# Inelastic collision dynamics of a single cold ion immersed in a Bose-Einstein condensate

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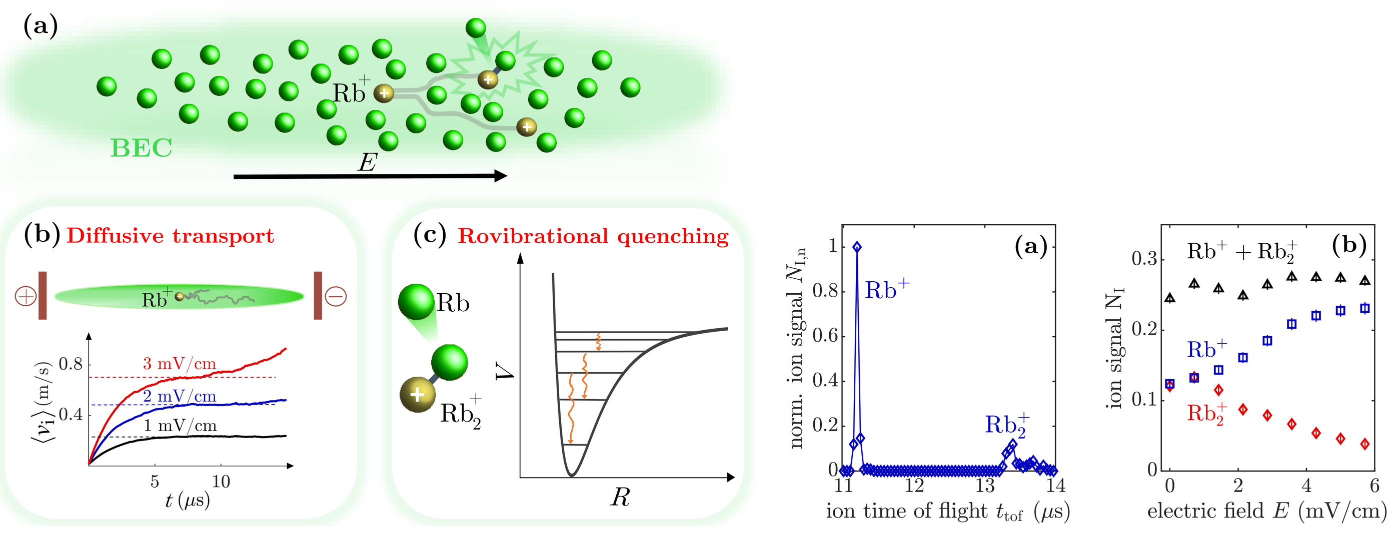
## Abstract

We create a single charged impurity inside a degenerate Bose gas from a single Rydberg excitation ionized by a sequence of fast electric field pulses. Due to high gas density and large ion-atom scattering cross section we can study the regime of frequent collisions and the resulting dynamics within tens of microseconds. In addition to diffusive transport properties we observe inelastic molecular ion formation via three-body recombination. We study the cold chemistry of these events and find evidence for subsequent rovibrational quenching collisions of the produced molecule.

## Hybrid ion-atom systems

- common approach: Paul trap for the ion and optically trapped atoms
- possible to reach $\sim 10-100\mu$K energies
- plenty of rf and optical fields making experiments quite complex
- here: direct production of an ion from a BEC
- Rydberg excitation in Rb gas and subsequent field ionization
- lower initial energy, dense gas, free ion
- very sensitive to stray electric fields



