A SINGLE ION IMMERSED IN AN ULTRACOLD GAS: FROM COLD CHEMISTRY TO IMPURITY PHYSICS

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A single ion in an ultracold gas is a versatile experimental platform to study interactions between charged and neutral particles in a controllable manner. When the gas density is large enough, a single ion can be viewed as an impurity in a sea of ultracold atoms or molecules. On the other hand, that single ion can also undergo a chemical reaction with atoms or molecules in the gas. This article discusses the dynamics of a charged impurity in an ultracold bath and the interplay between cold chemistry and impurity physics.

Co-trapping charged and neutral particles to sub-Kelvin temperatures brings a plethora of well-controlled scenarios in which interactions between charged and neutral particles can be studied and efficiently controlled [1,2]. As a result, in recent years, atomic, molecular, and optical physics has experienced a revolution around those experimental platforms paving the way for a new field of research: cold chemistry, *i.e.*, the study of chemical reactions at temperatures $\lesssim 1\mathrm{K}$ [1]. In the same vein, those systems provide a new avenue to study impurity physics in which the ion is considered an impurity in a bath of ultracold gas, either atomic or molecular.

When an ion approaches an atom or a molecule, the electric field of the ion induces a dipole moment on the neutral system, leading to a characteristic interaction potential, $V_{\mathrm{cn}} \propto R^{-4}$, where R is the atom-ion distance. This interaction has a longer range than the van der Waals dispersion force between neutral systems. A longer-ranged interaction translates into a larger characteristic length scale, approaching the typical interparticle distances in ultracold gases leading to the formation of a charged polaron [3], in which the ion is dressed with a cloud of virtual phonons or collective excitations of the gas. Similarly, a single ion in an ultracold bath can bind to several particles of the bath. It thus forms a mesoscopic molecular ion that can be regarded as a many-body bound state, *i.e.*, a cluster-like structure whose properties rely on an exchange of atoms from the bath [4].

From a few-body perspective, longer-ranged interactions result inexorably in larger collisional cross sections and thereby a more significant reaction rate. In other words, charged-neutral reactions are faster than neutral interactions under the same temperature, pressure, and density conditions. Consequently, despite being many-body systems, charged polarons and mesoscopic molecular ions are definitively affected by charged-neutral chemical reactions, *i.e.*, few-body processes.

A single ion in an ultracold atomic bath

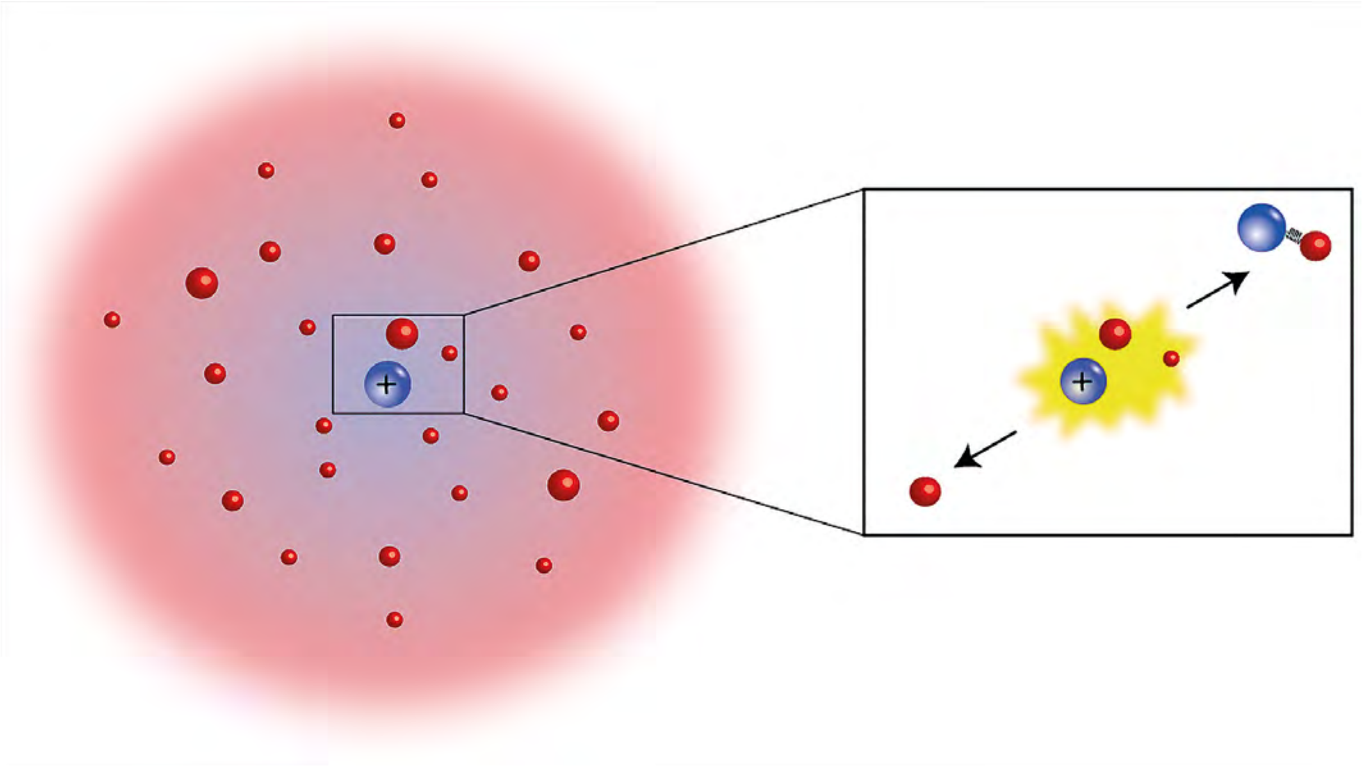
An ion A^+ reacts with the atoms of the atomic gas via ion-atom-atom three-body recombination (ternary association in chemistry): a three-body process in which two colliding partners combine into a bound molecule, as shown in Fig.1. There are two reaction products. One leads to the production of a molecular ion as

