Resonant antihydrogen formation in antiproton-positronium collisions

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Plan

- Motivations
  - Cross section phenomena in three body systems.
  - GBAR (Gravitational Behaviour of Antihydrogen at Rest) project.
- Theoretical framework,
  1. Merkuriev-Faddeev equations.
  2. Problem of the degeneracy of the excited states.
- Results.
- Summary.

Main motivations

- the aim of my work is to rigorously explore the cross sections of the $(e^-, e^+, \bar{p})$ system to:
    - do a more complete mapping of the cross sections
    - Highlight and study special phenomena linked to collision reactions:
        - Feshbach resonances
        - Gailitis oscillations

The GBAR project

- GBAR: Gravitational Behaviour of Antihydrogen at Rest.
- Experimental project supported by CERN (2012).
- International collaboration of 49 physicits from 14 different institutes.
- Equivalence principle verification : mesure the free fall of ultracold $\bar{H}$ to study the behavior of antimatter in a gravitational field.
- First experiments in 2017 testing proton collisions on Positronium.

The GBAR project

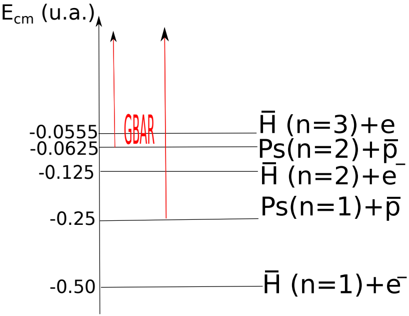
- $\bar{H}^+$ production controled by,

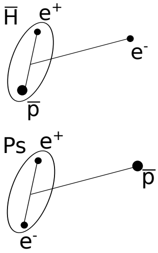
$$\bar{p} + Ps \rightarrow \bar{H} + e^-$$
$$\bar{H} + Ps \rightarrow \bar{H}^+ + e^-$$

- Looking for production beams optimisation.
- Experimental cross sections insufficiently known at the GBAR energy levels.
- Theoretical calculations needed. Benchmark contribution of ab-initio methods.

Generalities

$(\bar{p}, e^+, e^-)$ system thresholds.





n principal quantum number.

Up to now the GBAR experiment should be done above the $Ps(n = 2) + \bar{p}$ threshold.

Theoretical framework

Theoretical framework

- Hamiltonian considered to describe the 3-body system in the laboratory frame

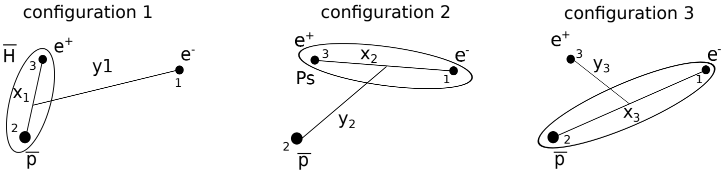
$$H_{lab} = \frac{\mathbf{p}_{\bar{p}}^2}{2m_{\bar{p}}} + \frac{\mathbf{p}_{e^+}^2}{2m_e} + \frac{\mathbf{p}_{e^-}^2}{2m_e} - \frac{\alpha\hbar c}{|\mathbf{r}_{e^+} - \mathbf{r}_{e^-}|} - \frac{\alpha\hbar c}{|\mathbf{r}_{\bar{p}} - \mathbf{r}_{e^+}|} + \frac{\alpha\hbar c}{|\mathbf{r}_{\bar{p}} - \mathbf{r}_{e^-}|}$$

α fine structure constant.

- We work in the center of mass frame.

$$H = H_{cm} + H^{int}$$

Theoretical framework, generalities



- Intrinsic coordinates defined with the Jacobi coordinates system
- The Hamiltonian can be written for each configuration,

$$H^{int} = H_0(\vec{x}_i, \vec{y}_i) + V_1 + V_2 + V_3.$$

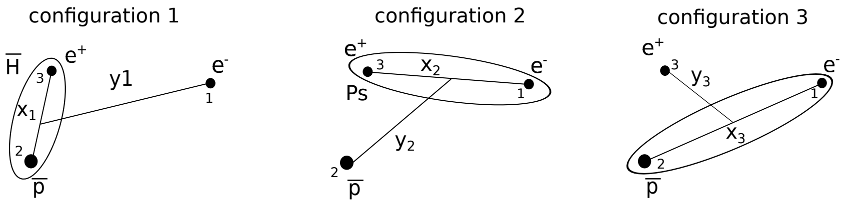
Theoretical framework

- The Merkuriev-Faddeev equations represent a mathematically rigorous ab-initio formulation of the scattering theory for 3-particle systems.
  In contrast to Schrödinger or Lippman-Schwinger equations, which fail to provide an unique solution for the multichannel scattering problem with N>2 particles.

