# Quantum physics of atoms and molecules

## Prof. Luigi Sangaletti

***COURSE AIMS AND INTENDED LEARNING OUTCOMES***

The quantum treatment of a few significant aspects of the structure of matter, with particular reference to:

- atomic physics.

- physics of many-atom physical systems, along a gradual path that starts from the simplest molecules and ends up with crystalline solids.

- radiation-matter interaction as the basis of experimental investigation into the physical systems covered by the course.

Intended learning outcomes.

At the end of the course, students will be able to:

- discuss the electronic properties of atoms, with reference to the Hamiltonian context in the presence of static electric and magnetic fields or electromagnetic fields;

- discuss the mechanisms underlying the magnetic properties of solids, from paramagnetism to ferromagnetism, both in classical and quantum terms;

- discuss the main aspects of matter-radiation interactions with both classical and quantum models;

- present the transition from the electronic properties of atoms to those of molecules, referring to the LCAO approach;

- calculate the electronic states of simple homopolar and heteropolar, linear and cyclic diatomic molecules;

- recognise the energy scales characteristic of electronic, vibrational and rotational excitations of molecules and their combinations, by referring to the Born–Oppenheimer approximation.

***COURSE CONTENT***

0- Matter-radiation interaction. Causality and dispersion relation. Kramers-Kronig transforms. Sum rules.

1- Complements of atomic physics.

Many-electron systems. Exchange interaction.

Central potential. Thomas-Fermi method. Hartree and Hartree-Fock methods.

Introduction to multiplet theory.

2- Atoms in a magnetic field: quantum treatment.

Quantum theory of the Zeeman and Paschen-Bach effects.

3- Atoms in an electric field.

Quantum theory of the linear and quadratic Stark effects. Crystal-field effects.

4- Nuclear spin and hyperfine structure.

Overview of nuclear spin and hyperfine structure.

Hyperfine structure in an external magnetic field.

5- Rudiments of magnetism.

Paramagnetism and the Brillouin function. Elementary theory of ferromagnetism.

7- Molecular physics. Born-Oppenheimer approximation.

8- Molecular hydrogen ion. Variational approach to the ground state calculation. The hydrogen molecule. LCAO method and Heitler-London method. Calculation of energy of the levels (sigma) as the distance between nuclei varies. Coulomb integral and exchange integral expressions.

9- Two-level systems. Exact solution of the eigenvalue problem and perturbation solution. Homopolar and heteropolar molecules. Ground state stabilization. Hückel approximation. Linear and cyclic molecules. Energy level filling in diatomic molecules. Heteronuclear diatomic molecules: ionic bond and semi-empirical potentials.

10 - Quantum mechanical two-body problem. Motion in a diatomic molecule. Vibrational and rotational energy levels.

Centrifugal distortion correction to rotational energy levels. Anharmonic effects.

Morse potential. Selection rules for rotational transitions. Selection rules for vibrational transitions. Franck-Condon principle. Vibronic transitions. Roto-vibrational spectra of diatomic molecules. Decay of excited states. Radiative and non-radiative de-excitation. Fluorescence and phosphorescence. Dissociation. Effects of temperature on the population of vibrational and rotational states. Vibrational modes and potential curves.

11- From molecules to solids. Introduction to electronic band structure.

Electronic levels of n-atom linear and cyclic molecules.

Calculation of energy eigenvalues with the Hückel method.

Statement of Bloch's theorem. Born-von Karman boundary conditions. Energy dispersion curves E=E(k). Density of states.

Trend of E=E(k) curves for s, p and d orbitals. Electronic band structure of a general two-dimensional system.

***READING LIST***

- B.H. Bransden - C. J. Joachain, *Physics of Atoms and Molecules,* Prentice-Hall, London (2003).

- Peter W. Atkins - Ronald S. Friedman, *Meccanica quantistica molecolare,* Zanichelli, Bologna.

- D. J. Griffiths, *Introduction to Quantum Mechanics,* Trad. Italiana, *Introduzione alla Meccanica quantistica*, Casa Editrice Ambrosiana, Milan (2005).

- Hermann Haken - Hans C. Wolf, *The Physics of Atoms and Quanta,* 7th edition, Springer Verlag, 2005.

- Franz Schawabl, *Meccanica quantistica,* Zanichelli, Bologna 1995.

***TEACHING METHOD***

Lectures. Focus seminars.

***ASSESSMENT METHOD AND CRITERIA***

Oral examination aimed to assess the level of knowledge of the main topics of the course, the ability to present them and the student’s mastering of these concepts to discuss problems in the field of atomic and molecular physics.

***NOTES AND PREREQUISITES***

Further information can be found on the course folder available on Blackboard