



# Bachelor in Physics (Academic Year 2024-25)

<b>Atomic and Molecular Physics</b>			<b>Code</b>	800524	<b>Year</b>	4 <sup>th</sup>	<b>Sem.</b>	1 <sup>st</sup>
<b>Module</b>	Fundamental Physics	<b>Topic</b>	Obligatory of Fundamental Physics		<b>Character</b>	Optional		

	Total	Theory	Exer. / Sem.	Lab.
<b>ECTS Credits</b>	6	4	2	
<b>Semester hours</b>	45	30	9	6

### Learning Objectives (according to the Degree's Verification Document)

- By the end of the course students will be able:
- To evaluate the main interactions within a many-electron atom, comprehending how they determine its description, properties, and energy levels.
  - To identify the effects of external factors (electric and magnetic fields, and collisions) on atoms.
  - To recognize the structure of diatomic and polyatomic molecules.
  - To understand the properties of radiation emission and absorption by atoms and molecules.
  - To comprehend the fluorescence and phosphorescence processes, and the basis of the main spectroscopic techniques.

### Brief description of contents

Many-electron atoms; electrostatic and spin-orbit interactions; angular momentum coupling; interaction with static external fields; molecular structure; diatomic and polyatomic molecules.

### Prerequisites

Quantum Physics I and II (basis of quantum mechanics, stationary perturbation theory, angular momentum coupling).  
Structure of Matter (Hydrogen atom, many-electron systems, central-field approximation, spin-orbit coupling, notions of molecular structure).

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### Theory/Excercises – Schedule and Teaching Staff

Group	Lecture Room	Day	Time	Professor	Period/ Dates	Hours	T/E	Dept.
B	1	We, Fr	14:00 – 15:30	Daniel Nieto Castaño	Full term	39	T/E	EMFTEL

T: Theory, E: Exercises

Office hours				
Group	Professor	Schedule	E-mail	Location
B	Nieto Castaño, Daniel	We,Fr:10:00-11:30 (rest online)	<a href="mailto:d.nieto@ucm.es">d.nieto@ucm.es</a>	03.228.0

COMPUTER LABORATORIES				
Group	Lecture Room	Sessions	Professor	Hours
L6	15	Tue 01/10 12:00-13:30 Tue 08/10 12:00-13:30	Nieto Castaño, Daniel	3.0

LABORATORY				
Group	Laboratory	Sessions	Professor	Hours
L12	Atomic Nuclear and Particle Physics Lab.	Thu 24/10 12:00-13:30 Thu 12/12 12:00-13:30	Nieto Castaño, Daniel	3.0

Syllabus
<p><b>Atomic Physics (60% approx.)</b></p> <ol style="list-style-type: none"> <li><b>Introduction to many-electron atoms</b> <ul style="list-style-type: none"> <li>Handling of antisymmetric wavefunctions                             <ul style="list-style-type: none"> <li>Configurations, degeneracy, periodic system</li> </ul> </li> <li>Approximation methods                             <ul style="list-style-type: none"> <li>Statistical and Hartree methods. Variational methods (Hartree-Fock)</li> </ul> </li> </ul> </li> <li><b>Corrections to the central field approximation</b> <ul style="list-style-type: none"> <li>Electrostatic interaction. Electrostatic terms and their determination                             <ul style="list-style-type: none"> <li>Calculation of corrections due to electrostatic interaction</li> </ul> </li> <li>Spin-orbit interactions                             <ul style="list-style-type: none"> <li>Total angular momentum <math>J</math> and eigenstates. Calculation of spin-orbit constants</li> </ul> </li> <li>Russel-Saunders approximation                             <ul style="list-style-type: none"> <li>Limits to <math>LS</math> coupling</li> <li>Other coupling models, <math>JJ</math> coupling, intermediate coupling, and their effects</li> </ul> </li> </ul> </li> <li><b>Atoms in external constant fields</b> <ul style="list-style-type: none"> <li>Magnetic fields. Zeeman and Paschen-Bach effects</li> </ul> </li> <li><b>Emission and absorption of radiation by atoms</b> <ul style="list-style-type: none"> <li>Interaction with the electromagnetic field. Einstein coefficients and their calculation</li> <li>Selection rules. Spectral lines.</li> </ul> </li> </ol> <p><b>Molecular Physics (40% approx.)</b></p> <ol style="list-style-type: none"> <li><b>Introduction to molecular structure</b> <ul style="list-style-type: none"> <li>Born-Oppenheimer approximation</li> <li>Structure of diatomic molecules</li> <li>Nuclear wave function. Vibrational and rotational states</li> <li>Electronic wave function. Potential curves</li> </ul> </li> <li><b>Emission and absorption of radiation by diatomic molecules</b> <ul style="list-style-type: none"> <li>Coupling of angular momenta</li> <li>Pure-rotational spectra</li> <li>Vibrational-rotational spectra</li> <li>Electronic transitions. Franck-Condon principle</li> </ul> </li> <li><b>Polyatomic molecules</b> <ul style="list-style-type: none"> <li>Molecular orbitals. Delocalization</li> <li>Rotational and vibrational states</li> <li>Spectroscopy</li> </ul> </li> </ol>

