GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2016-2017

Statistical Physics and Molecular Structure (E021520)

Course size (nominal values; actual values may depend on programme)

Credits 6.0	Study time 180 h	Contact hrs	60.0 h

Course offerings and teaching methods in academic year 2016-2017

A (semester 2)	Dutch	seminar: coached	30.0 h
		lecture	30.0 h

Lecturers in academic year 2016-2017

Van Speybroeck, Veronique	TW17	lecturer-in-charge
Lejaeghere, Kurt	TW17	co-lecturer

Offered in the following programmes in 2016-2017	crdts	offering
Bachelor of Science in Chemical Engineering and Materials Science	6	A

Teaching languages

Dutch

Keywords

Thermodynamics, Statistical Physics, Quantum Mechanics, Molecular symmetry, Spectroscopy

Position of the course

This course first aims at introducing the basic concepts of equilibrium thermodynamics and statistical physics. In the second part the experimental basis of quantum mechanics is presented, emphasizing the limits of the classical physics and the introduction of the quantum mechanics. The quantum mechanical postulates are introduced and the Schrödinger equation is solved for basic potentials (including the 1-dimensional harmonic oscillator and the hydrogen atom). In this course, applications are restricted to atoms and molecules. Finally symmetry groups are treated as tools for an adequate description of molecular modeling and spectroscopy.

Contents

- The main laws (HW) of thermodynamics: statistical view: HW I, Macrostate and microstate, Isolated systems in equilibrium, Systems in a heat bath, HW II, HW III
- Ensemble theory: Phase space, The ensemble concept, Partition functions (microcanonical, canonical, grand canonical), Boltzmann definition of entropy
- Statistical description of paramagnetics: canonical and micro-canonical description
- Specific heat of solids: Einstein theory, Debye theory
- The classical ideal gas: Maxwell-Boltzmann velocity distribution, Classical ideal gas, State equations, Joule's law, entropy, separation of degrees of freedom, translational, rotational, vibrational partition function, heat capacity
- Classical and quantum mechanical definition partition function
- Ideal quantum gases: Grand canonical distribution, Fermi-Dirac and Bose-Einstein distributions, Applications: electron gas, nuclear matter
- Low-temperature physics: Experimental low-temperature methods, Helium at low temperatures, Superconductivity, Bose-Einstein condensation
- Limits of classical physics and origin of quantum theory, wave-particle duality, discretization of orbital momentum and energy
- Schrödinger equation: stationary wave equation
- Postulates of quantum mechanics
- 1-dimensional potential problems: infinite potential well, harmonic oscillator
- 3-dimensional central potential: orbital momentum, spherical harmonics
- Hydrogen atom: energy spectrum and wave functions
- Symmetry groups in molecules and spectroscopy: generalities, molecular movements, infrared spectroscopy

Initial competences

Physics I, Physics II

Final competences

1 Master and apply the basic concepts of statistical physics.
2 Understand the relation between the macroscopic and microscopic description of matter.
3 Derive statistical quantities such as partition functions for simple and complex systems and apply them to determine macroscopically observable quantities.
4 Understand the various statistical distribution functions and apply them to systems with many degrees of freedom.
5 Understand the basic concepts of quantum mechanics (e.g. wave-particle duality, Schrödinger equation, orbital momentum, spherical harmonics).
6 Solve the Schrödinger equation for basic potential problems (1D or central).
7 Understand the need for a quantum mechanical description of phenomena at the atomic and molecular scale.
8 Master the quantum mechanical description of the hydrogen atom.
9 Understand the importance of symmetry for spectroscopy.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Lecture, seminar: coached exercises

Learning materials and price

Course notes

References

- Baierlein R., Thermal Physics, Cambridge University Press 1999 - ISBN 0-521-59082-5
- Kittel C., Kroemer H., Thermal Physics, W.H. Freeman 1980 - ISBN 0-7167-1088-9
- Mandl F., Statistical Physics, The Manchester Physics Series, 2nd edition, Wiley 1988 - ISBN 0-471-91533-5 (paperback)
- Veszprémi T., Fehér M., Quantum Chemistry - Fundamentals to Applications, Kluwer Academic/Plenum Publishing, 1999
- B. H. Bransden and G. J. Joachain, Introduction to Quantum Mechanics, Longman 1989

Course content-related study coaching

Lecturer and assistants are available before and after lectures or by appointment

Evaluation methods

end-of-term evaluation

Examination methods in case of periodic evaluation during the first examination period

Written examination, oral examination

Examination methods in case of periodic evaluation during the second examination period

Written examination, oral examination

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

Oral exam with a written preparation for the theory.
written closed-book exam for the exercises

Calculation of the examination mark