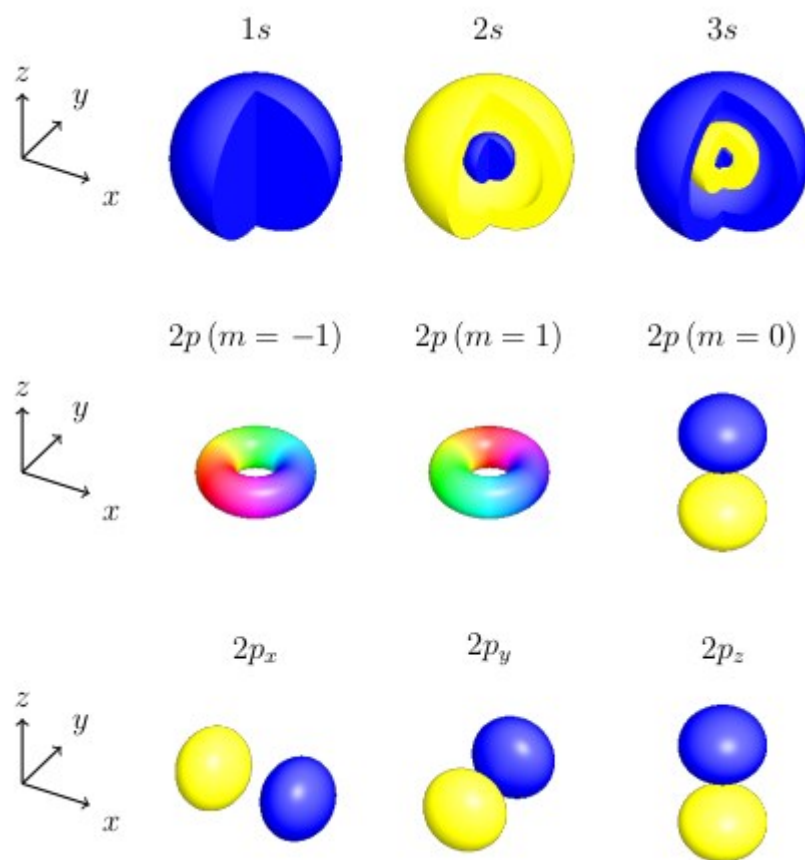




University
of Glasgow

School of Physics
& Astronomy



PHYS4002 Atomic Systems

1. Course Details

PHYS4002 Atomic Systems is a level 4 Physics Honours core course. It is a compulsory course for all students taking any of the Physics 4 degree options. It is composed of 18 lectures given in Semester 2.

Lecturer: Dr Dave Sutherland
Room 536, Kelvin Building
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Times: Normally Mondays and Wednesdays 10:00-11:00 am

Recommended text:

B.H. Bransden and C.J. Joachain, *Quantum Mechanics* (2nd edition),
Pearson Education Ltd., 2000.

More advanced:

B.H. Bransden and C.J. Joachain, *Physics of Atoms and Molecules* (2nd edition),
Prentice Hall.

Course notes and question sheets will be made available on Moodle.

2. Assessment

The course will be assessed via an examination in the April/May diet. It provides 10 Hlevel credits.

3. Required Knowledge

Students are expected to have completed the Level 3 course PHYS4025 Quantum Mechanics. They should be familiar with the concept of observables as operators and the role of commutators in Quantum Mechanics. They should be able to apply the Schrödinger Equation to a potential and calculate the energy levels and the wavefunctions of the system. They should be familiar with the quantum mechanical Simple Harmonic Oscillator (QHO) and the concept of angular momentum in Quantum Mechanics. We will assume a familiarity with mathematical concepts such as vector spaces and solving multivariate differential equations by separation of variables. This course will have some overlap with PHYS4026 Quantum Theory and PHYS4012 Mathematical Methods 2.