Theoretical framework

- In this frame work the Wave function is splited in 3 Merkuriev-Faddeev amplitudes,

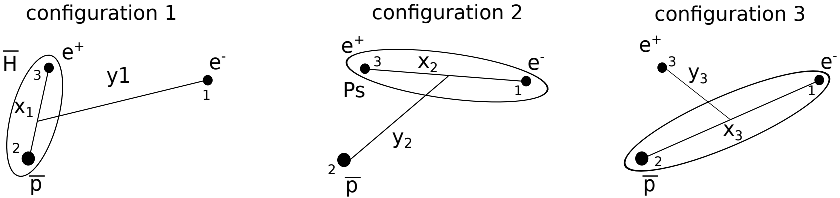
$$\Psi = F_1 + F_2 + F_3.$$



Theoretical framework

In the Merkuriev-Faddeev equations, potentials are separated in two parts, a long range part and a short range part,

$$V_i(x_i) = V_i^{(\ell)}(x_i, y_i) + V_i^{(s)}(x_i, y_i).$$



Merkuriev-Faddeev equations,

$$\begin{aligned}
(E - H_0 - V_1^{(\ell)} - V_2^{(\ell)} - V_3^{(\ell)})F_1 &= V_1^{(s)}(F_1 + F_2 + F_3) \\
(E - H_0 - V_1^{(\ell)} - V_2^{(\ell)} - V_3^{(\ell)})F_2 &= V_2^{(s)}(F_1 + F_2 + F_3) \\
(E - H_0 - V_1^{(\ell)} - V_2^{(\ell)} - V_3^{(\ell)})F_3 &= V_3^{(s)}(F_1 + F_2 + F_3)
\end{aligned}$$

The Schrödinger equation is the sum of the three equations.

$$\begin{aligned}
(E - H_0 - V_1 - V_2 - V_3)(F_1 + F_2 + F_3) &= 0 \\
\leftrightarrow (E - H_0 - V_1 - V_2 - V_3)\Psi &= 0
\end{aligned}$$

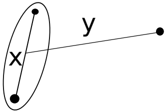
Theoretical framework

- Each Merkuriev-Faddeev amplitude is projected onto a partial wave basis,

$$F_i(\vec{x}_i, \vec{y}_i) \quad = \quad \sum_L F_i^L(\vec{x}_i, \vec{y}_i).$$

and $$F_i^L(\vec{x}_i, \vec{y}_i) \quad = \quad \sum_{\hat{\ell}_x + \hat{\ell}_y = \hat{L}} \frac{f^L_{i,\ell_x \ell_y}}{x_i y_i} \{ Y_{\ell_{xc}}(\hat{x}_i) \otimes Y_{\ell_{yc}}(\hat{y}_i) \}_{LM}$$

- where $\hat{L}$ is the total orbital momentum $\hat{\mathbf{L}} = \hat{\ell}_x + \hat{\ell}_y$



- Within this framework we are able to determine bound states, collision states and to compute cross sections (differential, partial, total).

Theoretical framework

- To compute the collision states, and cross sections we use an asymptotic interconnection in the numerical resolution (Kievsky method).

$$f_{i,\ell_x\ell_y}^{L,as}(x_i, y_i \to \infty) = \phi_c^{2b,bs}\left[j_{c'}(y_i)\delta_{c'c} + K_{c'c} f^{reg}(y_i)\eta_c(y_i)\right]$$

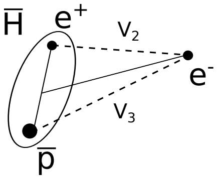
- $K \leftrightarrow S$ scattering matrix.

