PROGRAMME INTITUTS ET INITIATIVES

Appel à projet – campagne 2021

Proposition de projet de recherche doctoral (PRD)

IPhyInf - Initiative Physique des infinis

Intitulé du projet de recherche doctoral (PRD): Study of many-body dynamics in ion-ion collisions: a joint experimental and theoretical investigation

Directeur.rice de thèse porteur.euse du projet (titulaire d'une HDR) :

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Unité de Recherche :
Intitulé : Institut des NanoSciences de Paris
Code *(ex. UMR xxxx)* : UMR 7588

École Doctorale de rattachement de l'équipe (future école doctorale du.de la doctorant.e) : **ED564-Physique en IdF**

Doctorant.e.s actuellement encadré.e.s par la.e directeur.rice de thèse (préciser le nombre de doctorant.e.s, leur année de 1e inscription et la quotité d'encadrement) : aucun

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Intitulé : LCPMR
Code *(ex. UMR xxxx)* : UMR 7614

École Doctorale de rattachement : **ED388-ChimiePhysiqueChimieAnalytique ParisCentre**
Ou si ED non Alliance SU :

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Co-encadrant.e :

NOM : Prénom :
Titre : Choisissez un élément : ou HDR ☐
e-mail :

Unité de Recherche :
Intitulé :
Code *(ex. UMR xxxx)* :

École Doctorale de rattachement : **Choisissez un élément :**
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Study of many-body dynamics in ion-ion collisions: a joint experimental and theoretical investigation

Context

The understanding of energy transfer in various plasmas like stellar/interstellar plasmas, inertial confinement fusion plasmas, or, more generally, in ion-(hot or cold) matter interaction is a subject of interest since several years. The fundamental electronic mechanisms involved (such as loss / capture of electrons and excitation) play obviously a major role but their cross sections are notably lacking in the so-called intermediate velocity regime; a regime where the ion stopping power is at its maximum (the so-called Bragg's peak) leading, consequently, to the strongest effects in the irradiated matter. There, the most sophisticated theoretical calculations are at their limit of validity and no measurements are available. A significant test of theories can only be performed if the presence of numerous electrons can be avoided (beside the simplest case of a proton on hydrogen collision). Alternatively, the effect of other electrons participating to the processes must be explored. Such goals can only be achieved through ion-ion collision experiments with an ultimate control of the charge state of both ion beams (i.e. the number of electrons initially bound to each ion).

In this context and with the avenue of new generation accelerator facilities, the ASUR (*Agrégats et SURfaces sous excitations intenses*) team at INSP leads a Franco-German collaboration[1], named FISIC (**Fast Ion - Slow Ion Collisions**) for the development of an experimental program [1]. The intermediate velocity regime is reached when MeV/u ions collide with keV/u ions. We have then proposed a unique experimental crossed-beam arrangement for a wide range of collision combinations (in terms of atomic numbers and charge states) with an ultimate control of experimental conditions to measure absolute cross-sections of electronic processes. The goal of this experiment is to span from a pure three-body (a bare ion and a hydrogenic one) to a N-body problem with given charge states and electronic configurations of both ions. A systematic investigation as a function of the number of electrons and through iso-electronic series will allow studying in details various aspects of the dynamics, such as the effects of the inter-electronic interaction and its complementary role with nuclear attraction. From the theoretical side, the prediction of cross sections in the energy regime under consideration requires non-perturbative treatments of the electronic dynamics that imply close-coupling methods taking into account all couplings as well as interference effects between the different channels. In that respect, an emerging collaboration is taking place with the LCPMR and more precisely with A Dubois from the team "*Evolution temporelle de systèmes quantiques en champs intenses*"**.**

The doctoral project presented here is at the heart of this nascent collaboration between two laboratories – INSP (UMR 7588 UFR de Physique) and LCPMR (UMR 7614 UFR de Chimie) – of Sorbonne University.

Scientific approaches and objectives

The project presents two complementary components, with an experimental part of instrumental development and measurements, and a theoretical part for the feasibility proposal for collision systems and the interpretation of experimental campaigns.

Crossing two ion beams, under well controlled conditions, has always been a very challenging task, whatever the domain of physics under consideration. Indeed, many barriers have to be overcome like the charge state control of both ion beams, the control of the overlap between the two ion beams, the design of the collider chamber, the ultra-high vacuum conditions (10^{-11} mbar), the detection of the

[1] CIMAP (Caen), GANIL (Caen), GSI (Germany), Giessen University (Germany), Jena University (Germany) and INSP (Paris)

product ions and a fast acquisition system for coincidence measurements. The ASUR and its collaborators develop a dedicated platform, the low-energy FISIC platform designed to be easily transportable, that will provide a large variety of keV/u ion beams with a perfect control of their charge state from H to Xe. This platform must also easily connect to existing ion installations such as the SIMPA platform[2] at INSP that delivers keV/u ion beams and the CRYRING[3] storage ring at FAIR/GSI (Darmstadt) for MeV/u ion beams. The FISIC platform is divided into two parts. The first one, upstream the collision zone, is equipped with an ion source connected to a beam transport line well-adapted to shape the beam and clean it from the non-desired charge state thanks to a purification system recently developed [2]. This beam line has already been tested successfully [3] and the ion source is expected to be delivered beginning 2022.

