**B29QS Quantum Theory and Spectroscopy**

### COURSE DETAILS

**Course Code:** B29QS  
**Full Course Title:** Quantum Theory and Spectroscopy  
**SCQF Level:** 9  
**SCAF Credits:** 15  
**Available as Elective:** No

### DELIVERY LEVEL

<table>
<thead>
<tr>
<th>Undergraduate:</th>
<th>Yes</th>
<th>Postgraduate Taught:</th>
<th>No</th>
<th>Postgraduate Research:</th>
<th>No</th>
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### COURSE AIMS

This module aims to provide a fundamental course in the basic physics, concepts and techniques of quantum mechanics and spectroscopy.

### LEARNING OUTCOMES – SUBJECT MASTERY

- Appreciation of wave properties of particles and particle properties of waves.  
- Application of the Schrödinger equation to free and confined particles  
- Calculation of expectation values for observables  
- Appreciation of the Double slit experiment and interpretation of quantum mechanics.  
- Quantitative understanding of tunnelling and barrier penetration.  
- Familiarity with the harmonic oscillator  
- Basic knowledge of angular momentum in quantum mechanics.  
- Ability to reproduce elementary treatment of the Hydrogen atom.  
- To understand the concept of state vectors and to be able to relate this to qubits.  
- Ability to extract structural information from atomic and molecular spectra  
- Understanding why different types of spectra appear as they do  
- Simple understanding of atomic bonding  
- Appreciation of spectroscopy as a diagnostic tool  
- Appreciation of the timescales of molecular motion  
- Understanding of spectroscopic notation

### LEARNING OUTCOMES – PERSONAL ABILITIES

Personal abilities are embedded in the module. The module provides the opportunity to:

- Apply the advanced core knowledge expected of a professional physicist to gain professional level insights,  
- Communicate effectively with professional level colleagues  
- Interpret, use and evaluate critically a wide range of data to solve problems of both a familiar and unfamiliar nature  
- Manage time effectively, work to deadlines and prioritise workloads  
- Use a range of ICT skills with on-line materials and web links to support the learning process  
- Apply strategies for appropriate selection of relevant information from a wide source and large body of knowledge
B29QS Quantum Theory and Spectroscopy

SYLLABUS

Exercise significant initiative and independence in carrying out learning activities and researching information

SYLLABUS

Introduction to Quantum Theory:

• Comparison of classical theory (Rayleigh Jeans) and quantum theory (Planck)
• Photoelectric effect
• Bohr theory of the atom
• De Broglie principle and wave-particle duality
• Production and properties of x-rays
• Line spectra of atoms
• Compton scattering
• Electron diffraction

Quantum Theory:

• Wave vs. particle properties
• Schrödinger equation
• Free and confined particles
• Expectation values and observables
• Double slit experiment and interpretation of quantum mechanics
• Tunnelling
• The harmonic oscillator
• The rigid rotor and angular momentum
• The hydrogen atom.
• Entanglement
• The formalism of quantum mechanics: state vectors, Hilbert space and the density matrix.
• Quantum information processing: the two-level system and the qubit.

Spectroscopy:

• Common spectroscopic units of energy & notation
• Multi-electron atoms
• Angular momentum coupling
• Selection rules
• Atomic spectroscopy
• Timescales of atomic and molecular motion
• Rotational & vibrational spectroscopy of molecules
• Linear combinations of atomic orbitals & chemical bonding
• Introduction to molecular electronic spectroscopy
• Factors influencing spectral lines shapes & intensities
B29QS Quantum Theory and Spectroscopy

COURSE RELATIONSHIPS

N/A

<table>
<thead>
<tr>
<th>LOCATION AND ASSESSMENT METHODS</th>
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