DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Faculty	Center/Institute/ Department
Analytical Calculations Using Computer Algebra Systems (8 ECTS credits)	Physics N 002	Faculty of Physics	Institute of Theoretical Physics and Astronomy
Student's workload	Hours	Student's workload	Hours
Lectures		Consultations	20
Individual study	160	Seminars	20

Course annotation
The course deals with application of computer algebra system (Mathematica) and its application to a number of selected problems in physics. When solving scientific problem one often needs tools for analytical derivations of formulas, numerical calculations, graphical representation, solution of differential equations, etc. All these tools are provided by computer algebra systems (CAS). A vast variety of available tools ensure that scientists can concentrate on solving scientific problems and allow fast result checking without resorting to different and often incompatible software. Unfortunately, self-study of very complicated contemporary CAS would require much time and efforts, and this essentially motivates the existence of this course. The proposed course consists of three parts. The first part of the course (the first month) is devoted to the basics of CAS Mathematica. It introduces base syntax, most often used commands and suggestions on help system usage. This part is concluded with an overview of main programming paradigms, i.e. procedural, object oriented and functional programming styles. The second part is intended to demonstrate how one or another selected physical problem can be fully formulated, solved and presented using CAS Mathematica. The doctorate student can select the problem according to his/her interest and experience. The suggested list includes: electric circuits (two ports, transient processes, transient oscillations in LC contours), charged particle motion in electric and magnetic fields (both homogeneous and inhomogeneous), cyclotron resonance, Fermi-Dirac distribution and its application to electron density in semiconductors, interference of waves, Fourier transform and Fourier spectroscopy, digital filters, percolation, introduction to Monte Carlo method, Brusselator, nonlinear pendulum,

solitons (Burgers and KdV equations), quantum oscillator, quantum 2L system, quantum wells quantum barriers. Usually acquaintance with one or two problems are enough to understand potential and usefulness of CAS in solving physical problems.

The third part deals with the particular problem students want to solve. The suggested practice is that students themselves or their supervisors provide the problem for partial or full solution using Mathematica. The supervised work of students on the problem in hand constitutes the major part of the assessment in the exam.

List of literature

1. Michael Trott, “The Mathematica guidebook for symbolic”, 2006 (1453psl)
2. Michael Trott, “The Mathematica guidebook for numeric”, 2006 (1208psl)
3. Michael Trott, “The Mathematica guidebook for graphics”, 2004 (1340psl)
4. Andrey Grozin, “Introduction for Mathematica for physicists ”, 2014 (219psl)
5. Roman Schmied, “Using Mathematica for quantum mechanics (the student’s manual)”, 2019 (202psl)

Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
Gediminas Gaigalas	habil. Dr.	Prof.	1. G. Gaigalas, C. Froese Fischer, P. Rynkun, P. Jönsson, JJ2LSJ Transformation and unique labeling for energy levels // Atoms. ISSN 2218-2004. 2017, Vol. 5, p. 1-11. https://doi.org/10.3390/atoms5010006 2. J. Ekman, P. Jönsson, M. Godefroid, C. Nazé, G. Gaigalas, J. Bieroń, RIS4: A program for relativistic isotope shift calculations theory // Computer physics communications. ISSN 0010-4655. 2019, Vol. 235, p. 433-446. https://doi.org/10.1016/j.cpc.2018.08.017 3. C. Froese Fischer, G. Gaigalas, P. Jönsson, J. Bieroń, GRASP2018 – A Fortran 95 version of the general relativistic atomic structure package theory // Computer physics communications. ISSN 0010-4655. 2019, Vol. 237, p. 184-187. https://doi.org/10.1016/j.cpc.2018.10.032 4. G. Gaigalas, Coupling: The program for searching optimal coupling scheme in atomic theory // Computer physics communications. ISSN 0010-4655. 2020, Vol. 247, 106960, p. 1-9. https://doi.org/10.1016/j.cpc.2019.106960
Arturas Acus	Dr.	assoc. Prof.	1. A. Acus, E. Norvaišas, Ya. Shnir. Interaction of hopfions of charge 1 and 2 from product ansatz. EPL (Europhysics Letters) 110 1, 2015, psl. 10007.

			2. S-W Su, S-C Gou, I-K Liu, I B Spielman, L Santos, A Acus, A Mekys, J Ruseckas, G Juzeliūnas. Position-dependent spin–orbit coupling for ultracold atoms. New Journal of Physics 17 3, 2015, psl. 033045. 3. A. Dargys, A. Acus,"Cliffordo geometrinė algebra ir jos taikymai", monografija, ISBN**:** 9786094204371, Vilnius, Petro ofsetas, 2015, 386psl. 4. A. Dargys, A. Acus, Calculation of Quantum Eigens with Geometrical Algebra Rotors, Adv. Appl. Clifford Algebras (2017) 27: 241. https://doi.org/10.1007/s00006-015-0549-6 5. A. Acus, A., Dargys, „The Inverse of a Multivector: Beyond the Threshol p+q=5",Adv. Appl. Clifford Algebras (2018) 28: 65. https://doi.org/10.1007/s00006-018-0885-4 6. A. Matulis, A. Acus „CLASSICAL ANALOG TO THE AIRY WAVE PACKET", Lithuanian Journal of Physics, Vol. 59, No 3, pp. 121-129 (2019)
Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32			
Committee Chairman prof. S. Juršėnas			