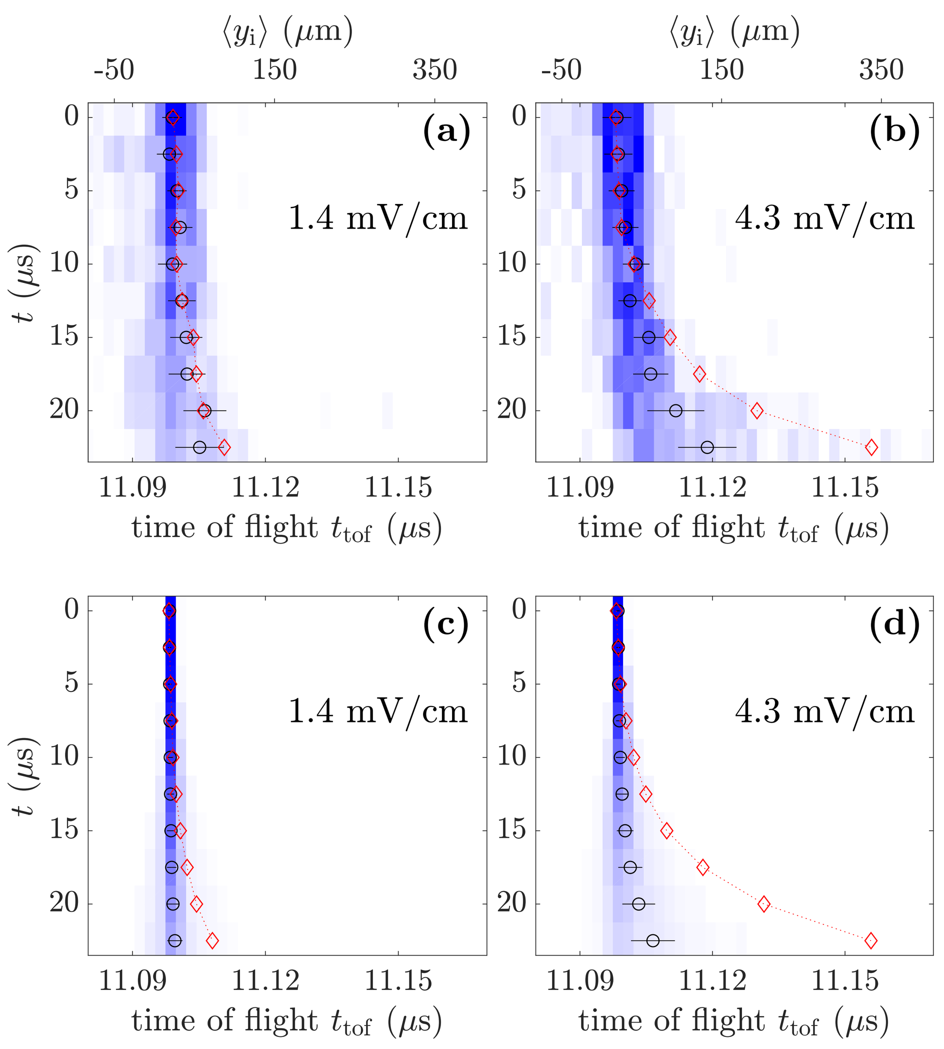

for review of the ion-atom field, see M. Tomza, KJ et al., Rev. Mod. Phys. 91, 035001 (2019)

## Two-body physics

- power-law interaction $V(r) = C_4/r^4$, length scale $R^\star = \sqrt{2\mu C_4/\hbar^2} \sim 1000a_0$, characteristic energy $E^\star = 1/2\mu(R^\star)^2 \sim \mu K$
- extended weakly bound states with $\sim R^\star$ size which can be comparable to the BEC healing length and interparticle distance
- s-wave pseudopotential $V(r) = \frac{4\pi a(k)}{\mu}\delta(r)$ needs to include finite range effects
- semiclassics works pretty well: Langevin collision rate $\gamma_L = 2\pi n\sqrt{C_4/\mu}$
- full differetnial cross sections can be calculated easily

## Stochastic modelling

- characterize the setup (stray fields, ion lens configurations etc) using ballistic reference data
- Monte-Carlo sampling of trajectories
- collisions with density-dependent rate and ballistic motion in between
- semiclassical and quantum cross sections agree
- no fitting parameters; takes into account stray fields and inhomogenous density profile
- disregards inelastic losses and atomic motion




Measured (top) and simulated (bottom) ion arrival times vs the transport time at different two different electric field values

