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

Project title: Collison-induced line-shape effects in molecular spectra

1.1. Project goals

- Development of new techniques of solving the Boltzmann equation for the velocity distribution of optical coherences
- Development of models of velocity-changing operators that are based one realistic intermolecular interactions
- Measurements of the collision-perturbed spectra based on the cavity-enhanced techniques
- Collision-perturbed spectra analysis and tests of the above-described theoretical developments

1.2. Outline

The collisional line-shape effects (including the beyond-Voigt effects [Wojtewicz2015]) play an important role in atomic and molecular physics. On the one hand they give an access to study the molecular interactions [Thibault2017,Wcislo2013] and dynamics [Wcislo2015], but on the other hand they deteriorate accuracy of optical metrology based on molecular spectroscopy [Wcislo2016]. In particular, the line-shape effects can limit the accuracy of atmospheric measurements of the Earth [Miller2005] and other planets [Feuchtgruber2013] and even modify the opacity of the exoplanetary atmospheres [Miller2008]. Therefore, it is crucial to develop new more accurate and numerically more efficient methods for describing the collision-induced shapes of molecular lines. Within this PhD project two aspects of this problem will be addressed:

- Development of new techniques of solving the Boltzmann equation for the velocity distribution of optical coherences (the transport-relaxation equation). We found a simple analytical way to express the derivatives of the collisional operators, which will enables us to use a multidimensional series-based formula not only to evaluate the line-shape function for an initial set of parameters but also to propagate the solution to entirely different physical conditions. In this sense we will obtain a global solution of the transport-relaxation equation.
- Calculations of the Boltzmann collisional operator for a realistic intermolecular potential. Till now, the most physical velocity-changing model implemented into the description of the collision-perturbed shapes of molecular lines was based on the power law intermolecular potential [Wcislo2013]. Within this PhD project the student will developed a calculation tools that will allow one, for the first time, to determine the velocity-changing collisional operator for a potential that possesses both a long-range attractive part and short-range repulsive part.

The important part of this PhD project is that the both theoretical developments will be tested on highly-accurate experimental spectra. The PhD student will perform the experiment that will be based on the cavity-enhanced spectrometers operating in the

Institute of Physics and KL FAMO. The PhD student will perform the analysis of the experimental spectra using the models that are based on the above described theoretical developments. This project will constitute experimental test of the most advanced and physically the most realistic line-shape model considered so far for isolated molecular lines.

1.3. Work plan

- Development of novel method of solving the transport-relaxation equation based on multidimensional series-based expansion
- Calculations of the Boltzmann operators for realistic intermolecular interactions and using them in collision-perturbed spectra simulations
- Measurements of the collision-perturbed spectra based on the cavity-enhanced techniques
- Spectra analysis and experimental validation of the above-described theoretical developments

1.4. Literature

[Feuchtgruber2013] H. Feuchtgruber, et al., A&A 551, A126 (2013)

[Miller2005] C. E. Miller, et al., C. R. Phys. 6, 876 (2005)

[Miller2008] E. Miller-Ricci, et al., Astrophys. J. 690, 1056 (2008)

[Thibault2017] F. Thibault, ..., P. Wcisło, J. Quant. Spectrosc. Radiat. Transfer 202, 308 (2017)

[Wcislo2013] P. Wcisło and R. Ciury lo, J. Quant. Spectrosc. Radiat. Transfer 120, 36 (2013)

[Wcislo2015] P. Wcisło, et al., Phys. Rev. A 91, 052505 (2015)

[Wcislo2016] P. Wcisło, et al., Phys. Rev. A 93, 022501 (2016)

[Wojtewicz2015] S. Wójtewicz, et al., J. Quant. Spectrosc. Radiat. Transfer 165, 68 (2015)

1.5. Required initial knowledge and skills of the PhD candidate

Skills and experience in experimental and theoretical 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 statistical, molecular and optical physics, laser technologies, and in molecular spectra analysis.

4. DECLARATION OF TECHNICAL/EXPERIMENTAL/FINANCIAL RESOURCES SUFFICIENT AND NECESSARY TO COMPLETE THE PROJECT

I declare that the optical and metrological infrastructure owned by the Institute of Physics and KL FAMO will be made available for the purpose of this project. I declare that any necessary additional equipment will be purchased from the 2018/31/B/ST2/00720 National Science Centre, Poland (OPUS) project.

5. DECLARATION CONCERNING THE AUTHORSHP OF PROJECT IDEA

I declare that the author of the idea for the doctoral project is:

Piotr Wcisło

6. DECLARATION CONERNING THE POSSIBILITY OF PUBLISHING THE CONTENT OF THE PROJECT

I declare that the description of the project submitted do the contest from point 1. can be published on the website of Doctoral School of Exact and Natural Sciences, Nicolaus Copernicus University in Toruń.

Toruń, 10.05.2020

place, date

Piotr Wcisło

signature of project submitter