3rd year Quantum Chemistry, NUIG: 2008-09, A.G. Ryder

8 CORE TOPICS (*ALL INTERLINKED*):

1. Failure of Classical Mechanics (~½L).
2. Schrödinger Wave Equation (~½L).
3. 1D Translational Motion (~½L).
4. Tunnelling (~½L).
5. 2D Translational Motion (~½L).
6. 3D Translational Motion (~½L).
7. Rotating Systems (~½L).
8. Vibrational motion (~½L).

Each topic builds on the preceding section, eventual goal to show how QChem is the fundamental basis for spectroscopy.

QUANTUM CHEMISTRY TEXTS:

- Atkins' *"Elements of Physical Chemistry"* 4th ed.: Chapter 12.
- Atkins' *"Physical Chemistry"* 8th ed.: Chapters 8 and 9 (up to Sec. 9.6 only).
- Introduction to Quantum Theory & Atomic Structure. P.A. Cox, Oxford Chemistry Primer. Chapters 1-3.
- Molecular Quantum Mechanics, Atkins & Friedman, 3rd edition. Introduction, Chapters 1-3.

QCHEM WEBSITES:

- www.quantum-chemistry-history.com/
- quantum.bu.edu/index.html
- vergil.chemistry.gatech.edu/notes/index.html
  - David Sherrill's website (Georgia Institute of technology):
  - Very detailed coverage of Quantum Chem.
  - vergil.chemistry.gatech.edu/notes/quantrev/quantrev.html
- www.quantum-physics.polytechnique.fr/index.html

DETAILED COURSE OUTLINE:	LEARNING OUTCOMES
1 Failure of Classical Mechanics: o Black Body Radiation & UV Catastrophe. o Heat Capacities. o Photoelectric Effect. o Spectroscopic evidence. o Diffraction of Electrons. o Wave-Particle Duality: De Broglie Relationship.	Understand and explain the evidence for quantum theory and the De Broglie Relationship.
1 Schrödinger Wave Equation: o Equation & Notation. o Wavefunctions & Probability. o Normalisation. o General properties of solutions. o Born Interpretation & Probability. o Uncertainty Principle.	Understand and be able to explain SWE, nature of wavefunctions, Born Interpretation, uncertainty principle.
1 Translational Motion: *1D simplest case* o Particle in a box. o Boundary Conditions. o Wavefunctions from de Broglie. o Zero Point Energy. o Energy Levels and Transitions. o Factors Influencing energies & wavefunctions.	Understand and be able to solve/use SWE for 1D case. Calculate and draw E-level diagrams / Wavefunctions.
1 Tunnelling: o Finite Potential wells. o Solutions. o Mass Effect. o Consequences of Tunnelling. o Radioactive Decay. o Scanning Tunnelling Microscopy.	Understand and explain the concepts involved and the practical consequences.
1 2D Translational Motion: *2D Box*. o Separation of Variables technique. o Solution to 2D SWE. o Energy level diagrams. o Degeneracy. o 2D Wavefunctions. o Simulation of 2D systems.	Generate and sketch E-level diagrams. Understand concept of degeneracy. Know how to use separation of variables technique to get SWE solution.
1 3D Translational Motion: *Quantum cubes*. o Separation of Variables technique. o Solution to 3D SWE. o Energy level diagrams. o Degeneracy & 3D Wavefunctions. o Quantum Dots.	Know how to use separation of variables technique to get SWE solution. Generate and sketch E-level diagrams. Explain Quantum Dots.
1 Rotational Motion: o Particle on a ring. o Angular Momentum & Moments of Inertia. o Boundary Conditions. o Rotational Energies. o SWE solution.	Know how to use separation of variables technique to get SWE solution. Generate and sketch E-level diagrams.
1 Vibrational Motion: *spectroscopy*. o Harmonic Oscillators. o Boundary Conditions. o Energy level diagrams / Zero-point energy. o Wavefunctions. o Probabilities.	Know how to draw and calculate energy level diagrams.