4. Intended Learning Outcomes

By the end of the course, students will be able to demonstrate a knowledge and broad understanding of quantum mechanics applied to atoms. They should be able to solve the Schrödinger equation and calculate the radial and angular parts of the hydrogen atom's wavefunctions. They should be able to apply perturbation theory to time-independent (Schrödinger) systems and derive the corrections to the energy levels of perturbed systems. They should be able to apply perturbation theory to determine the relativistic and magnetic properties of the hydrogen atom, including the effect of a magnetic field on the orbital and spin states and spin-orbit coupling in single electron systems. They should be able to calculate the Zeeman effect and the Landé g-factor. They should be able to calculate the effects of an electric field on the energy levels of the hydrogen atom (the Stark effect). They should be able to apply the addition of angular momenta to two electron systems and understand the ortho- and para- forms of the hydrogen molecule. They should be able to discuss the rotational spectra of molecules. They should be able to apply the Simple Harmonic Oscillator to determine the vibrational spectrum of diatomic molecules. They should be able to understand the properties of the periodic table of elements, the order of filling of electron orbits and its connection to atomic properties and energies. They should be able to relate electron-hole transitions to X-ray energies and to the empirical observations of Mosley. They should be able to describe optical spectra in 1-electron atoms and qualitatively determine shell energies in the cases of LS and jj coupling for multi-electron atoms.

5. Course Outline

5.0. Revision of Quantum Mechanics

We will review concepts in Quantum Mechanics: the wavefunction, Hermitian operators and orthonormality, eigenvalues and eigenfunctions, expectation values, commutators and compatible variables, the time-dependent and time-independent Schrödinger Equation.

5.1. Hydrogen atom

We will construct the time-independent Schrödinger Equation (TISE) for the Hydrogen atom, reducing the two-body (electron and nucleus) TISE into a one-body TISE in terms of the reduced mass and the $1/r$ electrostatic potential. We define the Rydberg energy and Bohr radius.

5.2. Solving the Hydrogen atom

We will solve the time-independent Schrödinger Equation for the $1/r$ potential using separation of variables, identifying the angular part of the solutions as spherical harmonics. We will identify the radial part as associated Laguerre polynomials. We will describe why boundary conditions imply that the associated quantum numbers (corresponding to angular momentum and energy) are quantised, applying this to the hydrogen atom to derive its energy levels and bound state wavefunctions, and discussing the properties of the solutions in contrast with classical expectations.

5.3. Angular momentum and spin

We will review the properties of orbital and spin angular momentum in the Hydrogen atom, including its quantum numbers, allowed values, the corresponding magnetic moments. We will describe an algorithm to construct eigenstates of a sum of two angular momenta, as relevant to the sum of orbital and spin angular momentum in the

Hydrogen atom.

5.4. Perturbation theory applied to the hydrogen atom

We will describe the basic formulation of time-independent perturbation theory, as well as the subtleties in its application in the degenerate case.

5.5. Internal perturbations

We will understand the origins of, and use perturbation theory to calculate the energy shifts resulting from, the three fine structure corrections to the Hydrogen atom: the relativistic correction, the spin-orbit coupling, and the Darwin term. We will describe more refined effects in the spectrum of hydrogen (hyperfine interactions and Lamb shift).

5.6. External perturbations

We will apply degenerate perturbation theory to the Stark effect, calculating energy shifts in Hydrogen orbitals under an applied electric field. We will discuss the strong field and weak field limits, the Landé g-factors and a calculation of the Zeeman effect for light atoms in weak and strong field limits.

5.7. The Elements

We will apply the concepts learned to understand the periodic table of elements and its relation to physical and chemical properties. We will illustrate the effects of electron screening and the order of filling of electron orbits. We will discuss the connection between the periodic table and atomic structure, ionisation energies, electron affinities.

5.8. Optical spectroscopy

We will describe optical spectra in series of 1-electron atoms and alkali atoms. We will describe multiple electron systems and the LS and jj coupling regimes. We will describe some basic features of atomic spectra (in light atoms) and selection rules.

5.9. X ray spectroscopy

We will discuss inner shell electron orbits in heavier atoms (ordering and energies). We will introduce the concept of electron-hole transitions and X-ray nomenclature. We will identify the allowed transitions and their characteristic spectra, discuss modifications of atomic energy levels due to electron screening and hence estimate X-ray energies. We will relate X-ray energies to the empirical observations of Moseley and their importance in determining atomic number.

5.10. Diatomic molecules

We will rederive the known eigenvalues of the Quantum Harmonic Oscillator (QHO) using ladder operators, and apply them to the vibrational spectrum of diatomic molecules. We will consider modifications to the QHO potential and illustrate the discussion with examples of rotational-vibrational spectra. We will discuss the two ortho- and para- forms of the hydrogen molecule and the determination of nuclear spin via Raman scattering. We will discuss the rotational spectra of molecules.