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Physique quantique et applications

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PhD thesis (for September 2017)
QED corrections in simple molecules

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The precise study of simple systems allows testing fundamental theories and evidencing possible deviations from the Standard Model of physics. If the agreement between theory and experiment is satisfactory, it can be exploited to determine physical fundamental constants. For example, high-precision spectroscopy of the hydrogen and deuterium atoms is used to determine the Rydberg constant and the charge radii of the proton and deuteron. However, there is currently an unexplained discrepancy, known as the « proton-radius puzzle », between the nuclear radii deduced from spectroscopy of conventional vs. exotic atoms where the electron is replaced by a muon [1].

New "players" in this game are the hydrogen molecular ions H_2^+ and its isotopes HD^+, D_2^+, which are the simplest molecules, made of two nuclei and one electron. These systems are sensitive to the same fundamental constants as their atomic counterparts H and D. In addition, they exhibit ro-vibrational transitions whose frequencies are very sensitive to the nuclear masses, allowing for an improved determination of the proton-to-electron mass ratio m_p/m_e [2]. It was recently shown that high-precision spectroscopy of H_2^+ and HD^+ could contribute to a resolution of the proton-radius puzzle [3]. For that aim the theoretical accuracy should reach a few parts in 10^{12}.

A few years ago, a systematic evaluation of QED corrections in three-body molecular systems was initiated, in collaboration with V. Korobov (JINR, Dubna, Russia). These corrections can be expressed in terms of a perturbative expansion in powers of the fine structure constant α. All terms up to the 5th order have been calculated [4], and work is in progress on 6th-order corrections. The objective of the PhD will be to improve the calculation of radiative corrections at this order and evaluate recoil corrections (linked to the motion of nuclei, and smaller by a factor of order m_e/m_p) at the 4th order.

Methods and techniques:

We follow the framework of "nonrelativistic Quantum Electrodynamics" (NRQED), meaning that correction terms are expressed in terms of effective operator mean values on the nonrelativistic (Schrödinger) wave function. The project implies both analytical calculations (derivation of the effective Hamiltonian) and their numerical implementation with wave functions obtained by a variational method.

[1] R. Pohl et al., *The size of the proton*, Nature **466**, 213 (2010).
[2] J. Biesheuvel et al., *Probing QED and fundamental constants through laser spectroscopy of vibrational transitions in HD$^+$*, Nature Communications **7**, 10385 (2016).
[3] J.-Ph. Karr, L. Hilico, J.C.J. Koelemeij, V.I. Korobov, *Hydrogen molecular ions for improved determination of fundamental constants*, Phys Rev. A **94**, 050501(R) (2016).
[4] V.I. Korobov, L. Hilico, J.-Ph. Karr, *$m\alpha^7$-Order Corrections in the Hydrogen Molecular Ions and Antiprotonic Helium*, Phys. Rev. Lett. **112**, 103003 (2014).