Theoretical framework

Using the Wronskian theorem,

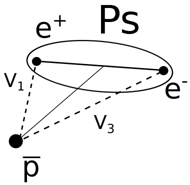
- Incoming channel in the $\bar{H} + e^-$ configuration.

$$K_{\alpha\beta} \propto < \psi^{(\beta)}_{Tot} \mid V_2 + V_3 \mid \psi^{in}_{\alpha} >$$



- Incoming channel in the $\bar{P} + Ps$ configuration.

$$K_{\alpha\beta} \propto < \psi^{(\beta)}_{Tot} \mid V_1 + V_3 \mid \psi^{in}_{\alpha} >$$



- The K matrix allows to calculate the cross sections.

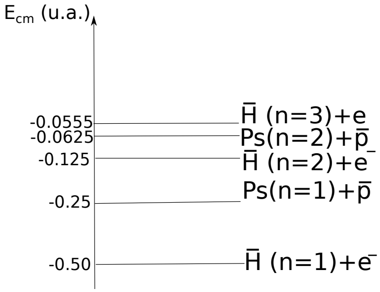
$$\sigma_{ij}^{L} = \frac{\pi a_0^2}{k_i^2}\frac{(2L+1)}{(2\ell_i+1)}\left|\left(\frac{2K_L}{1-iK_L}\right)_{ij}\right|^2$$

$$\sigma_{ij} = \sum_L \sigma_{ij}^{L}$$

$$\sigma_{ij}(\theta) = \frac{\pi a_0^2}{k_i^2}\left|\sum_L (2L+1)\left(\frac{2K_L}{1-iK_L}\right)_{ij} P_L(\cos(\theta))\right|^2$$

  - k_i relative momentum in the incoming channel.
  - ℓ_i angular monentum of the two body system in the incoming channel.

Problem of degeneracy of the excited states



- We focus mainly on the reactions above the $\bar{H}(n=2)$ threshold.
- One of the main technical difficulties comes from the treatment of the degeneracy.

Problem of degeneracy of the excited states

- The resolution of the Faddeev equations need the asymptotic functions of each channel.
- the determination of the asymptotic functions for the degenerate binary chanels leads to a system of coupled integro-differential equations,

$$(-\frac{\partial^2}{\partial y_i^2} + \frac{\ell'_y(\ell'_y+1)}{y_i^2} - k_{c'}^2)R_{c'}^{as} + \sum_c V_{c'c}R_c^{as} = 0,$$

where c and c' chanel indexes.

Problem of degeneracy of the excited states

$$(-\frac{\partial^2}{\partial y_i^2} + \frac{\ell'_y(\ell'_y+1)}{y_i^2} - k_{c'}^2)R_{c'}^{as} + \sum_c V_{c'c} R_c^{as} = 0,$$

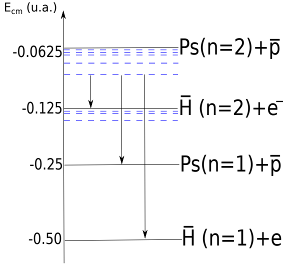
$V_{c'c}$ polarisation potential,

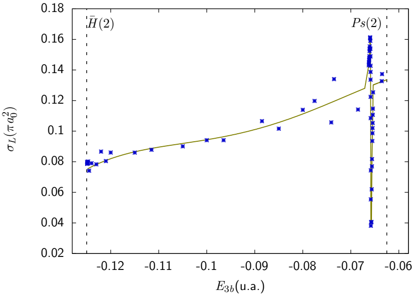
$$\begin{aligned} V_{c'c}(y_i) &= < \phi_{c'}^{2b,bs}\{c'\}_{LM} \mid V_2 + V_3 \mid \phi_c^{2b,bs}\{c\}_{LM} > \\ &\propto \frac{1}{y^2} \end{aligned}$$

where $\{c'\} = \{Y_{\ell_{x_{c'}}}(\hat{x}_i) \otimes Y_{\ell_{y_{c'}}}(\hat{y}_i)\}_{LM}$

Problem of degeneracy of the excited states-Feschbach resonances

- In the asymptotic region the coupling potential between the degenerate states has an $\frac{1}{y^2}$ behavior.
- The coupling potential generates effective attraction, this enables the formation three-body "long lived" or quasi-bound states. They take place just below the degenerate thresholds.