$$A^+ + B + B \rightarrow AB^+ + B, \qquad (1)$$

and another leads to the formation of a neutral molecule given by

$$A^+ + B + B \rightarrow B_2 + A^+. \qquad (2)$$

The formation of molecules via three-body recombination, either ionic or neutral, occurs in the short-range region where chemistry takes place. However, since the



▲ FIG. 1: A single ion in an ultracold atomic bath forms a charged polaron sketched by the blue cloud around the ion that identifies the portion of the bath directly affected by the ionic impurity. However, from a few-body perspective, the ion reacts with the particles or the gas via three-body recombination, shown in the zoom-in, with the subsequent formation of new reaction products.

charged-neutral interaction is longer-ranged than the van der Waals interaction, as shown in Fig.2, ion-atom-atom three-body recombination preferably forms molecular ions as a reaction product and its rate shows the temperature dependence as $k_3 \propto T^{-3/4}$ [5,6], which has been experimentally confirmed [7,8].

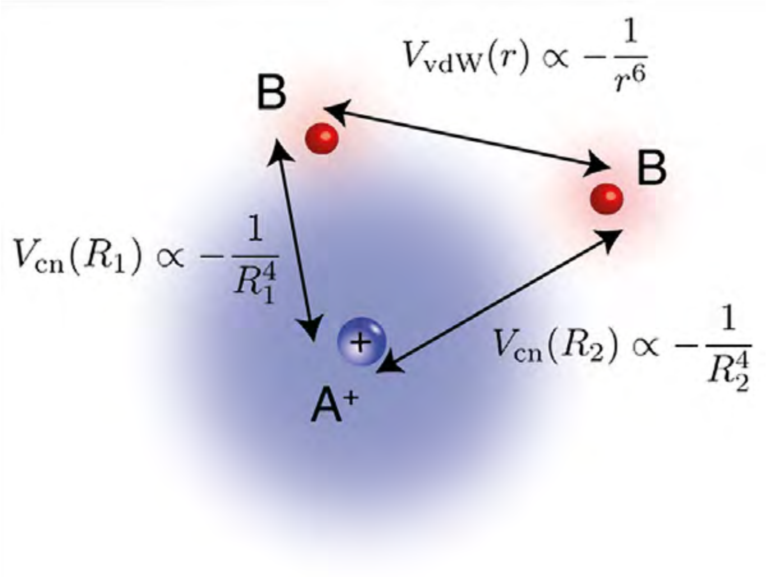
In many-body systems, reactive channels due to few-body processes may be considered decay channels when the particle treated as an impurity changes its nature as a result of the reaction, as is the case for ion-atom-atom three-body recombination. Every decay process has a characteristic lifetime, *i.e.*, the typical time-scale for the process to occur. In particular, the collision time gives the lifetime of the many-body decay channel: the typical time it takes the colliding bodies to reach the short-range region to react. For example, it is ~100μs for typical experimental conditions in atom-ion hybrid trap experiments [9].

