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

Project title: Collisions of simple molecules and atoms in fundamental studies

1.1. Project goals

The objective of the project are the quantum-scattering calculations for the simplest benchmark molecular systems for which many yet unsolved collisional problems wait to be analyzed theoretically from first principles and tested on highly-accurate experimental data:

- Calculations of the collisional effects for the self-perturbed molecular hydrogen and their application in ultra-accurate experimental determination of molecular hydrogen rovibrational structure (including the tests of the relativistic and QED corrections)
- Quantum scattering calculations for indistinguishable molecules and, for the first time, applying them to calculate the collisional line-shape parameters for indistinguishable molecules
- Quantum scattering calculations for two vibrating molecules with fully accessible vibrational and rotational inelastic channels including the exchange of vibrational excitation, which has not been done in the context of collisional line-shape modelling yet
- Quantum scattering calculations for molecular hydrogen that include the hyperfine structure; for the first time the hyperfine structure will be taken into account in the *ab initio* quantum scattering line-shape calculations

1.2. Outline

It has been demonstrated that the collisional line-shape calculations, based on the *ab initio* quantum scattering calculations, can be used for testing potential energy surfaces [Thibault2017], improving accuracy of ultra-accurate spectroscopy aimed at the tests of quantum electrodynamics [Wcisło2018], validating sophisticated statistical models based on Boltzmann-like equation [Wcisło2015] or generating spectroscopic databases [Stolarczyk2020]. It was shown, for the case of a simple benchmark system of H2-He, that the collision-perturbed spectra calculated from first principles remarkably well agree with highly-accurate measurements [Słowiński2020]. For a slightly more complex system of Ar-perturbed H2 (where the perturber-to-absorber mass ratio is much larger) an effect of strong competition between phase-/state-changing and velocity-changing collisions was theoretically predicted and validated on experimental spectra [Wcisło2015]. Recently, the accurate *ab initio* quantum scattering calculations were used to generate a comprehensive line-by-line database of beyond-Voigt line-shape parameters for the H2-He system [Wcisło2020]. It was shown, however, that the same methodology applied to a more complex system of self-perturbed D2 (i.e. the molecule-molecule case) resulted in a large discrepancy between theoretical and experimental shifts [Wcisło2018]. Within this

PhD project, the methodology will be significantly extended and new theoretical tools will be developed. The student will develop a quantum-scattering code for the molecule-molecule case that will include both vibrational and rotational inelasticity, develop a tools to handle the hyperfine structure in collisional calculations as well as a proper description of the quantum indistinguishability.

1.3. Work plan

- Analysis of the hyperfine structure for different isotopologues of molecular hydrogen and preparation of a proper basis for quantum-scattering calculations
- Development of the quantum-scattering codes for the case of molecular hydrogen that include the hyperfine structure
- Development of the quantum-scattering codes for molecule-molecule case that include the inelasticity in vibrations (and rotations as in usual approaches)
- Analysis of the problem of quantum distinguishability in the context of molecular scattering and collisional line-shape calculations
- Performing the quantum scattering calculations, evaluating the generalized spectroscopic cross sections, and the line-shape parameters

1.4. Literature

[Słowiński2020] M. Słowiński, ..., P. Wcisło, accepted in Phys. Rev. A
[Stolarczyk2020] N. Stolarczyk, ..., P. Wcisło, JQSRT 240, 106676 (2020)
[Thibault2017] F. Thibault, ..., P. Wcisło, JQSRT 202, 308 (2017)
[Wcisło2015] P. Wcisło, et al., Phys. Rev. A 91, 052505 (2015)
[Wcisło2018] P. Wcisło, et al., JQSRT 213, 41 (2018)
[Wcisło2020] P. Wcisło, et al., in preparation

1.5. Required initial knowledge and skills of the PhD candidate

Skills and experience in theoretical physics. Good knowledge of FOTRAN (also Matlab or Python). 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 physics, computer coding and numerical methods. Knowledge of quantum-scattering theory, molecular interactions and molecular spectroscopy.

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

I declare that computer resources needed for the calculations scheduled within this project (located at the NCU Institute of Physics and at our partners laboratories) will be made available.

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

signature of project submitter