The Exeter College Summer Programme
at Exeter College in the University of Oxford

Introduction to Quantum Mechanics

Course Description

Quantum mechanics is fundamental to many areas of chemistry, in particular our understanding of bonding and spectroscopy. This course provides an introduction to quantum theory from a chemist's perspective, focussing on the basics and spectroscopy of atoms; bonding is not discussed. An emphasis is placed on developing a clear understanding of quantum mechanical concepts such as the wavefunction and its connection to classical mechanics, as well as providing students with an understanding of essential concepts such as uncertainty and the Hamiltonian.

Prerequisites

Students should be confident in algebra and trigonometry and calculus involving basic differentiation. A general physical chemistry background is desirable, ideally in the form of an introductory physical chemistry course or thermodynamics.

Teaching Methods and Assessment

- 12 x 1.25hr Lectures (15hrs)
- 6 x 1.25hr Seminar Problem Classes (7.5hrs)
- 4 x 1.25hrs Tutorials (5hrs)

Performance Evaluation

Final examination: 60%
Problem sheets and Research project: 30%
Participation and attendance: 10%

Core Reading

The recommended texts for the course are:

P. Atkins and J. de Paula, *Physical Chemistry*, 2010, Oxford University Press. Chapter information below based on the 9th edition

P.A. Cox, *Introduction to Quantum Theory and Atomic Structure*, 1996, Oxford Chemistry Primers, Oxford Universityress

D.O. Hayward, Quantum Mechanics for Chemists, Royal Society of Chemistry, 2002

Lecture Schedule

1. **From waves to Photons**
    a. Waves in general
    b. Electromagnetic waves
    c. The photoelectric effect
    Reading: Cox – Ch1

2. **Wave-particle duality**
    a. Classical mechanics of a particle
    b. Low energy electron diffraction
    c. Young's slit
    Reading: Cox Ch2, Hayward Ch1

3. **Breakdown of classical physics**
    a. Black body radiation
    b. Heat capacities
    c. Atomic spectra
    Reading: Atkins Ch7

4. **Particle in a 1D box**
    a. Matter waves
    b. Boundary conditions
    c. Examples: quantum wells and p-electrons
    Reading: Hayward Ch1.4, Ch2

5. **The Schrödinger equation and wavefunctions**
    a. Time-dependent and time-independent Schrödinger equation
    b. The Hamiltonian operator
    c. Interpretation of the wavefunction
    Reading: Atkins Ch7.3-7.5

6. **The postulates of Quantum mechanics**
    a. The wavefunction postulate
    b. The form of the Hamiltonian
    c. The Schrödinger equation
    d. Expectation values
    e. Uncertainty principle
    Reading: Atkins Ch8

7. **Uncertainty arising from the wave nature of matter**

a. Diffraction of particles
b. Uncertainty for a particle in a box
c. The Heisenberg uncertainty principle
Reading: Hayward Ch3

8. Vibrational motion

a. The simple harmonic oscillator
b. The correspondence principle
c. Vibrational spectroscopy Reading:
Atkins Ch8.4-8.5, Cox Ch3.2

9. Rotational motion

a. The rigid rotor
b. Angular momentum
c. Rotational spectroscopy
Reading: Atkins Ch8.6-8.7, Cox Ch3.4

10. 1-electron atoms

a. The structure of 1-electron atoms
b. Quantum numbers
c. Radial distribution functions
Reading: Atkins Ch9.1-9.3

11. Multi-electron atoms

a. Orbital approximation
b. Penetration and shielding
c. Pauli principle
d. Spin-orbit coupling
Reading: Atkins Ch9.4-9.10

12. Quantum mechanical tunnelling

a. Basic concepts
b. Reflection and transmission probabilities
c. Barrier tunnelling
Reading: Atkins Ch8.3, Cox Ch3.1