Parity-dependent charge exchange in LiBa⁺ experiment

Xiaodong Xing[1], Pascal Weckesser[2], Romain Vexian[1], Ting Xie[1], Nadia Bouloufa-Maafa[1], Tobias Schaetz[2] and Olivier Dulieu[1]

[1] Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, Orsay, 91400, France.

[2] Albert-Ludwigs-Universitt Freiburg, Physikalisches Institut, Hermann-Herder-Strae 3, 79104 Freiburg, Germany.

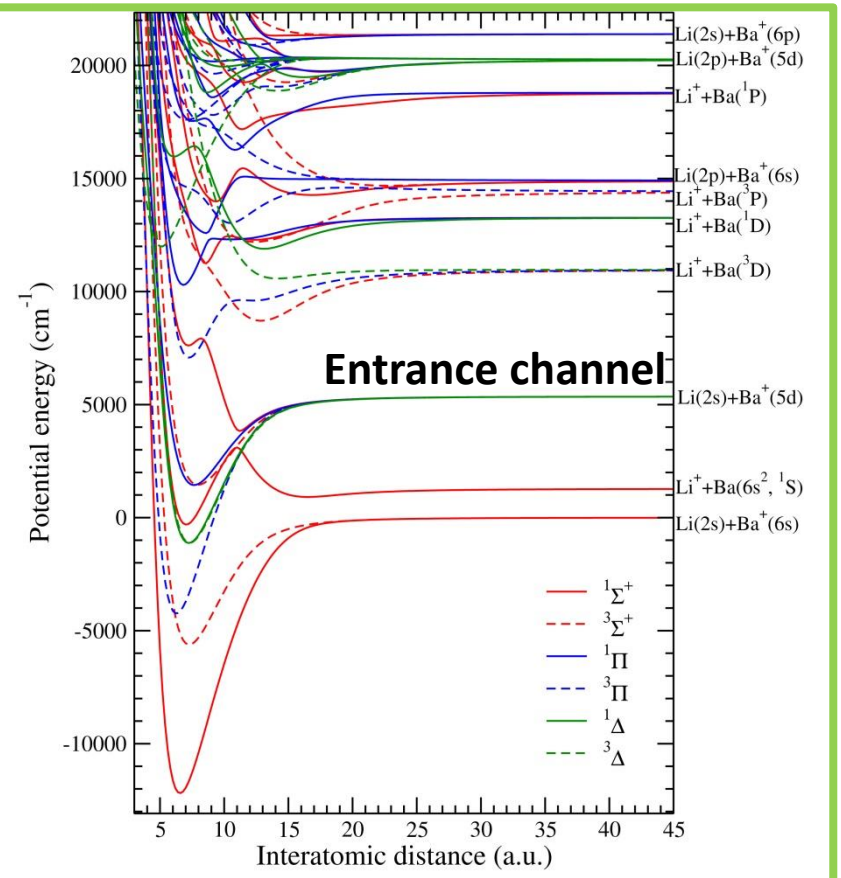
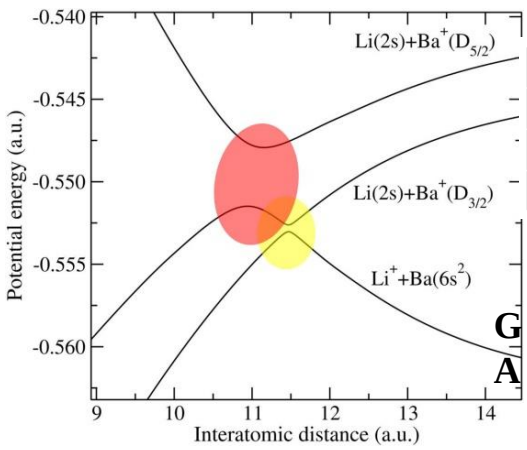


Figure 1: Potential energy surface for LiBa⁺.

Motivation

The charge exchange dynamic is one of the most essential and intuitive chemical reactions in atom-ion experiment [1,2]. In Freiburg, the experimental group build up a new experiment involving polarized ^{6}Li(2*s*) atoms and a single ^{138}Ba$^+$($5d^2D_{5/2;3/2}$) in optical trap and quadrupole trap, respectively. Based on the outcome of the loss events at the entrance $D_{5/2}$, they observe 66(5)% fine structure quenching and 44(5)% non-radiative charge exchange. Regarding the entrance $D_{3/2}$ they obtain 90.6(1.5)% non-radiative or radiative quenching and 9.4(1.5)% non-radiative charge exchange. We have developed several theoretical models of increasing complexity in order to identify the main interactions at play during these processes: a semi-classical Landau-Zener(LZ) model, a few-channel quantum scattering (FCQS) model with spin orbital couplings, and a multi-channel quantum scattering (MCQS) model considering spin-orbit couplings and rotational couplings.

