



COURSE UNIT DESCRIPTION

Course unit title	Code
ATOM THEORY	

Annotation

Lecturer(s)	Department, Faculty
Coordinating: Prof. Habil. Dr. Gediminas Gaigalas Other:	Physics Faculty, Institute of Theoretical Physics and Astronomy, Saulėtekio al. 3.

Study cycle	Type of the course unit
Second	Elective

Mode of delivery	Semester or period when it is delivered	Language of instruction
Lectures, seminars	2 nd semester	Lithuanian/English

Requisites	
Prerequisites: Courses in atomic physics and quantum mechanics completed.	Co-requisites (if relevant):

Number of ECTS credits allocated	Student's workload (total)	Contact hours	Individual work
5	140	64	76

Purpose of the course unit: programme competences to be developed		
To enhance the knowledge of postgraduate students in quantum mechanics and atomic physics, to introduce the main methods and ideas of modern atomic theory, and to provide them with the theoretical knowledge and practical skills needed to understand and theoretically analyse the electronic structure of atoms.		
Learning outcomes of the course unit	Teaching and learning methods	Assessment methods
After completing this course, the student: will acquire knowledge of: atomic properties, methods of their study and calculation, atomic particle impacts, atomic spectra and the information they provide; atomic research carried out in Lithuania, as well as a broader understanding of microworld phenomena and methods of their study will be able to: understand the electronic structure of atoms and analyse the information it provides.	Lectures, consultations, self-study, task solving, investigation of atomic and molecular compounds using computer codes, supercomputer.	Final evaluation consists of individual task solving results, written presentation of particular method and investigation and answering the questions.

Course content: breakdown of the topics	Contact hours	Individual work: time and assignments

	Lectures	Tutorials	Seminars	Workshops	Laboratory work	Internship/work	Contact hours,	Individual work	Assignments
1. Main atomic features. Atoms, atomic ions, their measurements. Atomic units' system. Schrödinger equation and atomic wave function.	1							4	Literature analysis
2. Single electron model. Spherical model of atomic single electron wavefunction. Electron orbitals. Atomic electronic states.	2							4	Literature analysis
3. Many electron atomic states and their description. Two electron atomic wavefunction, it's quantum numbers. Many electron atomic wavefunctions. Electronic shell, it's quantum numbers. Configurations with several open shells.	2			1	1			4	Literature analysis
4. Atomic structure, radial parts of wavefunctions. Methods for calculating radial wave functions. Electron collapse and electron occupation in shells.	2			1	1			4	Literature analysis, task solving
5. Main interactions in atom, coupling types.	2			4	4			6	Literature analysis
6. Computation of radial wavefunctions.	2			4	4			6	Literature analysis, task solving, task solving with computer programs
7. Computation of atomic parameters.	3			4	4			10	Literature analysis
8. Relativistic and correlation effects in atoms. Relativistic effects. Dirac equation and existents of spine. Methods for accounting correlation effects.	4			2	2			10	Literature analysis
9. Energy spectra.	3							4	Literature analysis
10. Interaction of the atom with electromagnetic field. Photoabsorbption.	2							4	Literature analysis
11. Emission spectra.	2							4	Literature analysis
12. Autoionisation of the atom and the Auger effect. Fluorescence efficiency.	2							4	Literature analysis
13. An atom in an electric and magnetic field.	2							4	Literature analysis
14. Atomic collisions with particles.	2							4	Literature analysis
15. New directions in atomic physics.	1							4	Literature analysis
Total	32			16	16			76	

Assessment strategy	Weight %	Deadline	Assessment criteria
Task solving, laboratory of computational tasks.	20	The end of each month.	Individual tasks solved (2 points);
Written presentation of the question, answering the questions.	80	The end of the module Atom theory.	Written exam or written presentation of particular method and individual investigation, answering the questions (8 points).

Author	Publishing year	Title	Issue of a periodical or volume of a publication; pages	Publishing house or internet site
Required reading				
1. A. Bandzaitis, D.Grabauskas.	1975	Kvantinė mechanika.		V.: Mokslas

2. J. Chmeliov, V. Butkus, L. Valkūnas.	2020	Kvantinė fizika.		Vilniaus universiteto leidykla, 620 p.
3. W.R. Johnson.	2007	Atomic Structure Theory: Lecture on Atomic Physics		Springer, Berlin, Heidelberg
4. K. Glemža.	1998	Atomų teorijos pradmenys (Paskaitų studentams konspektai). Pirma dalis.		Mokomoji knyga, 77 psl.
5. K. Glemža.	2004	Atomų teorijos pradmenys (Paskaitų studentams konspektai). Antra dalis.		Mokomoji knyga, 61 psl.
Recommended reading				
1. P. Jönsson, M. Godefroid, G. Gaigalas et al.	2023	An Introduction to Relativistic Theory as Implemented in GRASP	11, 7	<i>Atoms</i> , Atoms Free Full-Text An Introduction to Relativistic Theory as Implemented in GRASP (mdpi.com)
2. P. Jönsson, G. Gaigalas, Ch. F. Fischer et al.	2023	GRASP Manual for Users	11, 68	<i>Atoms</i> , Atoms Free Full-Text GRASP Manual for Users (mdpi.com)