

PhD thesis (for September 2019) QED corrections in one-electron 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, 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.

The hydrogen molecular ions (H_2^+ and its isotopes HD^+ , D_2^+) are very promising systems for such fundamental measurements. From a theory point of view, they are the next simplest systems after hydrogenlike atoms, so that their energy levels can be calculated with very high accuracy. They have ultra-narrow rovibrational transitions, the frequencies of which depend on the nuclear masses, allowing for improved determination of the proton-to-electron mass ratio m_p/m_e [1]. Spectroscopy of H_2^+ and HD^+ could also contribute to resolving the proton-radius puzzle [2].

For these aims, the theoretical accuracy, which has recently reached a level of $7.6 \cdot 10^{-12}$ [3], needs to be improved further by at least a factor of 2 or 3. The limitation comes from the one-loop self-energy of the bound electron (Fig. 1). So far, this correction has been calculated using a nonrelativistic expansion in powers of the binding potential. The objective of the PhD will be to achieve a fully relativistic calculation. The first step consists in solving numerically the Dirac equation for an electron in a two-center potential.

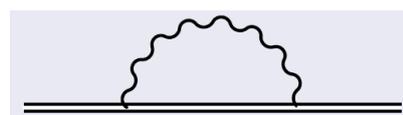


Fig. 1. One-loop self-energy diagram. The double line represents a bound electron.

[1] J. Biesheuvel et al., [Probing QED and fundamental constants through laser spectroscopy of vibrational transitions in \$HD^+\$](#) , Nature Commun. **7**, 10385 (2016).

[2] 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). [arXiv](#)

[3] V.I. Korobov, L. Hilico, J.-Ph. Karr, [Fundamental Transitions and Ionization Energies of the Hydrogen Molecular Ions with Few ppt Uncertainty](#), Phys. Rev. Lett. **118**, 233001 (2017). [arXiv](#)