<b>Bibliography</b>
<p><b>Basic:</b></p> <ul style="list-style-type: none"> <li>• B.H.Brandsen, C.J.Joachain, <i>Physics of atoms and molecules</i> (Pearson)</li> <li>• I.I.Sobelman, <i>Atomic Spectra and Radiative Transitions</i> (Springer Verlag)</li> <li>• G.K.Woodgate, <i>Elementary atomic structure</i> (McGraw Hill)</li> <li>• P.W. Atkins, <i>Molecular Quantum Mechanics</i> (Oxford Univ. Press)</li> <li>• F. Blanco Ramos, <i>Introducción a la Física de Átomos y Moléculas</i> (Amazon)</li> </ul> <p><b>Complementary:</b></p> <ul style="list-style-type: none"> <li>• H.G.Kuhn, <i>Atomic Spectroscopy</i> (Academic Press)</li> <li>• A.P. Thorne, <i>Spectrophysics</i> (Chapman and Hall)</li> <li>• B.W. Shore and D.H. Menzel, <i>Principles of Atomic Spectra</i> (John Wiley)</li> <li>• R.D.Cowan, <i>The theory of atomic structure and spectra</i> (Univ. California Press)</li> <li>• I.N. Levine, <i>Espectroscopía molecular</i> (Ed. AC, D.L.)</li> <li>• C. Sánchez del Río, <i>Introducción a la teoría del átomo</i> (Ed. Alhambra)</li> </ul>

<b>Online Resources</b>
<p>FAyM-didactic: programs for the numerical calculus practices (F. Blanco, J. Rosado, D. Nieto):  <a href="https://github.com/Pacobr/FAyM-didactic">https://github.com/Pacobr/FAyM-didactic</a></p> <p>Atomictools: a Python package to create and visualize atomic orbitals and more (A. Villar, J. Rosado):  <a href="https://github.com/JaimeRosado/atomictools">https://github.com/JaimeRosado/atomictools</a></p>

<b>Methodology</b>
<p>Theory lectures will be carried out using blackboard and computer presentations. The theoretical concepts explained will be reinforced with the solution to problems and exercises interspersed during the classes. The participation of the students in these exercises will be encouraged, and they may be requested to hand them in after the lecture.</p> <p>After each subject-matter is covered, a problem set will be delivered that will be solved completely or will come with partial indications so that the students can carry them out by themselves.</p> <p>There will be two numerical calculation practices in the computer room and two experimental laboratory practices. All the four practices are mandatory.</p> <p>Depending on the number of students enrolled, they may present to the class on topics relevant to the course contents. This activity may be carried out in groups or individually.</p>

<b>Evaluation Criteria</b>		
<b>Exams</b>	<b>Weight:</b>	70%
A final exam that consists of solving exercises of similar difficulty to those worked out during the course. The students will be allowed to consult their own notes, books, solved problems, etc/.		
<b>Other Activities</b>	<b>Weight:</b>	30%
Four compulsory practices. In addition, optional assignments may be proposed to increase marks..		
<b>Final Mark</b>		
<p>The final exam will include two parts, one corresponding to atomic physics, another one to molecular physics, that will be assessed separately. A mark lower than 3.5 over 10 in any of the two parts will be assigned as the final mark for the course, regardless of the rest of the marks. The marks of each part of the exam in the ordinary call may be kept for the extraordinary call.</p> <p>The four compulsory practices will contribute to the final mark with a weight of 30% of the total. If any of them are not done, the final mark for Other Activities will be 0.</p> <p>Optional assignments may be proposed to increase marks.</p>		