1
Number of Lectures: 28  Lecturer: Dr Charles Baily, Dr Michael Mazilu & Dr Aly Gillies
Academic Year: 2018-19

Overview
This module is only for those on the joint degree with chemistry and takes the form of PH3081 and about half of PH3080. Students take the same teaching and assessments as those in PH3081, as well as the same teaching and assessment from the first half of the computational physics module PH3080. The PH3081 module aims to develop mathematical techniques that are required by a professional physicist or astronomer. There is a particular emphasis on vector calculus, and on special functions that arise as solutions to partial differential equations that appear frequently in physics. Topics to be covered include: Fourier transforms, the Dirac delta function, the separation of variables method for solving partial differential equations, series solutions for second order ODEs, Hermite polynomials, Legendre polynomials and spherical harmonics. The vector calculus section covers definitions of the grad, div, curl and Laplacian operators, their application to physics, and their expressions in curvilinear coordinate systems. In the PH3080 section of the module students are introduced to the Mathematica package, and shown how this can be used to set up mathematical models of physical systems.

Aims & Objectives
- A better working knowledge and understanding of the mathematics used in other honours physics and astronomy modules.
- An improved ability to formulate problems relating to physical phenomena in mathematical language, starting from intuitive ideas.
- An ability to apply a range of mathematical techniques to the solution of such problems.
- An ability to discriminate between alternative methods of solution as to which is the most suitable for the task at hand.
- A significant enhancement of your problem solving ability as a practising physicist/astronomer.
- To develop a level of expertise in Mathematica and to introduce various common techniques used to solve and visualise physical problems; this includes both 2-D and 3-D graphical output and movies for visualising physics problems.
- Use of Fourier transforms.
- Solutions of first and second order differential equations.
- Introduction to symbolic programming.
- To introduce various numerical methods.

Learning Outcomes
You will have acquired the ability to program in Mathematica and be able to use Mathematica to solve, visualise and gain insight into a variety of physical problems. You will be aware of the advanced capabilities of Mathematica including symbolical and numerical equation solving.

By the end of the semester, Maths for Physicists students are expected to be able to:
- determine the components of a vector (or vector field) in Cartesian, cylindrical and spherical coordinates, write the fields in terms of appropriate unit vectors, and be able to translate an expression given in one coordinate system into either of the other two.
- state the definition of the Dirac delta function; and apply that definition to derive basic identities and compute integrals.
- represent functions as a discrete sum of orthonormal basis functions (e.g., sines/cosines, Hermite polynomials, Legendre polynomials, spherical harmonics, etc.), and apply the appropriate orthonormality relation to determine the series coefficients.
- compute the Fourier transform (or inverse transform) of simple functions, exploit basic relationships between transform pairs and use the convolution theorem to solve ordinary differential equations and compute integrals.
• solve second-order differential equations with non-constant coefficients using the method of Frobenius (power series solutions); this includes deriving recurrence relations, and determining closed-form expressions for the coefficients.

• sketch the first few Hermite polynomials, and derive explicit expressions when given a recurrence relation or a generating formula. Students should also be explain the relationship between the degree of a Hermite polynomial and its symmetry.

• state fundamental properties of solutions to Laplace’s equation in a bounded region of space (e.g., uniqueness of the solution, existence of local maxima or minima, etc.).

• describe the separation of variables technique, and use it to derive general solutions to second-order partial differential equations in Cartesian and spherical coordinate systems; then apply a given set of boundary conditions to determine a specific solution.

• compute line, surface and volume integrals in Cartesian, cylindrical and spherical coordinates.

• calculate the gradient or Laplacian of a scalar function, and the divergence or curl of a vector field, in Cartesian, cylindrical and spherical coordinates. Students should also be able to derive physical meaning from the resulting mathematical expressions, create and interpret visual representations of scalar and vector fields, and draw connections between them.

• apply Stokes’ theorem and the divergence theorem to convert between differential and integral equations, as well as interpret physical meaning from the resulting expressions.

• set up definite integrals of vector functions using Cartesian, cylindrical or spherical coordinates (as appropriate), and compute them for simple cases; this includes deriving expressions where all integration variables and limits are explicit (i.e., so that the integral could then be calculated by a computer).

Synopsis
For the part of the module overlapping with PH3081:-
Differential Equations
Dirac delta function
Fourier transforms
Series solutions, Hermite polynomials
Laplace’s equation in Cartesian and spherical coordinates
Legendre polynomials, spherical harmonics

Vector Calculus
Gradient, directional derivatives
Line and surface integrals
Divergence, divergence theorem
Curl, Stokes’ theorem
Helmholtz theorem, the Maxwell equations
Vector integration techniques

For the part of the module overlapping with PH3080:-
There are introductory programming labs teaching basic programming skills in Mathematica, different numerical methods and setting up physical problems. There are 5 case study labs and 3 assessed homework tasks. These are designed to provide case studies illustrating the use of Mathematica to solve and visualise a variety of Physics problems as well as introducing a number of advanced features in Mathematica. The case studies can vary from year to year but past case studies have included: Solving differential equations, Fourier transforms for filtering, chaotic motion, Mechanics and motion of coupled bodies moving in a potential, Analysis of periodic structures and Matrix and Tensor manipulation.

Indicative timetable: S1 weeks 1-2: introduction, S1 weeks 3-8: case studies, S1 week 9: class test

Pre-requisites
PH2012, MT2501 and MT2503, entry to MSci Chemistry and Physics degree programme.

Anti-requisites
PH3080, PH3081 or MT3506

**Assessment**
2-hour written examination = 60%, coursework = 40%

**Additional information on continuous assessment etc.**

Please note that the definitive comments on continuous assessment will be communicated within the module. This section is intended to give an indication of the likely breakdown and timing of the continuous assessment.

This module is formed from all of PH3081 Maths for Physicists and part of PH3080 Computational Physics. Two thirds of the module credit comes from the PH3081 part, and one third from the activities that are shared with PH3080. These two component parts are in the core JH programme, and as such there is a summary of deadlines etc. on the School’s Students and Staff web pages. Please see those module synopses for more details.

**Accreditation Matters**
This module contains material that is or may be part of the IOP “Core of Physics”. This includes
Three dimensional trigonometry
Vectors to the level of div, grad, and curl, divergence theorem and Stokes’ theorem
Fourier series and transforms including the convolution theorem

**Recommended Books**
Please view University online record:
http://resourcelists.st-andrews.ac.uk/modules/ph3082.html

**General Information**
Please also read the general information in the School’s honours handbook.