Problem of degeneracy of the excited states-Feshbach resonances

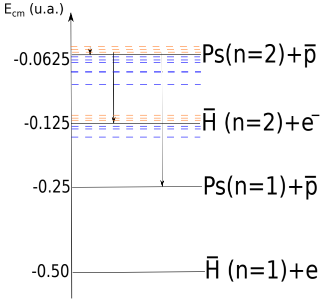
- The Feshbach resonances are characterised as S matrix poles.
- Their position can be determined via standard methods as the complex scaling method.

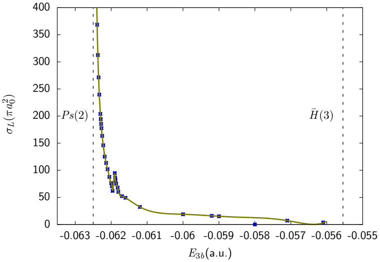
Problem of degeneracy of the excited states-Feshbach resonances

- The Gailitis phenomenon is characterised by dense oscillations wich can lead to divergences in the K-Matrix. They take place slightly above the degenerate thresholds. [1]
- Because of the divergencies in the K-Matrix elements these oscillations have already been referred to as resonances in some works [4][6].
- The position of such oscillations can not be determined via the usual methods.

[4] Inducted Long-Range Dipole-Field-Enhanced Antihydrogen Formation in the $\bar{p} + Ps(n = 2) \rightarrow e^{-} + H(n \leq 2)$ Reaction C.-Y. Hu, D. Caballero Phys. Rev. Lett 88.063401
[6]Low-energy anti-hydrogen formation differential cross sections from $Ps(n = 2)$via the modified Faddeev equations Chi-Yu Hu and David Caballero, J. Phys. B: At. Mol. Opt. Phys. 35 (2002) 3879–3886 [1] The influence of finite masses on the threshold behaviour of scattering in a three charged particle system, M Gailitis, J. Phys. B: At. Mol. Phys. 15 (1982) 3423-3440.

Problem of degeneracy of the excited states-Gailitis oscillations





- The "quasibound" states, below the degenerate channel, can be seen as bound states. In this case the Gailitis oscillations can be seen as a consequence of the Levinson theorem.

Numerical aspects

- x and y axis discretisation via Lagrange mesh method.
- The radial amplitudes core terms are approximated using the Lagrange-Laguerre basis functions.

$$
\begin{aligned}
f^{L}_{i,\ell_x\ell_y}(x_i, y_i) &= \sum_{i_x i_y}^{N_x, N_y} C_{i,\ell_x\ell_y,i_x,i_y} h_{i_x}(x_i) h_{i_y}(y_i) + f^{L,as}_{i,\ell_x\ell_y} \\
h_i &= (-1)^i c_i^{1/2} \frac{L_N(x/\eta)}{x/\eta - x_i} e^{-x/2\eta}
\end{aligned}
$$

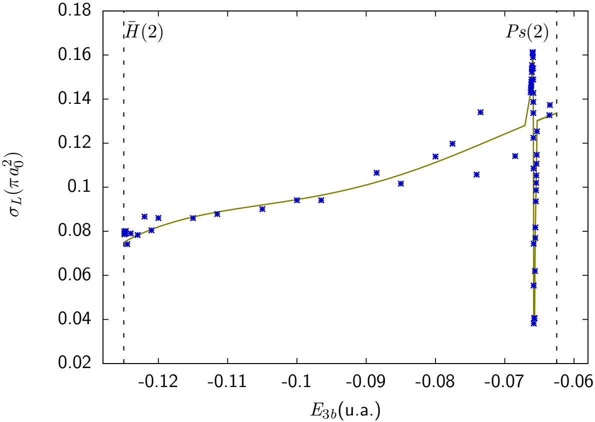
- The resolution of our system of equations becomes a linear problem, where the Laguerre-Lagrange coefficients are to be determined.
- Partial waves limited, $16 \leq \ell_x \leq 22$ $18 \leq \ell_y \leq 24$.

Numerical aspects

- Linear problem size $200000 - 300000$
- Numerical resolution is done on a supercomputer.
- Depending on the energy and the partial wave the time of the calculation varies between $2 - 18$ hours.
- In a first time, the linear problem is solved to determine the Lagrange-Laguerre coefficients.
- In a second time, The K matrix is computed.
- At last, the cross section are computed.

