MAPR1491 Supplements in physics

[30h+22.5h exercises] 4 credits

This course is taught in the 1st semester

Teacher(s): Jean-Christophe Charlier (coord.), Xavier Gonze, Luc Piraux, Gian-Marco Rignanese
Language: French
Level: First cycle

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.

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.

Content and teaching methods

Content :
Part 1 :
1.1. Review of basic notions of quantum mechanics : postulates, simple systems, kinetic moment.
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)
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)
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)
1.5. Harmonic oscillator
(Dirac's method : operators of creation and d'annihilation)
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)
1.7. Time-independent perturbation theory.
-
Part 2 :
2.1. Introduction: elements of statistical physics.
(Fundamentals, phase space and representative points, equiprobability principle, mean value of an observable, notion of ensemble)
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 ...)
2.3. Microcanonical ensemble
(Formalism: entropic représentation, ex: Einstein model for the lattice specific heat, counting techniques and high dimensionality)
2.4. Canonical ensemble
(Formalism: Helmholtz représentation, notion of partition function, notion of density of states, ex: Debye model for the lattice specific heat)
2.5. Grand-canonical ensemble
(Indiscernability principe, grand-canonical formalism, ex: adsorption of molecules on a surface)
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)
Methods :
Ex-cathedra courses and exercises.

Other information (prerequisite, evaluation (assessment methods), course materials recommended readings, ...)

Pre-requisite
FSAB 1104 Probability and statistics.

Other credits in programs

FSA12BA	Deuxième année de bachelier en sciences de l'ingénieur, orientation ingénieur civil	(4 credits)
FSA13BA	Troisième année de bachelier en sciences de l'ingénieur, orientation ingénieur civil	(4 credits)