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## CORRIGENDUM

Corrigendum:  $\bar{\text{H}}^+$  ion production from collisions between antiprotons and excited positronium: cross sections calculations in the framework of the GBAR experiment (2013 *New J. Phys.* 15 095022)P Comini<sup>1,\*</sup>, P-A Hervieux<sup>2</sup> and K Lévêque-Simon<sup>2</sup><sup>1</sup> CEA DRF/Irfu/DPhP, Centre de Saclay, 91191 Gif-sur-Yvette Cedex, France<sup>2</sup> Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67000 Strasbourg, France

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E-mail: [pauline.comini@cea.fr](mailto:pauline.comini@cea.fr)**Keywords:** antihydrogen, positronium, atomic collisions, cross sections

## 1. Introduction

In [1], we reported the CBA and CDW-FS calculations of partial and total cross sections for the formation of neutral and positively charged antihydrogen in charge exchange reactions involving excited states of positronium. Further work on the production of  $\bar{\text{H}}^+$  [2] lead us to reanalyse the calculations and to discover two errors that significantly change the published results. In the present *corrigendum*, we explicit these errors and present the corrected cross sections.

## 2. Corrections in the analytical formula and in the computation code

The discovered errors only affect the cross sections for the four-body reaction

$$\text{Ps}(n_p, l_p, m_p) + \bar{\text{H}}(n_h, l_h, m_h) \rightarrow e^- + \bar{\text{H}}^+, \quad (1)$$

which have been obtained by applying the detailed balance principle to the cross sections of the charge conjugated reverse reaction

$$e^+ + \text{H}^- \rightarrow \text{Ps}(n_p, l_p, m_p) + \text{H}(n_h, l_h, m_h). \quad (2)$$

In that case, CBA and CDW-FS are in fact identical and we will later refer to the model simply as CBA.

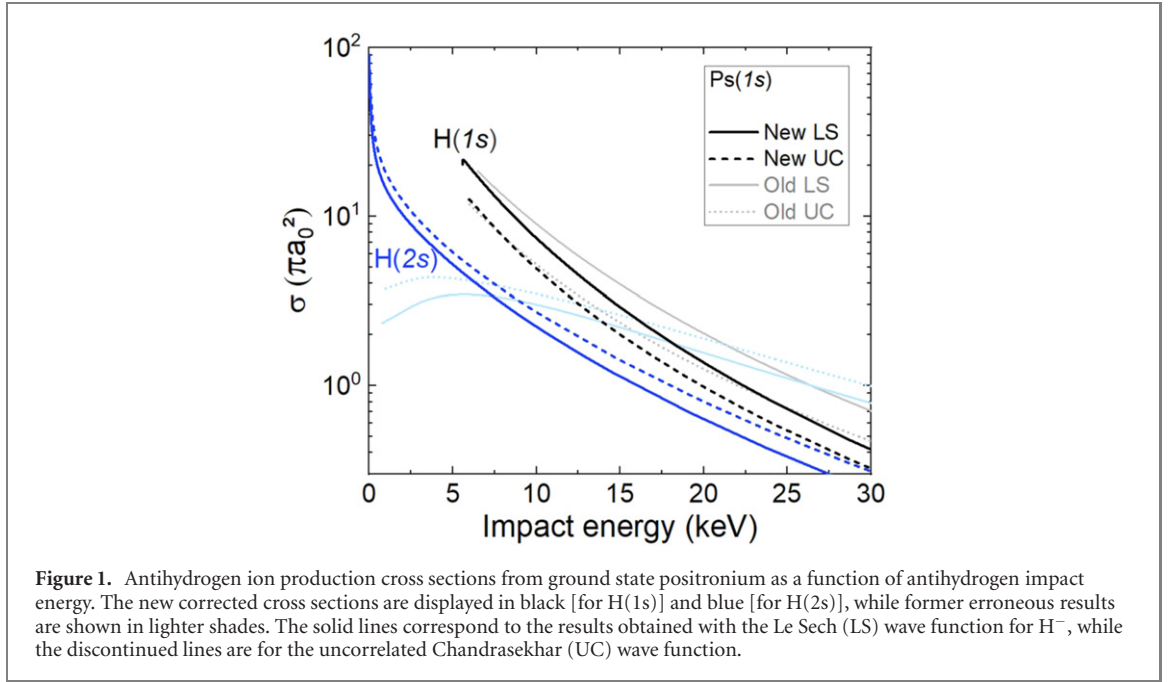
1. One error was found in the analytical expression of the cross-sections for reaction 2, in the *excitation* transition matrix element,  $t_{\text{exc}}$ , as defined by equation (25) in [1]. In order to compute  $t_{\text{exc}}$ , the interaction potential  $\left(\frac{1}{R} - \frac{1}{\rho}\right)$  is developed using the Laplace expansion of  $\frac{1}{\rho}$  (where  $\rho = \|\vec{R} - \vec{r}\|$ ; see figure 2 in [1] for the definition of the coordinates):