FCQS model



$1^1\sum^+$	0	0	$A_{1,4}$
0	$2^1\sum^+$	$G_{2,3}$	$A_{2,4}$
0	$G_{3,2}$	$3^1\sum^+$	$A_{3,4}$
$A_{1,4}$	$A_{4,2}$	$A_{4,3}$	$1^3\prod + A_{4,4}$

G is R-dependent Gaussian coupling.
A is R-dependent spin orbital coupling

Figure 2: Two strongly coupled avoided crossings at the short range. Diagonalizing this 4 by 4 matrix with relevant coulpings, we find out two close avoided crossings mutually interfere with each other. Due to the fact that LZ model employs a single non-adiabatic region, we build up a 4-channel FCQS model using close coupling theory to calculate the transition cross sections. The total cross sections are computed by the off-diagonal elements of S matrix as a sum over partial waves l:

$$\sigma(E) = \frac{\pi}{k_0^2}\sum_l (2l+1)|S(f \leftarrow i)|^2$$

where $k_0^2 = 2\mu E/\hbar^2$ with reduced mass μ and collision energy E.
i and f note the initial and final states.

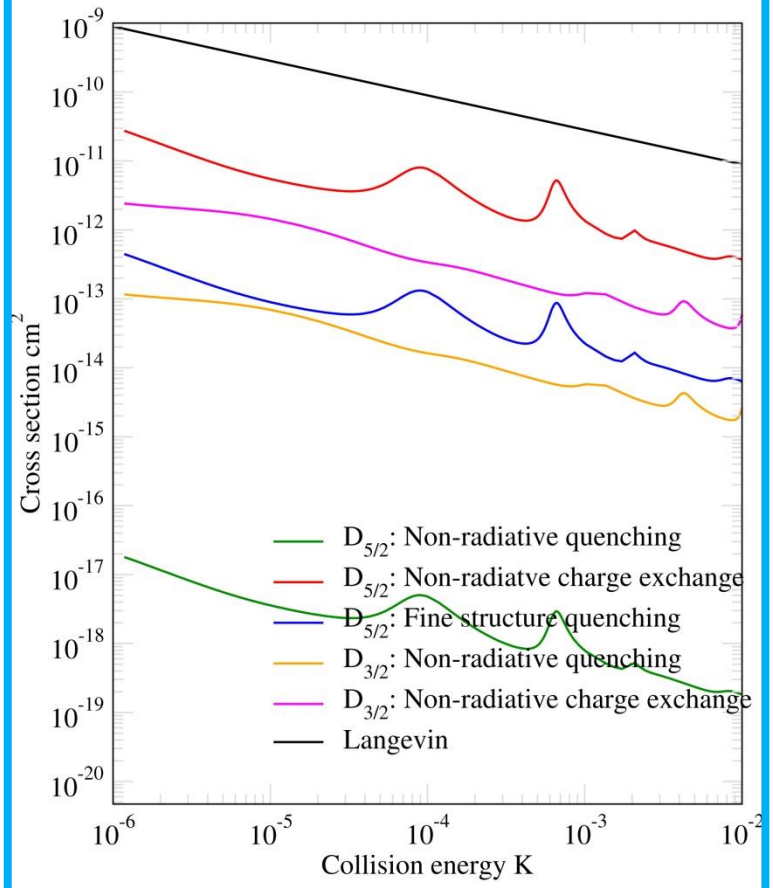


Figure 3: Cross section as a function of the collision energy. In FCQS model, our results show out the non-radiative charge exchange is dominated either in the entrance channel D5/2 or D3/2, which is the contrary of perspectives from experiments.

MCQS model

In the rigorous MCQS model, the full calculation includes the first 3 dissociation limits, 9 molecular states, the relevant R-dependent spin orbital couplings, R-dependent gaussian coupling and the corresponding rotational couplings. Then we can set up a 16 by 16 matrix based on $|\Omega| = 0^+, 0^-$ 1, 2, 3. The rotational coupling elements can be obtained by [3,4]:

$$< j_a j_b j l J|\Lambda S \Sigma J p > = (-1)^{l-\Omega-J}(2-\delta_{\Lambda,0}\delta_{\Sigma,0})^{-1/2}[1+(-1)^{L_a+L_b+l+p}(1-\delta_{\Lambda,0}\delta_{\Sigma,0})]$$
$$\times \sqrt{(2S+1)(2j_a+1)(2j_b+1)(2L+1)}$$
$$\times < l0|j-\Omega, J\Omega >< j\Omega|L\Lambda, S\Sigma >< L\Lambda|L_a\Lambda_a, L_b\Lambda_b >$$
$$\times \begin{Bmatrix} L_a & S_a & j_a \\ L_b & S_b & j_b \\ L & S & j \end{Bmatrix} < \Lambda_a\Lambda_b|\Lambda >$$

