Babeş–Bolyai University, Cluj-Napoca
Faculty of Physics
2011-2012 academic year
Summer semester

I. General information on the course

Title of the course: Models and numerical methods in atomic physics
Code: FMC0011
Credits: 7
Place:
Time:

II. Instructor

Name: Prof. Nagy Ladislau
Contact: lnagy@phys.ubbcluj.ro
Personal contact: Friday 10-12

III. The description of the course:

Objecives:
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.
Methods: Explication, problematization, multimedia projection, computer exemplification at the course. Problematization, case study, individual work at the laboratory.

IV. Compulsory bibliography:

1. Bransden and Joachain, Fizica atomului si a moleculei (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.

V. Laboratory equipement:

Multimedia projector
Computer laboratory

VI. The detailed schedule of the courses, laboratoy works and examinasion

Courses

No.	Topic	No. hours	Biblio-graphy
1.	Introduction. Approximation methods in atomic physics. The calculation of 2-electron matrix elements	2	[1]:36-57 302-310 [2]: 11-21
2.	Multielectron atoms. Independent electron appoximation. The coupling of angular momenta	2	[1]: 155-164 [2]: 69-76
3	Electrostatic corrections to the Hartree-Fock method. The dependence of the energy on the total spin and on the total angular momentum.	2	[1]: 395-408 [2]: 49-54
4.	Beyond the independent electron approximation. The configuration interaction method	2	[2]:36-40 [4]
5.	Time dependent perturbation theory. Transition probabilities.	2	[2]: 93-98
6.	Atomic collisions. Cross sections. The perturbational treatment of one-electron transitions	2	[2]:98-105 [3]: 271-275
7.	The treatment of the two-electron transitions.	2	[2]: 105-113 [3]: 275-280
8.	Transitions induced by the electromagnetic field. Optical transitions. The dipole approximation.	2	[1]: 187-202 [2]: 113-122
9.	Direct numerical solution of the time-independet Schrödinger equation	4	
10.	Direct numerical solution of the time dependent Schrödinger equation	4	

Laboratory work

In the first part: frontal progamming of the following problems

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 studend 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.

VII. The evaluation methods

The students are evaluated on the basis of their elaborated report (50%) and on the basis of an oral exam (50%)

VIII. Organization details:

The participation at the laboratory works and the elaboration of the report is compulsory

IX. Optional bibliography

1. L. Ixaru, Metode numerice pentru ecuatii diferentiale cu aplicatii, Ed. Academiei, Bucuresti, 1979
2. T. Beu, Calcul numeric in C, Ed. Albastra, Cluj, 2000
3. Haken and Wolf, The physics of atoms and quanta, Springer Verlag, 1994

Prof. Ladislau Nagy