$$\frac{1}{\rho} = \sum_{\Lambda m_\Lambda} \frac{4\pi}{\Lambda} \frac{r_{<}^\Lambda}{r_{>}^{\Lambda+1}} Y_{\Lambda m_\Lambda}(\hat{\mathbf{R}}) Y_{\Lambda m_\Lambda}^*(\hat{\mathbf{r}}). \quad (3)$$

The radial part of this expansion appears in the term  $\tilde{\mathcal{L}}_{n_h l_h}^{\Lambda l_t}(r_1, R)$  of equation (29). This is where a sign inversion occurred. The correct expression for  $\tilde{\mathcal{L}}_{n_h l_h}^{\Lambda l_t}(r_1, R)$  is:

$$\tilde{\mathcal{L}}_{n_h l_h}^{\Lambda l_t}(r_1, R) = \frac{1}{\Lambda} \int_0^\infty dr_2 r_2^2 R_{n_h l_h}(r_2) \left( \frac{\delta_{\Lambda 0}}{R} - \frac{r_{<}^\Lambda}{r_{>}^{\Lambda+1}} \right) \tilde{h}_{l_t}(r_1, r_2). \quad (4)$$

The effect of the error is a change of sign of  $t_{\text{exc}}$ . Since the cross sections are proportional to the square of the transition matrix element (see equation (31) in [1]), this error only contributes significantly through the cross terms ( $t_{\text{exc}}^* \times t_{\text{cap}}$  and  $t_{\text{cap}}^* \times t_{\text{exc}}$ ) when  $t_{\text{exc}}$  and  $t_{\text{cap}}$  are of the same order of magnitude. When the



hydrogen is in its ground state, this first correction accounts for less than 20 % to the new cross section values near the reaction thresholds; the effect is larger toward higher energies. When the hydrogen atom is in the 2s state, this correction changes the behavior of the cross-sections toward very low energies, leading to new cross sections higher by more than an order of magnitude close to the thresholds (see section 3 below).

2. The second error was found in the code used to compute the four-body reaction cross sections. It affects the *capture* terms  $t_{\text{cap}}$  only [see equation (26)]. The code was written for a special case when  $l_p \neq 0$  while  $l_h = 0$ . We therefore ask the reader to refer also to appendix B.1 of [1]. The error occurred in the part of the code computing the term  $\mathcal{U}_{i\mathcal{L}}$  [equation (B.2)] and concerned the imaginary part of this term, which originates from the partial wave expansion of the Coulomb wave functions (see equation (10) in [1] for the expansion). We highlight it in red characters in the analytical formula of  $\mathcal{U}_{i\mathcal{L}}$  reproduced below:

$$\sum_{l_f l' l' \lambda} i^{-l-l_f} e^{i(\delta_l + \delta_{l_f})} \mathcal{B}_{l\mathcal{L}}^{l_f l' l' \lambda} \mathcal{R}_{l_f l' \lambda l_i}^{l_h=0}. \quad (5)$$