## Field dissociation

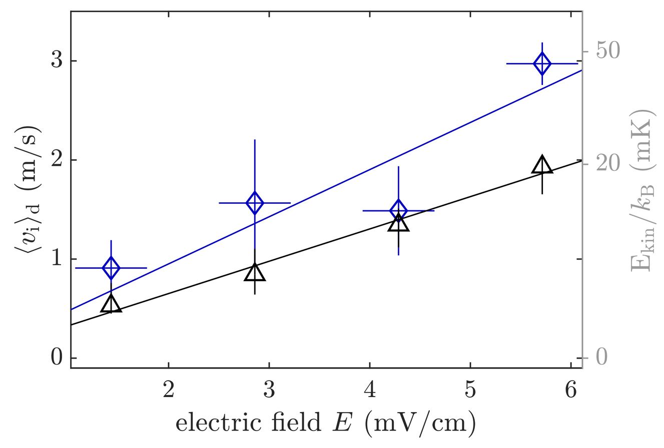
- relating the binding energy and dissociating field
- semiclassical over-the-barrier model

$$V_{\rm tot}(R) = -\frac{C_4}{2R^4} - \frac{1}{2}qE_{ex}R$$

- dissociation enabled if the barrier height is lowered by the field
- average over the orientation and diabatic field ramp (classical trajectory simulations)

## Transport properties

- simulation points to diffusive transport
- extract drift velocity $\langle v\rangle(E)$
- ion mobility $\mu = \frac{\partial\langle v\rangle}{\partial E}$
- exp. result $(47 \pm 16)\cdot 10^3\mathrm{cm}^2/(\mathrm{Vs})$ vs simulated one $(33 \pm 3)\cdot 10^3\mathrm{cm}^2/(\mathrm{Vs})$

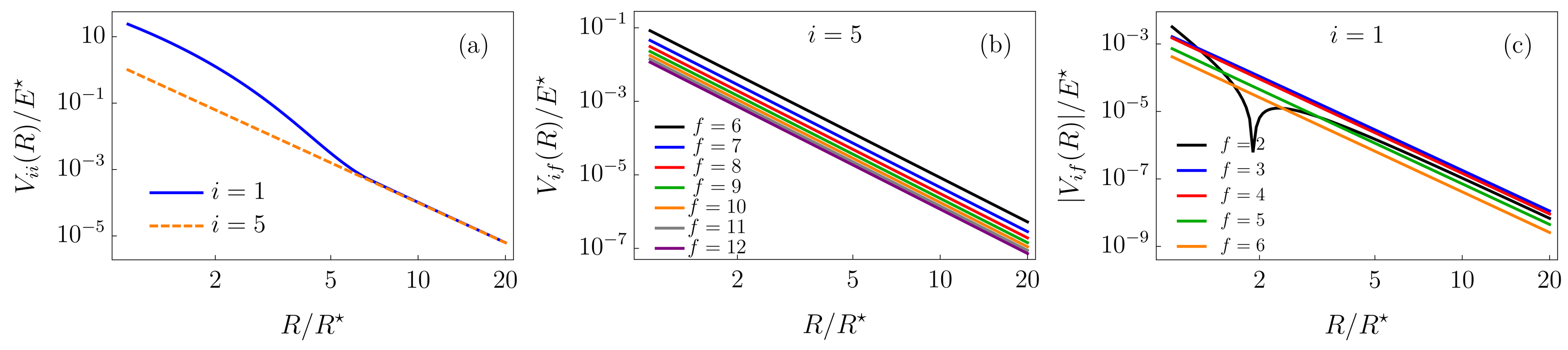



## Atom-molecule collisions

- three-body problem, Jacobi coordinates **r** (internal molecular), **R** (center of mass-to-atom)
- weakly anisotropic three-body potential surface
- decompose into asymptotic channel states with the molecular ion in state $v, j$ and a free atom
- close-coupled equations with interaction potential

$$W_{vj,v'j'}(R) = \left(\frac{2\mu}{\hbar^2}E_{vj} + \frac{\ell(\ell+1)}{R^2}\right)\delta_{vv'}\delta_{jj'} + \frac{2\mu}{\hbar^2}V_{vj,v'j'}(R)$$

