

Introduction to Atomic and Molecular Physics (C000919)

Course size (nominal values; actual values may depend on programme)
Credits 6.0 Study time 180 h Contact hrs 52.5 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	Dutch	seminar: coached	20.0 h
		exercises	
		demonstration	2.5 h
		lecture	30.0 h

Lecturers in academic year 2018-2019

Smet, Philippe	WE04	lecturer-in-charge
Vrielinck, Henk	WE04	co-lecturer

Offered in the following programmes in 2018-2019

	crdts	offering
Bachelor of Science in Physics and Astronomy	6	A
Preparatory Course Master of Science in Physics and Astronomy	6	A

Teaching languages

Dutch

Keywords

Quantum modeling of atomic structure, group theory applied to molecules

Position of the course

The aim of this course is (i) to construct the quantum-mechanical formalism required for the theoretical interpretation of atomic spectra and (ii) to apply group theory to molecular systems to obtain a basic insight in the relation between the symmetry of molecules and molecular spectra.

Contents

- Coupling of angular momenta (Clebsch-Gordon coefficients).
- Approximation techniques: time-independent perturbation theory (for degenerate and non-degenerate levels); variation theory (Rayleigh ratio, Rayleigh-Ritz method); Hellman-Feynman theorem; time dependent perturbation theory.
- Atomic structure and spectra of hydrogen: interpretation of the analytic solution to the non-relativistic, spin-free Hamiltonian; expectation value of the radial coordinate; perturbative treatment of spin-orbit coupling and relativistic effects (fine structure); influence of magnetic field, both weak (Zeeman effect), strong (Paschen-Back effect) and intermediate; magnetic and electric dipole transitions.
- Atomic structure and spectra of helium: Coulomb integral; exchange integral; excited states; Pauli principle; Slater determinant.
- Polyelectronic atoms and ions: shielding, perturbative treatment of Coulomb interaction and spin-orbit coupling in Russell-Saunders coupling and jj-coupling; micro states, term symbols, configuration labels; Hund's rules; diagonal-sum rule; influence of external magnetic fields (Zeeman effect) and electric fields (Stark effect).
- Introduction to group theory: symmetry operations and elements; symmetry classification of molecules; multiplication tables; matrix representations; characters and classes; irreducible representations; great and little orthogonality theorems; reduction of representations; symmetry-adapted bases; symmetry transformation of orbital functions; decomposition of a direct-product base; electronic transition probabilities, dipole moments, overlap integrals.
- Introduction to molecular physics.

Initial competences

Non-relativistic quantum physics - electromagnetism

Final competences

- 1 Knowing the physical core concepts and applying them at an appropriate level of abstraction.
- 2 Mastering firm basic knowledge of major domains in physics and astronomy (including quantum mechanics, wave and optics, electromagnetism), required for the study of atomic and molecular physics.
- 3 Possessing extended knowledge of mathematics, and being able to apply it when solving problems in physics.
- 4 Knowing standard techniques and models in atomic and molecular physics, and applying them within the relevant application areas.
- 5 Being able to critically analyse classic and modern scientific resources.
- 6 Being able to select, synthesize and process relevant data, in a structured way.
- 7 Using physical terminology in a correct way.

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

Demonstration, lecture, seminar: coached exercises

Learning materials and price

Syllabus (226 p) available for download via Minerva, or via student organization.
Solution of exercises via Minerva.

References

P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, fourth edition, price : £35.99 (Paperback) ISBN-10: 0-19-927498-3 ; ISBN-13: 978-0-19-927498-7
Publication date : 23 December 2004 ; 608 pages

Course content-related study coaching

Interactive support via Minerva (forums), e-mail or personal contact with teacher (after making an appointment).

Evaluation methods

end-of-term evaluation

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

Written examination with open questions, open book examination, oral examination

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

Written examination with open questions, open book 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

Open book exam ; theory : oral ; exercises : written

Calculation of the examination mark

5/20 points: theory

15/20 points: exercises (3 exercises)