Master 2: *International Centre for Fundamental Physics*

INTERNSHIP PROPOSAL

(One page maximum)

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Thesis possibility after internship: YES
Funding: Not yet; If YES, which type of funding:ED Paris-Saclay

The statistics of ultracold chemical reactions

Summary (half a page maximum)

New advances in producing and trapping species at temperatures below 1 mK have made ultracold chemistry a reality. For the first time, we can explore reactions in the regime where resonances, tunnelling, quantum degeneracy and other quantum effects dominate the dynamics. In addition, external fields may be used to favour or disfavour typical and exotic reaction mechanisms, to "tailor" interactions and study the consequences of confinement upon reactivity. A series of exciting experiments at JILA, Colorado, started addressing many of these issues [1], while Quéméner and Bohn [2], Idziaszek *et al.* [3] and Gao [4] developed quantum models for interpreting the observed reaction rates.

The most important open question is that of product-state distributions. These are far more sensitive than reaction rates to the details of the reaction dynamics, and provide a deeper understanding of the underlying physics. Rigorous quantum-mechanical calculations [5] are impractical for most cases of interest. This is partly due to the huge number of states involved in low-energy collisions [6]. There is, however, a more fundamental reason for this: Ultracold reactions span the most widely-different energy, length and time scales explored in chemistry to date, and hence pose an unprecedented challenge to chemical collision theory. We recently exploited these scale differences to connect statistical theories [7] and ultracold collision theory [8] into a framework for calculating statistical product-state distributions for ultracold reactions in fields (see link in Ref. [9]); we call it the *statistico-dynamical approach* (SDA) [9].

The goal of this project is to develop and use SDA to solve exciting new challenges in ultracold chemistry. We will focus on two key objectives: (1) To develop a new SDA formalism for many-body capture problems; and (2) To study ion-neutral reactions. The student will learn about ultracold physics and the statistical formalism, and how to use the STATFIELDS program [10] to calculate statistical properties for prototypical ultracold reactions. Successful achievement of these goals will lead to high-impact publication(s) in international journals.

Good knowledge of *Atomic and Molecular Physics* is required, knowledge of *Reaction Dynamics* is a plus. Good programming skills (*e.g.*, Fortran, C/C++, Python) are desirable.

[1] S Ospelkaus *et al. Science* **327**, 853 (2010); K-K Ni *et al. Nature* **464**, 1324 (2010); MHG de Miranda *et al. Nat. Phys.* **7**, 502 (2011)
[2] G Quéméner and JL Bohn *Phys. Rev. A* **81**, 022702 (2010) ; *ibid*, *Phys. Rev. A* **81**, 060701(R) (2010)
[3] Z Idziaszek and PS Julienne *Phys. Rev. Lett.* **104**, 113202 (2010) ; Z Idziaszek *et al. Phys. Rev. A* **82**, 020703 (2010)
[4] B Gao *Phys. Rev. Lett.* **105**, 263203 (2010) ; B Gao *Phys. Rev. A* **83**, 062712 (2011)
[5] TV Tscherbul and RV Krems *J. Chem. Phys.* **129**, 034112 (2008)
[6] M Mayle, BP Ruzic and J. L. Bohn *Phys. Rev. A* **85**, 062712 (2012); M Mayle *et al. Phys. Rev. A* **87**, 012709 (2013)
[7] W Hauser and H Feshbach *Phys. Rev.* **87**, 366 (1952); WH Miller *J. Chem. Phys.* **52**, 543 (1970)
[8] RV Krems, B Friedrich and WC Stwalley, eds., *Cold Molecules: Theory, Experiment, Applications* (Taylor & Francis, London, 2009)
[9] ML González-Martínez, O Dulieu, P Larrégaray and L Bonnet *Phys. Rev. A* **90**, 052716 (2014);see http://community.dur.ac.uk/m.l.gonzalez-martinez/files/downloads/2014_mlgm_CCMI_Reactions_poster.pdf
[10] ML González-Martínez; STATFIELDS computer program, version 0.9 (2015)

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: NO Macroscopic Physics and complexity: NO
Quantum Physics: YES Theoretical Physics: YES