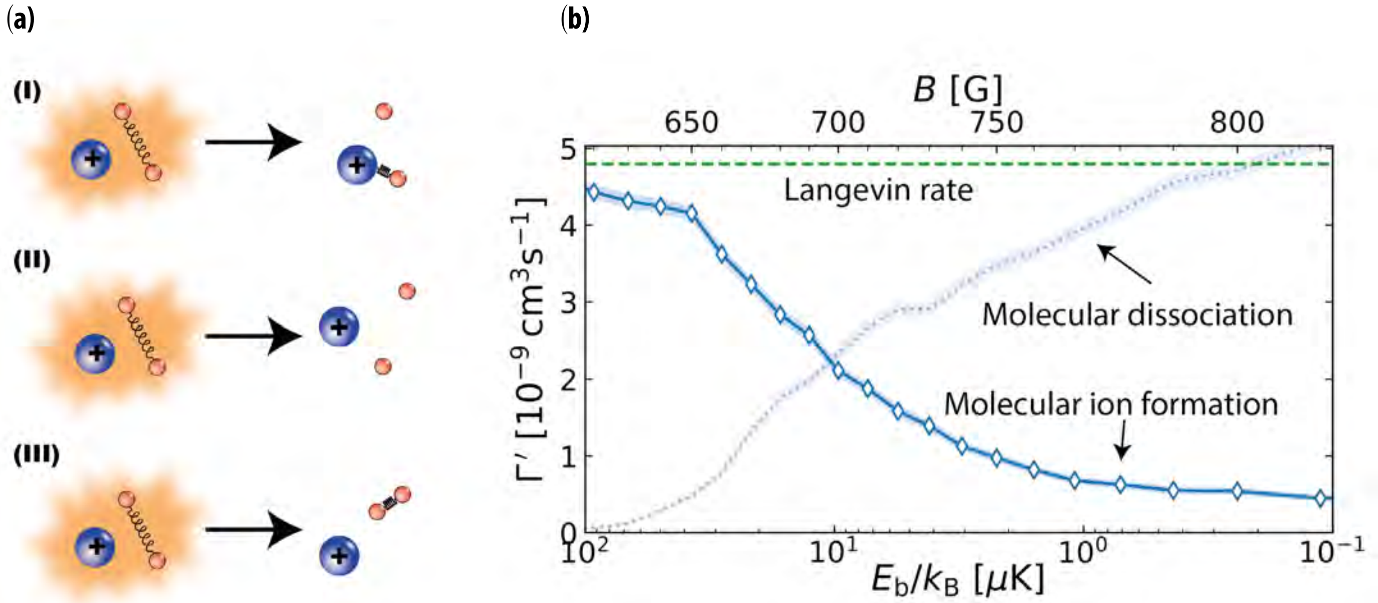
A single ion in an ultracold molecular bath

When a single ion is brought into contact with an ultracold gas of molecules, the ion can be considered an impurity in a bath with internal degrees of freedom. As a result, new and intriguing many-body phenomena may occur. Nevertheless, very little has been developed in this direction. On the contrary, such a scenario has been studied theoretically and recently experimentally from a few-body perspective [11].

An ion interacting with a molecule could react to form a molecular ion, as depicted in panel (I) of Fig.3. Furthermore, at energies above the binding energy of the molecule, the ion may dissociate the molecule, as depicted in panel (II) of Fig.3. Finally, the ion may induce a change in the internal state of the molecule, known as vibrational quenching, as shown in panel (III) of Fig.3. However, at temperatures $\lesssim$ 1 mK, vibrational ● ● ●

▼ FIG. 2: Ion-atom-atom three-body interactions. The shaded blue represents the characteristic length scale for charged-neutral interactions, whereas the red color stands for van der Waals interactions. reaction products.