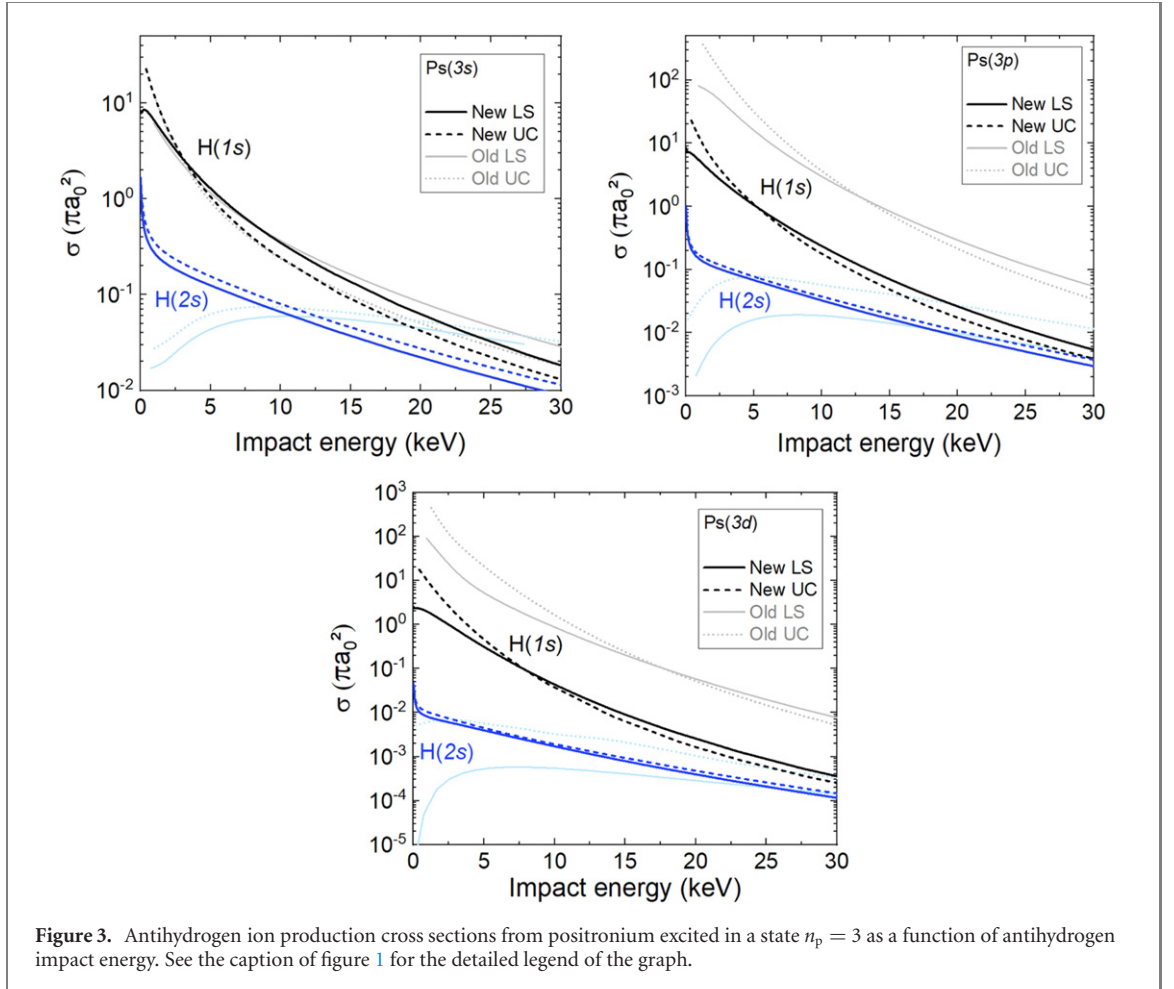
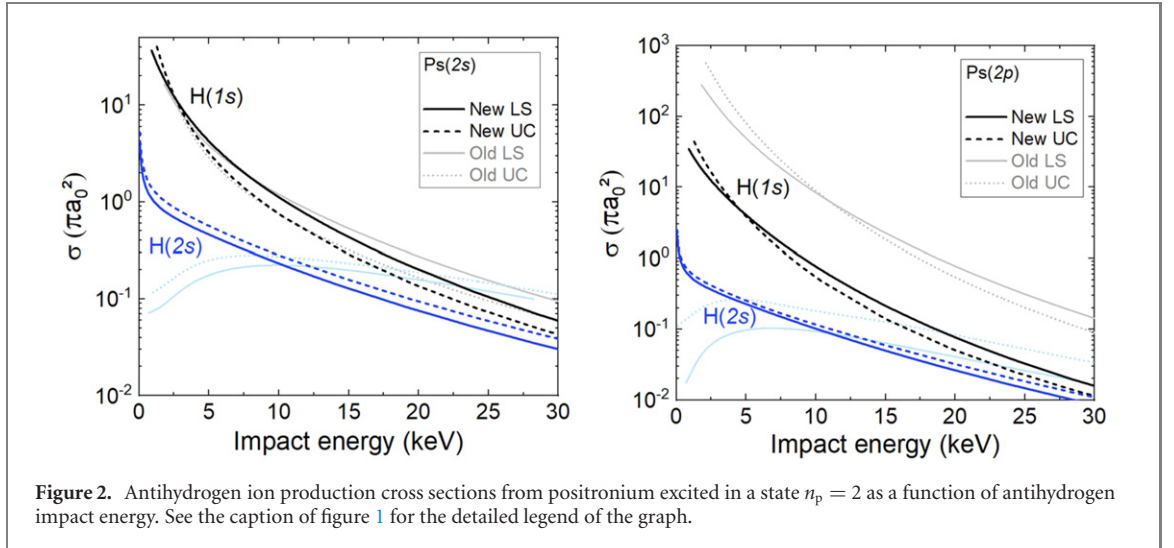
The index  $l$  comes from the partial wave expansion of the Coulomb wave function used to describe the exchanged electron that is going out of the target, within the formed positronium atom. In the code,  $l$  has been mistakenly swapped with  $l'$ . When the positronium is in a state with orbital angular momentum  $l_p = 0$ , then  $l' = l$ . Thus this error does not affect the  $l_p = 0$  states. On the contrary, for  $l_p \neq 0$ ,  $l$  and  $l'$  are linked. Indeed, for a fixed value of  $l$ ,  $l'$  is varied between  $|l - \lambda|$  and  $|l + \lambda|$ , with  $\lambda$  being itself varied from 0 to  $l_p$  ( $\lambda$  is introduced in the treatment of the spherical harmonic  $Y_{l_p m_p}(\hat{\rho})$  of the positronium bound state wave function). This index exchange is the error generating the most dramatic change to the computed cross sections for excited states of positronium, leading us to reconsider some conclusions of the original article.

