1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Testing the quantum theory for molecules with ultra-accurate molecular beam spectroscopy

1.1. Project goals

- Development of an experimental setup for accurate spectroscopy of HD molecule in molecular beam,
- Ultra-accurate measurements of HD rovibrational energies in its ground electronic state (the goal is to reach accuracy corresponding to quantum electrodynamic correction tests at higher than fifth meaningful digit level)

1.2. Outline

The progress in accurate measurements of the rovibrational structure of H_2 (and isotopologues) in its ground electronic state has dramatically accelerated following the incorporation of optical frequency combs (OFCs). The incorporation of OFCs has coincided with a theoretical breakthrough. The unprecedented accuracy in calculating the nonrelativistic contribution to the rovibrational energy [Pachucki2018] (the dominant contribution), sets the further rapid progress to be expected on the theory side in the upcoming years.

The most accurate measurements of the rovibrational lines in molecular hydrogen were obtained with infrared-ultraviolet double resonance spectroscopy in molecular beams [Fast2020] and cavity-enhanced spectroscopy: for HD, the sub-Doppler saturation technique was implemented [Cozijn2018, Tao2018], while for homonuclear isotopologues, due to the lack of dipole transitions, Doppler-limited techniques were used [Wcisło2018, Zaborowski2020] (the Doppler-limited technique was also used for HD [Fasci2018, Castrillo2021]). The highest accuracy, 13 kHz, was obtained for the HD isotopologue [Fast2020]. The factors that limit the accuracy depend on the approach used. For instance, for HD molecular beam experiments, the accuracy is limited by the residual first-order Doppler shift to the 12 kHz level [Fast2020].

The relative accuracy of the best measurements for the hydrogen molecule is at the 10^{-10} level [Fast2020], while the relative accuracy of the best spectroscopic measurements is 10^{-18} [Bothwell2019, Brewer2019]. The fundamental limitation for HD rovibrational spectroscopy is estimated at the 10^{-24} level. This shows an enormous (8 orders of magnitude) gap between the present best accuracy for molecular hydrogen and the present best accuracy of laser spectroscopy and an even larger (14-orders of magnitude) gap when compared with the fundamental limitation for HD.

The goal of this project is to improve the previous best experiment [Fast2020] at several steps, starting from molecular beam generation and geometrical arrangement, through the efficiency of HD+ ion production and detection up to the efficiency of HD excitation on the spectroscopy transition.

1.3. Work plan

- Development of HD source and beam geometry alignment
- Development of UV ionizing laser and HD+ ion detection system
- Development of spectroscopy laser
- Ultra-accurate measurements of HD rovibrational line
- Theoretical simulations/estimations and experimental data analysis

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate)*

[Bothwell2019] T. Bothwell, et al., Metrologia 56, 065004 (2019)
[Brewer2019] S. M. Brewer, et al., Phys. Rev. Lett. 123, 33201 (2019)
[Castrillo2021] A. Castrillo, et al., Phys. Rev. A 103, 022828 (2021)
[Cozijn2018] F. M. J. Cozijn, et al., Phys. Rev. Lett. 120, 153002 (2018)
[Fasci2018] E. Fasci, et al., Phys. Rev. A 98, 022516 (2018)
[Fast2020] A. Fast, S.A. Meek, Phys. Rev. Lett. 125, 023001 (2020)
[Pachucki2018] K. Pachucki, J. Komasa, Phys. Chem. Chem. Phys. 20, 247 (2018)
[Tao2018] L.-G. Tao, et al., Phys. Rev. Lett. 120, 153001 (2018)
[Wcisło2018] P. Wcisło, et al., J. Quant. Spectrosc. Radiat. Transfer 213, 41 (2018)
[Zaborowski2020] M. Zaborowski, et al., Opt. Lett. 45, 1603 (2020)

1.5. Required initial knowledge and skills of the PhD candidate

Skills and experience in experimental physics. Good knowledge of Matlab, LabView or Mathematica (or equivalent) software. Excellent problem-solving and communication skills. Written and verbal communication skills and presentation skills. Teamwork ability. Good command of the English language.

1.6. Expected development of the PhD candidate's knowledge and skills

Knowledge, skills and experience in molecular and optical physics, laser and cryogenic technologies, and in molecular spectra analysis.