INTERNSHIP PROPOSAL

Laboratory name: Laboratoire Kastler Brossel CNRS identification code: UMR 8552
Internship director: KARR Jean-Philippe
e-mail: karr@lkb.upmc.fr Phone number: 01 44 27 60 79
Web page: https://www.lkb.upmc.fr/iontrap/3bodyqs/
Internship location: campus Pierre et Marie Curie, 4 place Jussieu, 75005 Paris

Thesis possibility after internship: YES Funding: NO

QED calculations in the simplest molecules

The theory of quantum electrodynamics (QED) allows for very accurate predictions. Comparison between experimental and theoretical values of QED-related quantities can be used for stringent tests of the Standard Model and to determine the values of fundamental physical constants. Well-known examples are the electron's anomalous magnetic moment (related to the fine-structure constant α) or the spectrum of the hydrogen atom (related to the Rydberg constant and proton charge radius).

Recently, measurements of ro-vibrational transition frequencies in hydrogen molecular ions (H_2^+, HD^+…), the simplest molecules in nature, have reached a record 12-digit accuracy [1]. Owing to the dependence of ro-vibrational energy levels on particle masses, comparison of experimental results with theoretical predictions [2] has led to an improved determination of the proton-electron mass ratio m_p/m_e [3]. It has also contributed to setting constraints on hypothetic new interactions beyond the Standard Model [4], where the added value of molecular systems resides in their sensitivity to interactions between nucleons. The burgeoning experimental activity in this field gives strong motivation to improve further the theory of hydrogen molecular ions by computing higher-order QED corrections.

Two main theoretical approaches can be used, depending on the type of correction. One is to perform a fully relativistic calculation, using as a starting point a high-precision numerical resolution of the Dirac equation [5]. The other possibility is the Non Relativistic QED (NRQED) framework, where QED corrections are described by effective Hamiltonians in a nonrelativistic (Schrödinger) formalism.

Several topics are envisaged for the internship, to be discussed further with the applicant and adapted to his preferences between theoretical and numerical work:
- improve the theoretical hyperfine structure in HD+ by computing the proton-deuteron spin-spin interaction coefficient in the NRQED framework;
- implement a new basis set ("B-spline" basis functions) to solve numerically the Dirac equation with high accuracy, which will be useful to perform a fully relativistic calculation of the one-loop self-energy correction.

[1] S. Patra et al., Science **369**, 1238 (2020).
[2] V.I. Korobov, L. Hilico, and J.-Ph. Karr, Phys. Rev. Lett. **118**, 233001 (2017).
[3] Recommended values of fundamental constants can be found at https://pml.nist.gov/cuu/Constants/.
[4] M. Germann et al., Phys. Rev. Research **3**, L022028 (2021).
[5] H.D. Nogueira and J.-Ph. Karr, Phys. Rev. A **107**, 042817 (2023).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: NO
Soft Matter and Biological Physics: NO
Quantum Physics: YES
Theoretical Physics: YES