### 3. Corrected four-body results with the UC and LS wave functions

In this section, we provide the corrected cross sections for  $\bar{H}^+$  formation and compare them to the old erroneous values by updating the figures of section 3.2 in [1]. Only the uncorrelated Chandrasekhar wave function (UC) and the Le Sech wave function (LS) for  $H^-$  are presented for the clarity of the figures but the authors can provide the cross section for the correlated Chandrasekhar wave function upon request. Figures 1–3 replace respectively figures 15–17 of [1], while figure 4 replaces both figures 12 and 18.

Most of the general conclusions drawn in [1] remain unchanged:

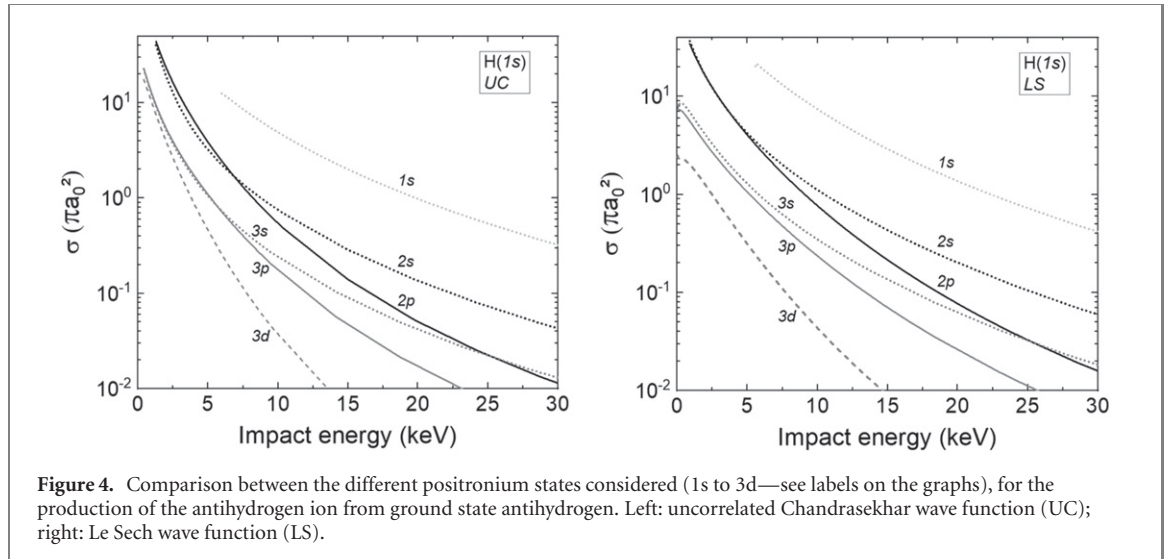
- (a) the production of the antihydrogen ion is mostly favored when the antihydrogen in the entrance channel is in its ground state and,
- (b) it tends to greatly increase toward the thresholds.



