

4.0 credits	30.0 h + 22.5 h	1q
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Teacher(s) :	Rignanese Gian-Marco ; Charlier Jean-Christophe (coordinator) ; Gonze Xavier ; Piraux Luc ;
Language :	Français
Place of the course	Louvain-la-Neuve
Main themes :	The course is divided into 2 parts. In the first part, centred on quantum mechanics, one reviews basic notions, and completes the exposition of these. Then, one examines the harmonic oscillator (Dirac's method), some basics of molecular physics, and perturbation theory. In the second part, centred on statistical physics, one presents basic notions, the kinetic theory of gases, the different statistical ensembles, and quantum fluids.
Aims :	This module aims at completing the student formation in physics, in view of the understanding of the properties of molecules, solids and nanostructures. At the end of the module, the student will be able to use quantum mechanics to understand the cohesion of such systems, and their response to perturbations, as well as to use statistical physics to forecast their energetical behaviour as a function of temperature. <i>The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".</i>
Content :	<p>Content :</p> <p>Part 1 :</p> <p>1.1. Review of basic notions of quantum mechanics : postulates, simple systems, kinetic moment.</p> <p>1.2. Fundamental theorems and general properties. (Hermitian operators, normalisation of wave functions, basis of eigenfunctions associated with an hermitian operator, orthogonality of basis functions, classical approximation of the Schrödinger equation)</p> <p>1.3. Measure theory. (Statistical distribution of the results of the measure of an observable, ideal measure, compatible and uncompatible observables, Heisenberg uncertainty relations, application to the kinetic moment)</p> <p>1.4. Matrix mechanics and representation theory. (Linear combination of basis vectors, change of basis of functions, real space and momentum space, wavefunctions as vectors, operators as matrices, transformation laws, closing relation, projectors)</p> <p>1.5. Harmonic oscillator (Dirac's method : operators of creation and d'annihilation)</p> <p>1.6. Electronic structure of molecules (Variational principle, atom with many electrons, linear combination of atomic orbitals - tight binding - core/valence orbitals, binding and anti-binding orbitals, s and p orbitals, -charge transfer and non-binding orbitals, sp3 bonds, sp2+ p bonds, applications to diatomic molecules, water, ethane, ethene)</p> <p>1.7. Time-independent perturbation theory.</p> <p>-</p> <p>Part 2 :</p> <p>2.1. Introduction: elements of statistical physics. (Fundamentals, phase space and representative points, equiprobability principle, mean value of an observable, notion of ensemble)</p> <p>2.2. Kinetic theory of gases. (Definition of an ideal gas, speed distribution function, Maxwell-Boltzmann statistics, properties of an ideal gas - pressure, kinetic energy ...)</p> <p>2.3. Microcanonical ensemble (Formalism: entropic représentation, ex: Einstein model for the lattice specific heat, counting techniques and high dimensionality)</p> <p>2.4. Canonical ensemble (Formalism: Helmholtz représentation, notion of partition function, notion of density of states, ex: Debye model for the lattice specific heat)</p> <p>2.5. Grand-canonical ensemble (Indiscernability principe, grand-canonical formalism, ex: adsorption of molecules on a surface)</p> <p>2.6. Quantum fluids (Notion of fermions, bosons, ideal Fermi fluid, Fermi-Dirac statistics, electronic specific heat, ideal Bose fluid, Bose-Einstein statistics, notion of BE condensation, ex : superfluidity and supraconductivity)</p> <p>Methods : Ex-cathedra courses and exercises.</p>
Other infos :	Pre-requisite FSAB 1104 Probability and statistics.

<p>Cycle and year of study :</p>	<p>> Bachelor in Engineering > Master [120] in Biomedical Engineering</p>
<p>Faculty or entity in charge:</p>	<p>FYKI</p>