From the experimental point of view, the doctoral project concerns mainly the development of the second part of the FISIC platform that includes the collision chamber and an ion spectrometer. Ion trajectory simulations [4] have already been performed but further investigations are needed to complete the final design. For instance, the crossing point of the two ion beams has to be surrounded by a metallic interaction zone which can be put on high voltage to energetically ‘tag’ the product ions issued from the true ion-ion collision events so as to eject signals from ion-residual gas interactions. The last functional unit of the platform is an ion spectrometer to separate the different ion charge states originating from the ion-ion collisions. This will be accomplished by a 90° electrostatically cylindrical deflector which guides the product ions and the initial ion beam toward a position sensitive detection system. Very recently this ion spectrometer has been manufactured and a first version of a detection system has been tested on the SIMPA facility in July 2020. To fully validate this ensemble, beam time was recently obtained on ARIBE/GANIL[4] in close collaboration with the CIMAP laboratory at Caen.

As soon as the different elements will be ready, the complete FISIC platform from the ion-source up to the low-energy ion spectrometer will be tested in real conditions by performing ion-ion collisions first in the keV/u energy collision domain. Indeed, the FISIC platform will be connected to the existing SIMPA platform. Beyond the possibility of testing and characterizing the FISIC platform, we will be able to obtain novel results with multi-charged ions (with one or two electrons) of light to medium atomic numbers (Z=1, 6 and 18 scheduled for the first campaigns). In the longer term, the platform can be moved on CRYRING for the first measurements in the high-energy domain.

The theoretical and numerical simulation component of our project concerns the modeling of electronic processes within the framework of a non-perturbative semi-classical approach: the relative motion between nuclei target and projectile is described classically while the electronic dynamics are treated by solving the time dependent Schrödinger equation (TDSE). This approach makes possible to deal with collisions in a very wide range of energy impact, typically from 0.1 to 2000 keV/u and in the close-coupling regime, i.e. when the processes of capture, excitation and ionization are likely and strongly coupled. The originality of the code lies in the possibility of having up to four active electrons and of considering *ab initio* the coulombic electronic repulsion in a static and dynamic "configuration interaction" approach. This permits at the same time to overcome approximations such as "independent electrons", "independent events" and methods with pseudopotential or model potential but also to test them when they are becoming unavoidable as soon as *ab initio* approaches are too demanding in computing resources.

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[2] SIMPA (Source d’Ions Multichargés de Paris): http://www.insp.upmc.fr/-La-source-d-ions-muticharges-de,421-.html
[3] CRYRING storage ring: https://www.gsi.de/work/forschung/appamml/atomphysik/anlagen_und_experimente/cryringesr.htm
[4] ARIBE: http://cimap.ensicaen.fr/spip.php?rubrique153

In the framework of this project, and before the experiments at CRYRING in Germany, we may consider quasi-symmetrical ion-ion systems as benchmarks with 1, 2 or 3 active electrons, located on one or both centers in the keV/u regime where the LPCMR team has a long expertise [5-7]. Very recently, this approach has demonstrated its versatility and reliability for ion-ion systems and for multi-charged ionic projectiles [8-10] in the MeV energy domain. The work of the doctoral student would not only be to use the adequate code available in the group but also to develop small codes (i) to build the bases of atomic states necessary for the description of the systems (crucial phase of our calculations) and (ii) for the interpretation of the experimental results. After normal initial training, the first task of the student will be to investigate – prior to experiments – the first collision systems envisioned experimentally.

Finally, this doctoral project will benefit from a new collaboration between two SU teams from two different UFR. The integrated experiment-theory approach can have its limits but is an essential tool in current scientific activity. It will enrich the experience and expertise of each team while giving the doctoral student a double competence.

Relevance to IPI's theme

With the FISIC platform under consideration in this application, we propose to perform ion-ion experiments in a hitherto unexplored collision regime, where the ion stopping power is maximum, to measure absolute cross sections of electronic processes. These processes are responsible for the ion energy transfer into stellar/interstellar plasmas and also in inertial confinement fusion plasmas.

The platform FISIC will be also valuable to determine astrophysical nuclear reactions at CRYRING between bare ions avoiding hence the potential effect of the electron screening. In consequence, the FISIC collaboration has been recently enlarge to the community of astrophysical nuclear physics[5].