Results between the $H(n = 2)$ and $Ps(n = 2)$ thresholds

$L = 0$ partial cross section $Ps(1s) + \bar{p} \rightarrow \bar{H}(2s, 2p) + e^-$



- Partial cross section σ_L in πa_0^2 units (a_0 is the bohr Radius).
- New resonance in the S partial wave cross section.

Results

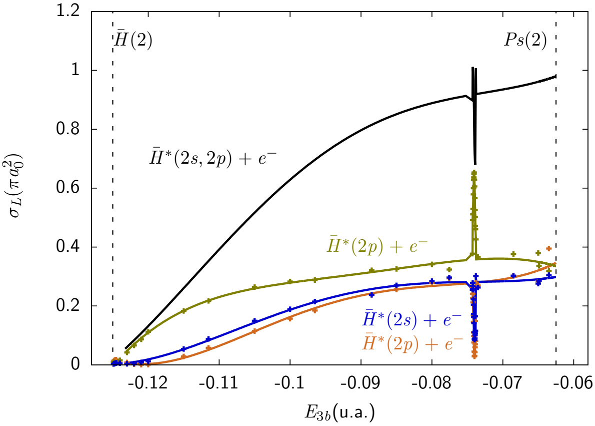
The position of the resonances is calculated using the complex scaling method ([2]).

Threshold	-Res(E_{res}) a.u.	$\Gamma/2$ a.u.
$H(n=2)$	0.128622631	3.3283[-5]
-0.124932	0.1251318	1.82[-6]
$Ps(n=2)$	0.07513977	1.67290[-4]
-0.25	0.0658293	8.127[-5]
	0.0633866	2.494[-5]
	0.06274	6.9[-6]

- Good agreement in the energy position, $\Delta(E_{res}) = 1 \times 10^{-5}\ a.u.$

[2] Resonant antihydrogen formation in antiproton–positronium collisions R Lazauskas, P-A Hervieux, M Dufour and M Valdes. J.Phys. B: At. Mol. Opt. Phys. 49(2016)094002

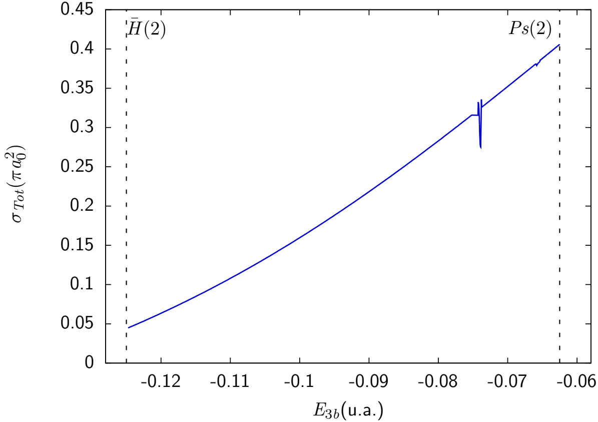
$L = 1$ partial cross section, $Ps(1s) + \bar{p} \rightarrow \bar{H}(2s, 2p) + e^-$



New resonance in the P partial wave in agreement with M. Umair *et al [7].*

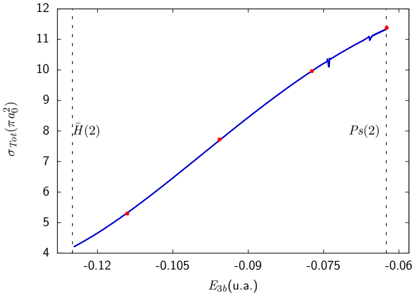
[7] Natural and unnatural parity resonance states in positron–hydrogen scattering M Umair and S Jonsell J. Phys. B: At. Mol. Opt. Phys. 47 (2014) 225001 (7pp)

Total cross section
$\bar{H}(1s) + e^- \rightarrow H(2s, 2p) + e^-$



- The S wave resonance can be seen in all the reactions.