Case (a) $(^S\Lambda_\Omega)$		Case (c) (Ω)		Case (e) (j_1, j_2, j, l)	
e	f	e	f	e	f
$^1\Sigma_0^+$	$^3\Sigma_0^+$	0^+	0^-	(1/2,3/2,2,J+2)	(1/2,3/2,2,J+1)
$^3\Sigma_1^+$	$^3\Sigma_1^+$	0^-	0^-	(1/2,3/2,2,J)	(1/2,3/2,2,J-1)
$^1\Pi_1$	$^1\Pi_1$	1	1	(1/2,3/2,2,J-2)	(1/2,3/2,1,J+1)
$^3\Pi_0$	$^3\Pi_0$	1	1	(1/2,3/2,1,J)	(1/2,3/2,1,J-1)
$^3\Pi_1$	$^3\Pi_1$	1	1	(1/2,5/2,3,J+2)	(1/2,5/2,3,J+3)
$^3\Pi_2$	$^3\Pi_2$	1	1	(1/2,5/2,3,J)	(1/2,5/2,3,J+1)
$^1\Delta_2$	$^1\Delta_2$	2	2	(1/2,5/2,3,J-2)	(1/2,5/2,3,J-1)
$^3\Delta_1$	$^3\Delta_1$	2	2	(1/2,5/2,2,J+2)	(1/2,5/2,3,J-3)
$^3\Delta_2$	$^3\Delta_2$	2	2	(1/2,5/2,2,J)	(1/2,5/2,2,J+1)
$^3\Delta_3$	$^3\Delta_3$	3	3	(1/2,5/2,2,J-2)	(1/2,5/2,2,J-1)

Table 1: Good quantum numbers for s+d limit

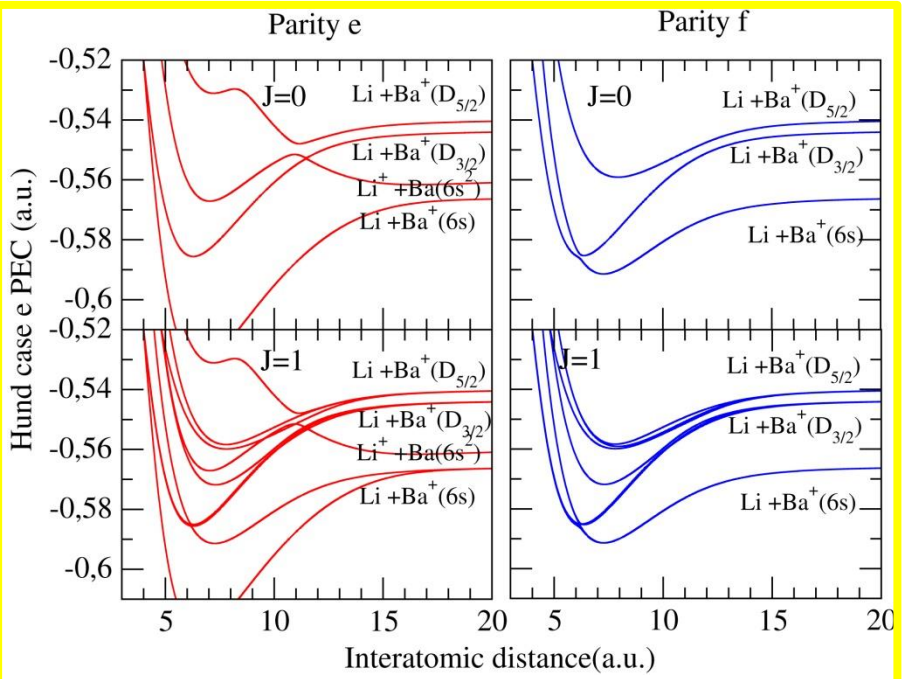


Figure 4: Parity-dependent potential energy surface for J=0 and 1. Here, it is clearly to notice that ***charge exchange happens only at Parity e*.**