Role of the two project leaders

E Lamour and A Dubois will equally (50%-50%) supervise the doctoral project.

E Lamour is used to performed experiments on large scale facilities such as GANIL and GSI and is responsible for the SIMPA platform at INSP where the low-energy FISIC beam line is already running. She will take care of the new ion source that will be mounted and tested in 2022. She is the scientific coordinator of the FISIC collaboration and is in close contact with the atomic physics group of CRYRING/FAIR/GSI installation.

A Dubois is one of the co-authors of several original codes to solve the TDSE non perturbatively for atomic collisions. He has a long expertise in the modeling of electronic processes for collisions between weakly charged ions and/or low-Z atoms or molecules. He has also already started investigating the MeV energy range for which he is developing further the codes. He will be in charge of the theoretical and numerical training of the student and will supervise the computational investigations.

Related publications

[1] F. Aumayr, K. Ueda, E. Sokell, S. Schippers, H. Sadeghpour, F. Merkt, T. Gallagher, B. Dunning, P. Scheier, Olof Echt, T. Kirchner, S. Fritzsche, A. Surzhykov, X. Ma, R. Rivarola, O. Fojon, L. Tribedi, **E. Lamour**, J. R Crespo López-Urrutia, Y. A Litvinov, V. Shabaev, H. Cederquist, H. Zettergren, M. Schleberger, R. A Wilhelm, T. Azuma, P. Boduch, H. T Schmidt and T. Stöhlker; *Roadmap on photonic, electronic and atomic collision physics: III. Heavy particles: with zero to relativistic speeds - Chapter 3 - Collisions involving heavy projectiles;* J. Phys. B: At. Mol. Opt. Phys. 52 171003 (2019).

[5] Collaboration with C.G. Bruno et al from the *School of Physics and Astronomy, University of Edinburgh.*

[2] D. Schury, A. Kumar, A. Méry, J.-Y Chesnel, A. Lévy, S. Macé, C. Prigent, J-M Ramillon, J. Rangama, P. Rousseau, S. Steydli, M. Trassinelli, D. Vernhet, and **E. Lamour**; *An electrostatic in-line charge-state purification system for multicharged ions in the kiloelectronvolt energy range;* RSI 90, 083306 (2019).

[3] D. Schury, A. Méry, J.M Ramillon, L. Adoui, J-Y Chesnel, A. Lévy, S. Macé, C. Prigent, J. Rangama, P. Rousseau, S. Steydli, M. Trassinelli, D. Vernhet, A. Gumberidze, T. Steohlker, A. Brauning-Demian, C. Hahn, U. Spillmann and **E Lamour**; *The low energy beamline of the FISIC experiment: current status of construction and performance*; J. Phys.: Conf. Ser.1412 162011 (2020)

[4] A. Kumar, A. Méry, L. Adoui, JY. Chesnel, A. Lévy, S. Macé, C. Prigent, J.M. Ramillon, J. Rangama, JP. Rozet, P. Rousseau, S. Steydli, M. Trassinelli, D. Vernhet and **E. Lamour**; *Numerical simulations of purification and final charge state analysis of the slow ion beam for the FISIC project;* Journal of Physics: Conf. Series 875 (2017)

[5] J.B. Wang, J.P. Hansen, and **A. Dubois**; *Spin anisotropy for excitation in collisions between two one-electron atoms;* Phys. Rev. Lett. 85, 1638-1641 (2000).

[6] J. Caillat, N. Sisourat, **A. Dubois**, I. Sundvor, and J.P. Hansen; *On orientation effects in He2+ − H2+ collisions at intermediate collision energies;* Phys. Rev. A, 73, 014701/4 (2006).

[7] N. Sisourat, J. Caillat, **A. Dubois**, and P. D. Fainstein; *Coherent electron emission from H2 molecules induced by swift ion impact;* Phys. Rev. A 76, 012718/9 (2007).

[8] J.W. Gao, Y. Wu, JG. Wang, **A. Dubois**, and N. Sisourat; *Double electron capture in H+ + H- collisions;* Phys. Rev. Lett. 122, 093402/5 (2019).

[9] I. Madesis, A. Laoutaris, T.J.M. Zouros, E.P. Benis, J.W. Gao, and **A. Dubois**; *Pauli shielding and break-down of spin statistics in multi-electron, multi-open-shell dynamical atomic systems*; Phys. Rev. Lett. 124, 113401/7 (2019).

[10] T. J. M. Zouros, S. Nikolaou, I. Madesis, A. Laoutaris, S. Nanos, A. Dubois, and E.P. Benis; *Radiative cascade repopulation of 1s2s2p 4P states formed by single electron capture in 2-18 MeV collisions of C4+(1s2s 3S) with He;* Atoms 8, 61/21(2020).