**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**

| Undergraduate: | Yes | Postgraduate Taught: | No | Postgraduate Research: | No |

**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
• 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 theory and spectroscopy:

- 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

COURSE RELATIONSHIPS

N/A

LOCATION AND ASSESSMENT METHODS

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