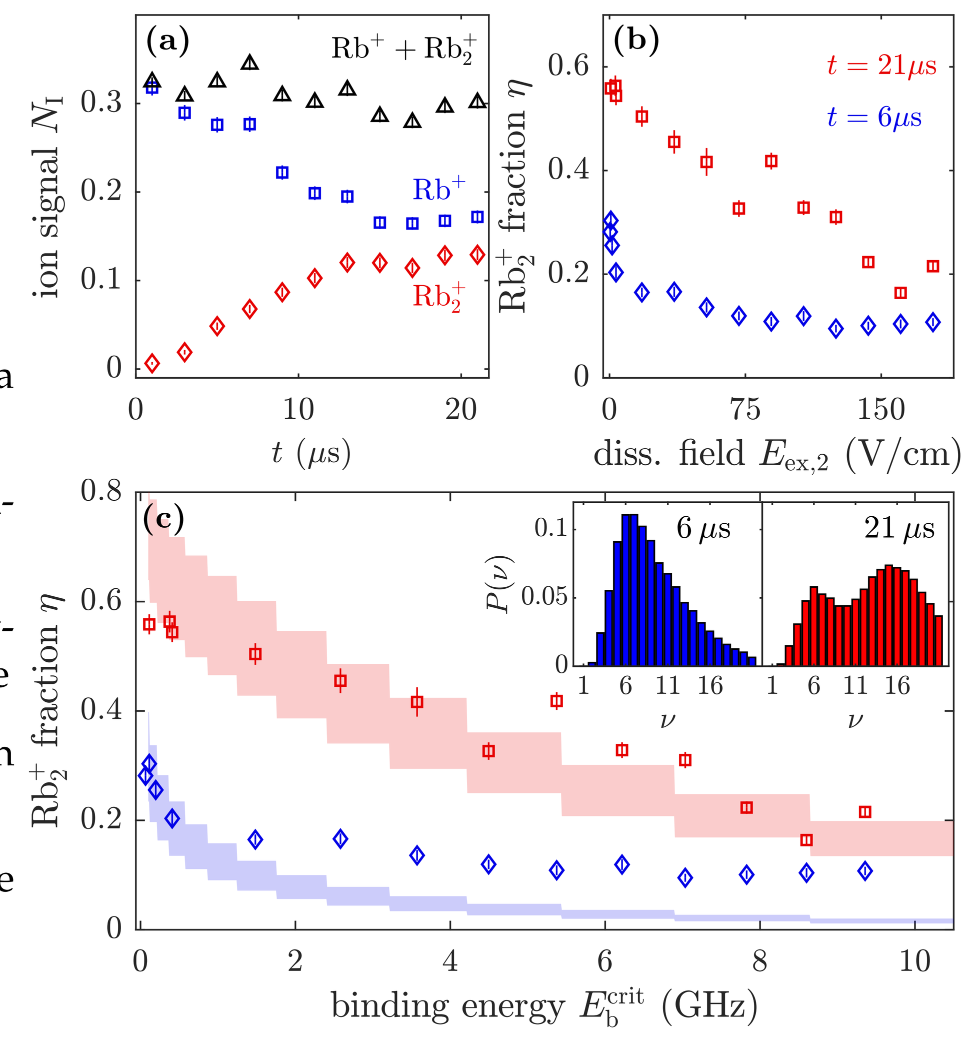
- effective potential asymptotically reaches $1/R^4$ form, off-diagonal couplins generally weak
- calculate the inelastic state-to-state collision rates




Effective atom-molecule potentials. Left: diagonal part for two vibrational states, middle: off-diagonal couplings for the $v = -1$ state, right: same for $v = -5$.

## Vibrational quenching

- three-body recombination creates a molecular ion
- subsequent collisions can change the internal state
- binding energy can be measured by trying to dissociate the incoming molecule
- extended stochastic model with built-in vibrational relaxation
- clear redistribution of vibrational state population




Three-body recombinationand vibrational quenching. (a) $Rb^+$ and $Rb_2^+$signal. (b) Fraction of molecules as a function of the dissociating field. (c) Same as a function of binding molecule energy. Inset: distribution of bound states at two different transport times.

## Outlook

- observation of diffusive dynamics of a charged impurity in a BEC
- formation of weakly bound molecular ions and subsequent vibrationally inelastic collisions
- simple models based on classical trajectories and two-body events
- prospects for strong impurity-medium interactions, polaron physics, controlled ultracold chemistry

Dieterle *et al.* Phys. Rev. A 102, 041301(R) (2020)
Dieterle *et al.* Phys. Rev. Lett. in press
K. Jachymski, F. Meinert, Appl. Sci. 10, 2371 (2020)