PhD subject proposal – 2022

Title: Modeling the energy spectrum of laser-cooled lanthanide atoms

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Scientific department: ICQ
Research group: SMPCA

Co-supervisor: Maxence LEPERS

General scientific context:

Due to temperatures very close to the absolute zero, laser-cooling of atoms allows to probe intriguing features of quantum matter like Bose-Einstein condensation. The obtained ultracold gases are also promising platforms for quantum technologies or quantum simulation of condensed-matter physics. Atoms possessing a dipole moment are particularly interesting, as their long-range and anisotropic interactions open the possibility to design systems with strong interparticle correlations. In this context, atoms belonging to the lanthanide family, which possess a strong magnetic moment in their ground level, have attracted growing attention in the last 15 years, which led for example to the observation of supersolidity with erbium atoms (see e.g. Nat. Phys. **17**, 1349, 2021). This strong magnetic moment comes from their unpaired 4f electrons; but the latter also induce a rich energy spectrum, with many levels and many available optical transitions in the visible and infrared frequencies. Knowing the energy and the strength of those transitions is crucial to determine the feasibility of laser-cooling and trapping of atoms, not only in the ground level but also in well-chosen excited levels. However, only a small proportion of those transition strengths have been measured experimentally, and so their calculation is required.

The SMPCA team of Laboratoire ICB possesses an internationally recognized knowledge in the fields of atomic spectroscopy, molecular spectroscopy and molecular reaction dynamics. The team also possess a strong expertise in software and database developments. Regarding the present project, its co-supervisor possesses a well-established expertise in the spectroscopy of ultracold lanthanide atoms, which he investigated with world-leading experimental groups (see e.g. Phys. Rev. Research **3**, 033256, 2021). Moreover, a new atomic database has recently been set up: the Calculated Database of Dijon for AtomiC Spectra (CaDDiAcS, see the search form at https://vamdc.icb.cnrs.fr/caddiacs/).

Objectives:

The objective of the present project is to calculate energy levels and Einstein coefficients for spontaneous emission – a quantity characterizing the transition strength –, for lanthanide atoms relevant in current-day ultracold experiments, including erbium, dysprosium, thulium or neodymium. Therefore, this theoretical project will be held in relationship with experimental groups working on ultracold lanthanide atoms. The computed atomic properties will be useful to characterize the efficiency of laser-cooling and trapping, for instance through the dynamic dipole polarizabilities in various energy levels. Lanthanide atoms can present up to several tens of thousands of lines in the visible and infrared windows; the Einstein coefficients calculated in this project will be published in the CaDDiAcS database hosted in Dijon.

Proposed work:

The atomic-structure calculations performed during the project comprise two steps during which the computed quantities are adjusted to their known experimental counterparts. Firstly, energy levels are calculated using a combination of *ab initio* and least-square fitting techniques implemented in the open-source suites of codes Cowan. Secondly, a similar combination is used to calculate Einstein coefficients with the code FitAik, that has recently been developed in our team. In addition to their interest for cold atoms, our calculations will also serve to test the performances of the code FitAik. Therefore, calculations with other species presenting a methodological interest, such as lanthanide

singly-ionized ions, will also be performed. As for polarizabilities and other derived quantities, they can be calculated with codes written by the future student.

Required knowledge:
Solid knowledge in quantum mechanics, in particular atomic physics and angular-momentum theory, and in computer programming (in particular in Fortran).

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