Conclusion

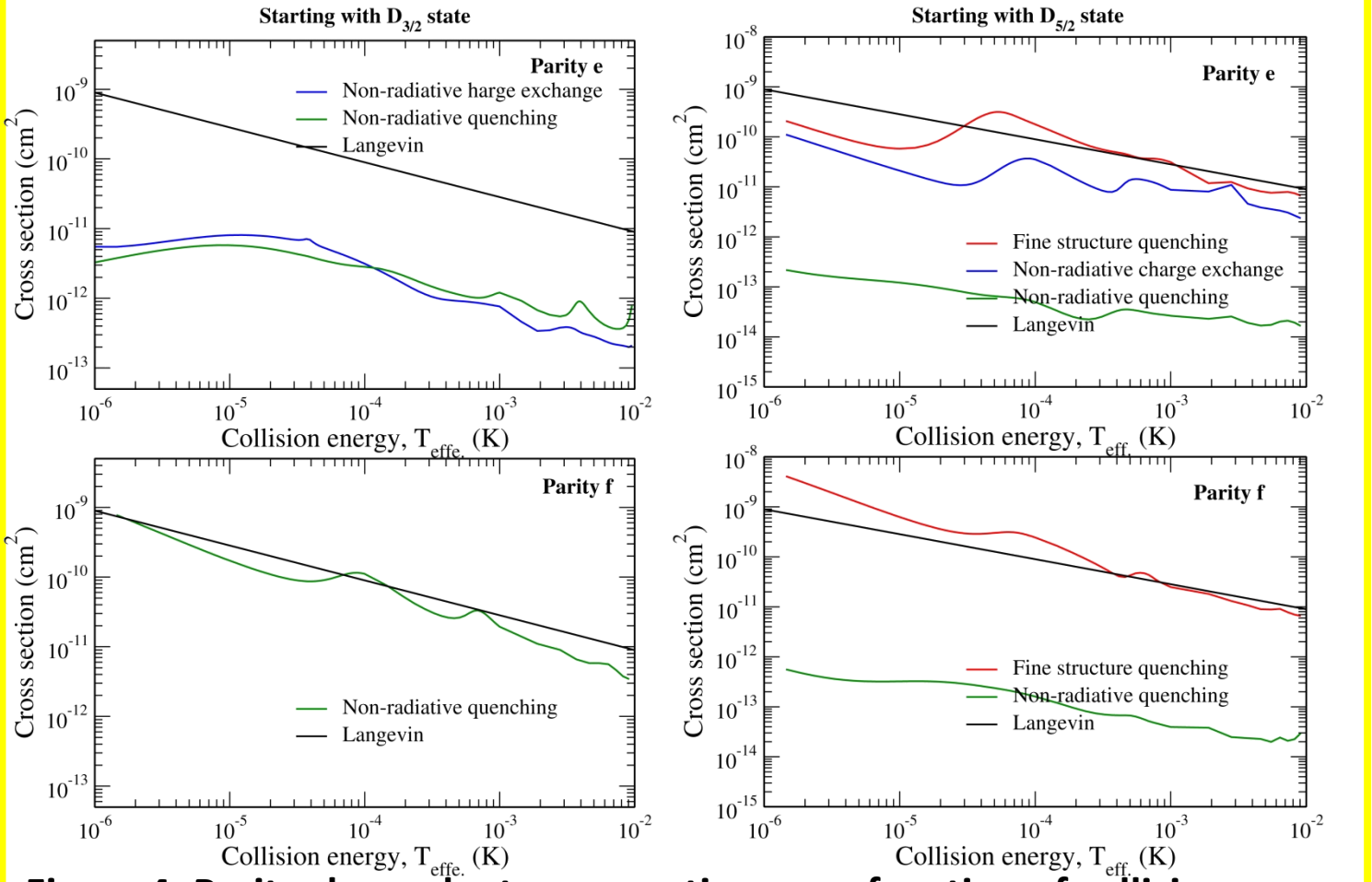


Figure 4: Parity-dependent cross sections as a function of collision energy. The calculated energy-dependent cross section approaches the Langevin prediction, while we also predict the presence of a shape resonance around 100 microkelvin. The rigorous MCQS model is found necessary to qualitatively reflect the experimental findings. Again, the non-radiative charge exchange is solely found at Parity e.

By comparing the theoretical FCQS and MCQS models, we realize that with or without the rotational couplings can completely reverse final results. Although the parity cannot be distinguished in experimental measurements, our in-depth theoretical designed model demonstrates such particular parity-dependent quantum effect for non-radiative charge exchange dynamic. Due to the temperature uncertainty of Ba^+ ion in the course of collisions, however, comparisons at the numerical level need further study.

[1] Sikorsky, T. *et al.* **Nat. commun.** 2018, 9, 920
[2] Ben-shlomi, R. *et al.* **Phys. Rev. A** 2020, 102, 031301(R)
[3] Singer, J. *et al.* **J. Chem. Phys.** 1983, 79, 6060.
[4] Parlant, G. *et al.* **J. Chem. Phys.** 1999, 110, 363