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Report on the PhD dissertation

Quantum effects in ultracold collisions of atoms, ions, and molecules

by Mr. Dariusz Wiater

Thematic classification

The doctoral thesis "Quantum effects in ultracold collisions of atoms, ions, and molecules" by Mr. Dariusz Wiater has been conducted at the Faculty of Physics of the University of Warsaw under the supervision of Prof. D. Sc. Michał Tomza. The thesis describes the modeling and analysis of collisions in ultracold systems consisting of ions and atoms.
The contributions of the author have been essential for the successful realization of two landmark experiments:

- The experiment conducted in Amsterdam with Ytterbium ions and Lithium atoms demonstrates the successful buffer gas cooling of a single ion in a Paul trap down to the quantum regime [1].
- In the experiment conducted in Freiburg with Barium ions and Lithium atoms it was shown that it is possible to observe and manipulate Feshbach resonances between a single ion and ultracold atoms [2].

The calculations done by the author have been essential for guiding the experiments and in the interpretation of the results.
Parts of the results have been published in two articles:

[1] T. Feldker, H. Fürst, H. Hirzler, NV Ewald, M. Mazzanti, D. Wiater, M. Tomza, R. Gerritsma, "Buffer gas cooling of a trapped ion to the quantum regime", Nature Physics 16, 413–416 (2020).
[2] P. Weckesser, F. Thielemann, D. Wiater, A. Wojciechowska, L. Karpa, K. Jachymski, M. Tomza, T. Walker, T. Schaetz, "Observation of Feshbach resonances between a single ion and ultracold atoms", Nature 600, 429–433 (2021).

It should be mentioned that the two articles are published in the journals Nature and Nature Physics. Both journals are among the highest ranked journals in Physics.

Content and contributions of the work

The thesis is written as a monography. It starts with two chapters (Chapters 1 and 2) about ultracold atoms and ions and their interactions. This part describes the physical background and sets the motivation behind the choice for the two ion-atom systems (Yb^+ / Li and Ba^+ / Li), that are considered in this thesis. In addition the construction of potential energy curves and the main concepts from quantum scattering theory, including Feshbash resonances, are described.

The next three chapters (Chapters 3 - 5) are devoted to the description of the experimental techniques for cooling atoms and ions and more specifically to the experimental setups in Amsterdam (Yb^+ / Li system) and Freiburg (Ba^+ / Li system).

The largest part of the thesis (Chapters 6 - 8) describes of the calculations done by the author and presents the results. This part contains a lot of material which is not included in the two manuscripts, but which has been important for conducting the experiments in Amsterdam and Freiburg.

Chapter 6 is devoted to study of buffer gas cooling in the system Yb^+ / Li to the quantum regime. Parts of this project are published in manuscript [1]. The main result of this project is the determination of the spin-exchange rate as a function of the collision energy, which is presented in Figure 40. The figure shows a good agreement between the experimental results from the Amsterdam group and the theoretical results, which were obtained by the author. In the classical regime the rate should be independent from the energy. However, the rate shows a strong dependence on the collision energy. This can be considered as a proof, that the system is in the quantum regime. The calculation of the rate is not trivial, because it is very sensitive to the values of the singlet and triplet scattering lengths and the number of Langevin collisions. An additional difficulty is that the results from ab initio calculations are not accurate enough. The author found an elegant solution to this problem by a careful χ^2 analysis and convolution with the energy distribution of the ions. In addition the author calculated the dependence of the position of the Feshbach resonances on the strength of the magnetic field. The part about the Feshbach resonances is not included in manuscript [1].

Chapter 7 shows the investigations of the Feshbach resonances in the system Ba^+ / Li. Parts of this project have been published in manuscript [2]. Figure 85 shows the detection of Feshbach resonances as a function of the magnetic field. The experimental results have been obtained by the group in Freiburg using ion-loss spectroscopy. The author computed the position of four s-wave resonances. These are in very good agreement with the experiments. The experiments show additional resonances, which were not further assigned. For the estimation of the Feshbach resonances the author computed the hyperfine structure of Ba^+ / Li mixtures and spin-orbit couplings. Furthermore he constructed the potential energy curves and performed quantum scattering calculations and determined the position of Feshbach resonances and bound states.

In Chapter 8 the author derives the equations for the analytic calculation of atom-molecule collisions with the help of pseudo-potentials. Unfortunately this chapter is not written in a clear way. Many symbols in the equations are not explained. The cited literature in this chapter deals only with atom-atom interactions, but not with atom-molecule interactions. In addition it seems that the author neglects all internal degrees of freedom of the molecule (for example: electronic, vibrational and rotational state). However, the equations in this chapter are useful for general potentials with anisotropic parts.

The thesis ends with a summary in Chapter 9 and four appendices, which contain additional derivations for Chapter 8.

Summary assessment

Mr. Dariusz Wiater made significant contributions to two important publications in the field of ultracold ion-atom systems. His calculations made it possible that the quantum regime has been reached for an ion in a buffer gas in the experiments, which were conducted in Amsterdam [1]. Furthermore his calculations has been essential in the search for Feshbach resonances in the experiments on a single Barium ion in a ultracold gas of Lithium atoms, which were conducted in Freiburg [2]. In addition the calculations by Mr. Wiater have been important in the interpretation of the results of both experiments. In summary, this PhD-thesis is excellent.

Mr. Wiater has shown a deep understanding of experimental, theoretical and computational techniques for ultracold systems. The techniques, which were developed by him, can be applied in other emerging fields of Physics, like quantum simulations, quantum computing or the investigation of quantum gases.

I suggest to award Mr. Dariusz Wiater the PhD degree on summa cum laude level (with highest distinction).

Jan Franz

Jan Franz, Gdańsk, 6. February 2023