Babeş–Bolyai University, Cluj-Napoca
Faculty of Physics
2008-2009 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.	The review of the models in atomic physics. Classical models, the planetary model. The Bohr and Bohr-Sommerfeld models. The quantum model.	2	[1]:36-57 125-150
2.	Methods for treating the hydrogen atom. Multielectron atoms. The necessity of the approximation methods. Independent electron appoximation	2	[1]: 155-164 [2]: 69-76
3.	The variational method. The Rayleigh-Ritz method. One-parameter method for the helium atom. The Hylleras wavefunctions	2	[1]: 131-140 302-310 [2]: 11-21
4.	The Hartree and the Hartree-Fock approximations. The self consistent field method.	2	[1]:371-395 [2]: 22-35
5.	Beyond the independent electron approximation. The configuration interaction method	2	[2]:36-40 [4]
6.	The stationary perturbational method. The ground states and the excited states of the helium.	2	[1]:310-327 [2]: 40-48
7.	The perturbational treatment of the electrostatic corrections. The dependence of the energy on the total spin and on the total angular momentum.	2	[1]: 395-408 [2]: 49-54
8.	The perturbational treatement of the spin-orbit interaction	2	[1]: 233-246 [2]: 54-58
9.	The atom in magnetic field. The Zeeman effect. The application of the perturbation method for different strengths of the field	2	[1]: 246-258 434-437 [2]:58-63
10.	Te atom in electric field. The Stark effect.	2	[1]:259-270 [2]:64-68
11.	Time dependent perturbation theory. Transition probabilities.	2	[2]: 93-98
12.	Atomic collisions. Cross sections. The perturbational treatment of one-electron transitions	2	[2]:98-105 [3]: 271-275
13.	The treatment of the two-electron transitions.	2	[2]: 105-113 [3]: 275-280
14.	Transitions induced by the electromagnetic field. Optical transitions. The dipole approximation.	2	[1]: 187-202 [2]: 113-122

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