


5.00 credits

30.0 h + 30.0 h

Q1

Teacher(s)	Charlier Jean-Christophe ;Gonze Xavier ;Piroux Luc ;Rignanese Gian-Marco ;
Language :	French
Place of the course	Louvain-la-Neuve
Main themes	<p>Quantum physics : non-relativistic quantum mechanics postulates ; measure theory ; hydrogen atom ; polyelectronic atoms ; harmonic oscillator ; spin ; variational principle (Ritz) ; formation of the chemical bonds.</p> <p>Statistical physics : basic notions, the kinetic theory of gases, the different statistical ensembles (microcanonical, canonical and grand-canonical), and quantum fluids (fermions and bosons)</p>
Learning outcomes	<p>At the end of this learning unit, the student is able to :</p> <p>Contribution of the course to the program objectives Axis N°1 :1.1</p> <p>Specific learning outcomes of the course At the end of their classes, the students are expected to be able:</p> <ol style="list-style-type: none"> 1. To explain the postulated and basic equations of the non-relativistic QM including the measure theory. 2. To apply MQ to the treatment of different simple systems. 3. To compute the mean values of simple observables for wavefunctions with one electron, their fluctuations, to check Heisenberg uncertainty relationship, and to build the matrix representation of an operator. 4. To build a molecular orbital diagram for a simple specific molecule, and to deduce from it the physical characteristics (bond order, total spin). 5. To explain the basic principles of statistical physics. 6. To compute the thermodynamical properties of a perfect gas, and to use Maxwell-Boltzmann statistics. 7. To work with the different statistical formalisms : microcanonical (e.g. study lattice specific heat - Einstein model), canonical (e.g. Debye model), and grand-canonical (e.g. to derive Fermi-Dirac and Bose-Einstein statistics) 8. To predict the temperature-dependent behaviour of systems (specific heat, internal energy, mean number of particules, superfluidity, superconductivity) thanks to statistical ensembles.
Evaluation methods	The students are evaluated individually, in a written examination, on the basis of the above-mentioned learning outcomes (questions will focus on their knowledge, their understanding, their ability to apply the concepts explained during the lecture, the latter being developed during the exercise sessions). The statistical and quantum parts have the same weight. Concerning quantum fluids, a tasting session is organized.
Teaching methods	Ex cathedra lectures and exercice sessions.
Content	<ol style="list-style-type: none"> 1 Quantum physics <ol style="list-style-type: none"> 1.1. Introduction/Reminders 1.2. Postulates 1.3. Operators 1.4. Measure theory (including Heisenberg uncertainty principle) 1.5. Hydrogen atom 1.6. Polyelectronic atoms 1.7. Matrix mechanics 1.8. Harmonic oscillator (creation and annihilation operators) 1.9. Spin 1.10. Variational principle 1.11. Tight-binding method (understanding of the electronic structure and cohesion of diatomic molecules) 2 Statistical Physics <ol style="list-style-type: none"> 2.1. Introduction: Elements of Statistical Physics 2.2. Kinetic Theory of Gases and , and billiard game theory 2.3. Microcanonical Ensemble 2.4. Canonical Ensemble 2.5. Grand-Canonical Ensemble 2.6. Quantum Fluids

Inline resources	Moodle UCL
Faculty or entity in charge	FYKI

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Minor in Applied Chemistry and Physics	MINOFYKI	5		
Specialization track in applied Chemistry and Physics	FILFYKI	5		