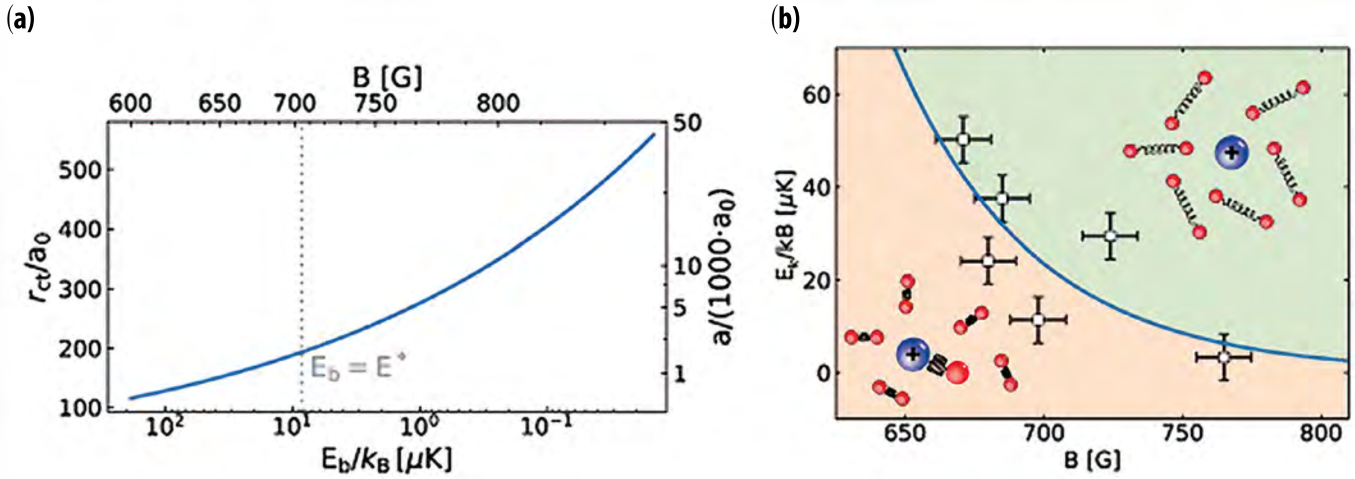
▸ **FIG. 3:** Few-body dynamics of an atomic ion colliding with a molecule. Panel (a) shows the possible reaction channels: (I) molecular ion formation; (II) molecular dissociation; (III) vibrational quenching. Panel (b) shows the reaction rate for the molecular dissociation and the molecular ion formation channel as a function of the binding energy in units of temperature (kB is the Boltzmann constant). The reaction is for Yb^+ interacting with a Li_2 molecule at a collision energy of 11 µK. The green-dashed line depicts the Langevin rate. Figure adapted from Ref. [10].

quenching is negligible due to the dominant nature of charged-neutral interactions. Therefore, there are only two possible outcomes: a molecular ion or two atoms and one free ion.

The relevance of each of these reaction products for a given collision energy depends on the molecular binding energy, as shown in panel (b) of Fig.3 for Yb^+-Li_2 collisions. In particular, the dominant reaction channel is molecular ion formation for deeply bound molecules (in comparison to the collision energy), whereas for weakly bound molecules molecular dissociation is the most relevant reaction channel [10]. Furthermore, the molecular ion formation rate saturates to the Langevin rate (the maximum possible rate for a charged-neutral interaction), which has been experimentally confirmed [11]. Therefore, by tuning the binding energy of the ultracold molecular gas, it is possible to control whether the ion reacts to form a molecular ion or, on the contrary, stays unchanged.

Feshbach molecules are weakly bound molecules whose binding energy depends on the applied external magnetic field, as shown in panel (a) of Fig. 4 for the Li_2 molecules. Therefore, controlling the collision energy and the external magnetic field, it is possible to draw a phase diagram for a charged impurity in an ultracold molecular gas, as shown in panel (b) of Fig.4 for the particular

▾ **FIG. 4:** Panel (a) shows the relationship between the binding energy of the molecule and the applied external field channeled by the presence of a broad Feshbach resonance in Li-Li scattering. Vertical-axes represent the Li-Li scattering length, a, and the classical turning point (the classical size of the molecule), r_{ct}, in atomic units of distance, *i.e.*, Bohr radii, a_0=0.529177×10^{-10}m. Panel (b) shows the "phase-diagram" of a single ion in an ultracold bath of weakly bound molecules. Figure adapted from Ref. [10].



> **As a result, to preserve the charged impurity, we need to have a gas of weakly bound molecules and as large collision energies as possible.**

case Yb^+ in an ultracold gas of Li_2 Feshbach molecules. As a result, to preserve the charged impurity, we need to have a gas of weakly bound molecules and as large collision energies as possible.

Outlook

A single ion in an ultracold gas is a platform to study many-body systems such as charged polarons and mesoscopic molecular ions. However, due to the very reactive nature of ion-atom interactions, it is required to approach the same system from a few-body physics standpoint. Therefore, it is necessary to work synergetically between many-body and few-body physics to reveal the true nature of many-body processes in atom-ion hybrid traps.

About the author

Jesús Pérez Ríos is an Assistant Professor at the Department of Physics and Astronomy of Stony Brook University (USA). His research focuses on the study of fundamental atomic and molecular processes at the interplay between atomic, molecular, and optical physics and other disciplines of physics and chemistry such as high energy physics, condensed matter physics, and chemical physics.

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