SYLLABUS

1. Information regarding the programme

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| 1.1 Higher education institution | **Babes-Bolyai University** |
| 1.2 Faculty | **Physics** |
| 1.3 Department | **Physics** |
| 1.4 Field of study | **Physics** |
| 1.5 Study cycle | **Master** |
| 1.6 Study programme / Qualification | **Computational physics** |

2. Information regarding the discipline

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|---|---|---|---|---|---|---|---|
| 2.1 Name of the discipline | **Numerical computations in atomic physics** | | | | | | |
| 2.2 Course coordinator | **Ladislau Nagy** | | | | | | |
| 2.3 Seminar coordinator | **Ladislau Nagy** | | | | | | |
| 2.4. Year of study | 1 | 2.5 Semester | 2 | 2.6. Type of evaluation | E | 2.7 Type of discipline | Speciality |

3. Total estimated time (hours/semester of didactic activities)

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|---|---|---|---|---|---|
| 3.1 Hours per week | 4 | Of which: 3.2 course | 2 | 3.3 seminar/laboratory | 2 |
| 3.4 Total hours in the curriculum | 56 | Of which: 3.5 course | 28 | 3.6 seminar/laboratory | 28 |
| Time allotment: | | | | | hours |
| Learning using manual, course support, bibliography, course notes | | | | | 22 |
| Additional documentation (in libraries, on electronic platforms, field documentation) | | | | | 20 |
| Preparation for seminars/labs, homework, papers, portfolios and essays | | | | | 32 |
| Tutorship | | | | | 10 |
| Evaluations | | | | | |
| Other activities: .................. | | | | | |

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| 3.7 Total individual study hours | 84 |
| 3.8 Total hours per semester | 140 |
| 3.9 Number of ECTS credits | 6 |

4. Prerequisites (if necessary)

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| 4.1. curriculum | • |
| 4.2. competencies | • quantum mechanics, atomic physics, numerical methods |

5. Conditions (if necessary)

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| 5.1. for the course | • |
| 5.2. for the seminar /lab activities | • |

6. Specific competencies acquired

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| **Specific competences** | **• Using in-depth knowledge of physics, mathematics, and programming in various multi- and inter-disciplinary fields.**<br>**• Applying atomic physics to understand of complex scientific phenomena.**<br>**• Making effective use of in-depth knowledge of physics, mathematics in solving real problems in atomic physics**<br>**• Using advanced information technology and electronic communication in order to analyse, model, simulate, and aggregate data from various branches of physics or other related fields.**<br>**• Solving advanced problems of atomic physics by means of field-related mathematical and computer instruments (analytical, numerical, or statistical tools).**<br>**• Communicating complex scientific ideas, experiments or outcomes of a scientific project.** |
| **Transversal competences** | **• Accomplishment of professional tasks in an effective and responsible manner, in compliance with the field-specific legislation and code of ethics.**<br>**• Implementation of effective interdisciplinary teamwork methods at various hierarchical levels.**<br>**• Effective use of information sources, as well as communication and professional-assisted training resources in both mother tongue and English.** |

7. Objectives of the discipline (outcome of the acquired competencies)

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| 7.1 General objective of the discipline | • The students should acquire basic knowledge about numerical methods used in atomic physics. |
| 7.2 Specific objective of the discipline | • The students should become familiar with the approximation methods used in atomic physics and other fields, such as the variational method, the stationary and time dependent perturbational methods. The students should form their skills for programming the applications of these methods. They should be able to solve problems and perform numerical calculations by computer individually |

8. Content

| 8.1 Course | Teaching methods | Remarks |
|---|---|---|
| Introduction. Approximation methods in atomic physics. The calculation of 2-electron matrix elements | Explication, problematization, multimedia projection, computer exemplification. | |
| Multielectron atoms. Independent electron appoximation. The coupling of angular momenta | | |
| Electrostatic corrections to the Hartree-Fock method. The dependence of the energy on the total spin and on the total angular momentum. | | |
| Beyond the independent electron approximation. The configuration interaction method | | |
| Time dependent perturbation theory. Transition probabilities. | | |
| Atomic collisions. Cross sections. The perturbational treatment of one-electron transitions | | |
| The treatment of the two-electron transitions. | | |

| | | |
|---|---|---|
| Transitions induced by the electromagnetic field Optical transitions. The dipole approximation. | | |
| Numerical solution of the one dimensional Schrodinger equation. Continuum states | | |
| Numerical solution of the one dimensional Schrodinger equation. Bound states | | |
| Direct numerical solution of the time-independent Schrödinger equation in 3 dimensions | | |
| Direct numerical solution of the time dependent Schrödinger equation in 3 dimensions | | |

Bibliography


1. Bransden and Joachain, The physics of atoms and molecules, Editura Tehnică, Bucureşti, 1998.
2. L. Nagy, Numerikus es kozelito modszerek az atomfizikaban (Numerical and approximate methods in atomic physics), Scientia Cluj, 2002
3. L. Nagy, Two-electron processes in fast collisions with charged particles, Nucl. Instr. Meth. B, 124 (1997), 271-280.
4. L. Nagy, Multi-electron processes in atomic collisions – Theory, Nucl. Instr. Meth B154 (1999) 23-130.
5. L. Ixaru, Metode numerice pentru ecuatii diferentiale cu aplicatii, Ed. Academiei, Bucuresti, 1979
6. T. Beu, Calcul numeric in C, Ed. Albastra, Cluj, 2000
7. Haken and Wolf, The physics of atoms and quanta, Springer Verlag, 1994


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| 1. The numerical calculation of a one-electron Hamiltonian matrix element. | | |
| 2. The numerical calculation of a two-electron Hamiltonian matrix element | | |
| 3. Application of the Hartree-Fock method | | |
| In the second part: each student receives an individual problem to solve. He/she studies the theoretical background, peforms the analytical calculations, writes the computer code for the numerical part and elaborates a report on the problem. The presentation should follow the structure of a scientific paper. | | |

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

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10. Evaluation

| Type of activity | 10.1 Evaluation criteria | 10.2 Evaluation methods | 10.3 Share in the grade (%) |
|---|---|---|---|
| 10.4 Course | Knowlidge, understanding and capacity of application of numerical methods in atomic physics | Oral exam | 50 |
| 10.5 Seminar/lab activities | Individual work | Written report | 50 |
| | | | |
| 10.6 Minimum performance standards | | | |
| 55% | | | |

| Date | Signature of course coordinator | Signature of seminar coordinator |
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| ..26.09.2017……….. | ........................................ | ........................................... |

| Date of approval | Signature of the head of department |
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