



04/05/2026 – 19/06/2026

**Title of the project: Calculating the energy levels of the helium atom**

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Laboratory / Department / Team: ICB / ICQ / MARS

**Collaborations:**

**Summary:**

This project is an initiation to the modeling of atomic energy spectra, which was the first historical purpose of quantum mechanics. It will focus on helium (He), the simplest multi-electron atom, where the Coulombic repulsion between the two electrons plays an important role.

The first goal of the project is to learn how to build the Hamiltonian of He, expressing it in a basis of hydrogenic wave functions. Then, the energy levels of the atom will be calculated by diagonalizing the Hamiltonian using a computer code in Octave/Matlab. The student will tune the parameters of that code which is already written. The computed energies will be compared to the experimental values, and their variation with for example the number of basis wave functions will be examined. The Hamiltonian eigenvectors will also be calculated, in order to understand the role of atomic symmetry and its relation to electronic spin.

**Type of project (theory/experiment): theory**

**Required skills:**