- (c) Always with ground state antihydrogen, the highest cross sections are obtained when the positronium is excited in a state  $n_p = 2$ .
- (d) The two previously identified energy regions of interest emerge once again: right above the threshold of the  $\bar{H}(1s) + \text{Ps}(1s)$  channel, around 6 keV, and then below 2 keV, with the case  $\text{Ps}(2s, 2p)$  peaking at the threshold around 1 keV.

To these conclusions, nuances have to be added in the light of the corrected results for  $\bar{H}(2s)$ :

- (a) in the case of ground state positronium, the cross section for antihydrogen being in the metastable state 2s actually exceeds the one with  $\bar{H}(1s)$ , although for energies below 500 eV;



- (b) for all the considered Ps states, the channels with  $\bar{H}(2s)$  now exhibit a resonant behavior toward zero energy;
- (c) the highest cross section values are obtained for the  $\bar{H}(2s) + \text{Ps}(1s)$  channel, with already  $35 \pi a_0^2$  at 150 eV, which is comparable to the maximum values obtained at 1 keV for  $\bar{H}(1s) + \text{Ps}(2s, 2p)$ .

Finally, some of the most important conclusions from [1] have to be revised. Indeed, the new cross sections for  $\text{Ps}(2p, 3p)$  are, for instance at 1 keV, lower by roughly an order of magnitude and for  $\text{Ps}(3d)$  by a factor 50 than originally published. Therefore, these corrected results strongly diminish the interest of positronium excitation for reaction 1, as can be seen on figure 4 which compares the different states of positronium. Indeed, even with positronium in a state  $n_p = 2$  at 1 keV, the gain due to the cross sections would be at best a factor 2 compared ground state positronium at 6 keV, requiring an highly efficient scheme to produce these states of positronium. In an experimental context where the antihydrogen atoms have first been produced by charge exchange between antiprotons and positronium atoms, positronium excitation remains useful to enhance the antihydrogen production. In particular, the cross sections increase toward low energy and with the antihydrogen principle quantum number  $n_h$  (as shown in the original article [1] and more recent publications, for instance [3]). However, for  $n_p = 3$  states of positronium, the enhanced excited antihydrogen production insufficiently compensates for the much lower corrected cross sections for  $\bar{H}^+$  production from ground state antihydrogen.

Further comments and perspectives. For the calculations of the corrected cross sections, we decided to push a little further toward the reaction thresholds. The newly found resonant behavior for  $\bar{H}(2s)$  deserves consideration, in particular in the case of ground state positronium since it provides the highest CBA cross section for  $\bar{H}^+$  production. This could motivate experimental efforts to work at impact energies lower than 1 keV and to optimise the  $\bar{H}(2s)$  fraction in the beam. Another interesting feature appearing in the corrected results is the suppression of the nearly resonant behavior toward the  $n_p = 3$  threshold when electronic correlations are introduced in the wave function describing  $\text{H}^-/\bar{H}^+$ . We are aware of the limitations of perturbation theory at low energies and are looking forward to future *ab initio* calculations (as for instance the recent coupled rearrangement channels (CRC) calculations [4]) that could investigate both features highlighted here.

#### 4. Accounting for the spin of the particles

To conclude this *corrigendum*, we would like to point at a rightful comment made by Swann *et al* [5]:

*“it appears that in figure 19 the cross sections of McAlinden *et al* [64] are shown incorrectly and should be reduced by a factor 4”*

Reference [64] in the article of Swann *et al* being reference [19] in our original article. In figure 19 of [1], we compared our CBA results with other available theoretical calculations. However, in our calculations and in applying the detailed balance principle, we did not include the spin states (and this remark applies for the corrected cross sections presented above as well), while McAlinden *et al* did.

If we are to compare the cross sections taking into account the spin states, then the cross sections for the direct reaction 1 should be summed over the spin states of  $H^-$  ( $S = 0$ ) and positron ( $S = \frac{1}{2}$ ) in the exit channel (the average over the spin states of the incoming particles leaves the cross sections unchanged). This implies a multiplication by a factor 2.

In the article of McAlinden *et al*, the results for the reverse reaction 2 already include the summation over the spin states of hydrogen ( $S = \frac{1}{2}$ , 2 states) and positronium (with  $S = 0$  para-Ps and  $S = 1$  ortho-Ps, 4 states). The ‘no-spin’ cross sections are therefore retrieved by dividing by a factor 8. After applying the detailed balance principle combined with the aforementioned factor 2 multiplication for the direct reaction, the McAlinden *et al* cross sections for reaction 1 should indeed be reduced by a factor 4.

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