Total cross section
$Ps(1s) + \bar{p} \rightarrow \bar{H}(1s, 2s, 2p) + e^-$

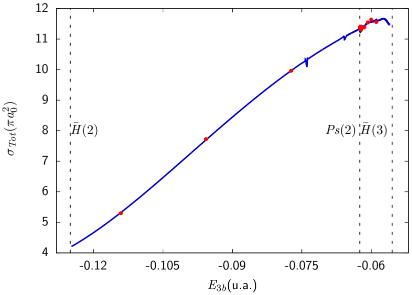


- Total cross section, maximum total angular momentum $L_{max} = 7$.
- The bigger contributions come from the $L = 2(D)$, $L = 3(F)$ and $L = 4(G)$ partial waves.
- The dots in this figure come from the calculations done by A.S. Kadyrov *et al.* [3] with the two-center convergent close-coupling method.

[3] Antihydrogen Formation via Antiproton Scattering with Excited Positronium A. S. Kadyrov, C. M. Rawlins, A. T. Stelbovics, and I. Bray., M. Charlton PHYSICAL REVIEW LETTERS, 183201 (2015)

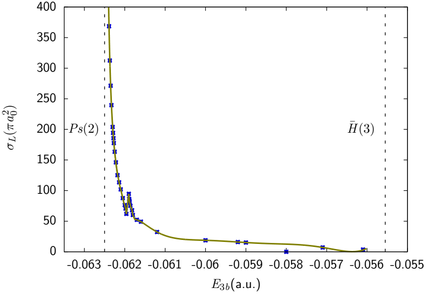
Results between the $Ps(n=2)$ threshold and $H(n=2)$ threshold

Total cross section $Ps(1s) + \bar{p} \rightarrow \bar{H}(1s, 2s, 2p) + e^-$



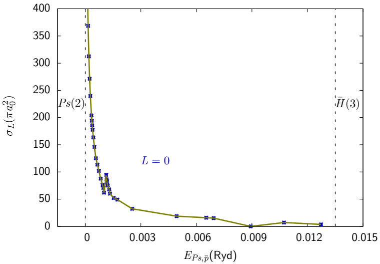
- extension of the precedent results, $L_{max} = 7$.
- The bigger contributions come from the $L = 2(D)$, $L = 3(F)$ and $L = 4(G)$ partial waves.
- The dots in this figure come from the calculations done by A.S. Kadyrov *et al.* [3] with the two-center convergent close-coupling method.

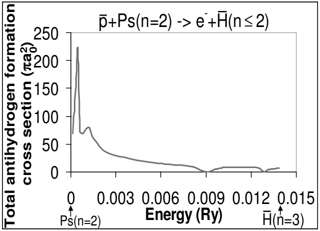
$L = 0$ partial cross sections
$Ps(2s, 2p) + \bar{p} \to \bar{H}(1s, 2s, 2p) + e^-$



- Our calculations show the existence of two so called Gailitis oscillations in the S partial wave.
- One of them seems to have no consequence on the partial cross section.

$L = 0$ partial cross sections $Ps(2s, 2p) + \bar{p} \rightarrow \bar{H}(1s, 2s, 2p) + e^-$





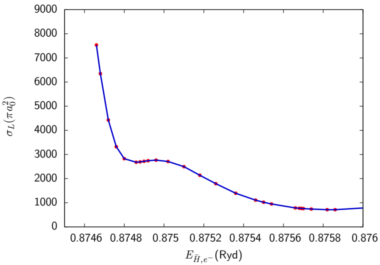
Chi-yu Hu *et al* [4]

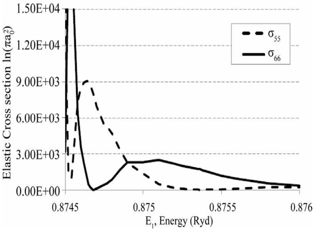
- Resonance in the $\bar{H}$ production near the $Ps(n = 2)$ threshold for the S wave.

[4] Inducted Long-Range Dipole-Field-Enhanced Antihydrogen Formation in the

$\bar{p} + Ps(n = 2) \rightarrow e^- + H(n \leq 2)$ Reaction C.-Y. Hu, D. Caballero Phys. Rev. Lett 88.063401

$L = 0$ partial elastic cross sections $Ps(2s, 2p) + \bar{p} \rightarrow Ps(2s, 2p) + \bar{p}$



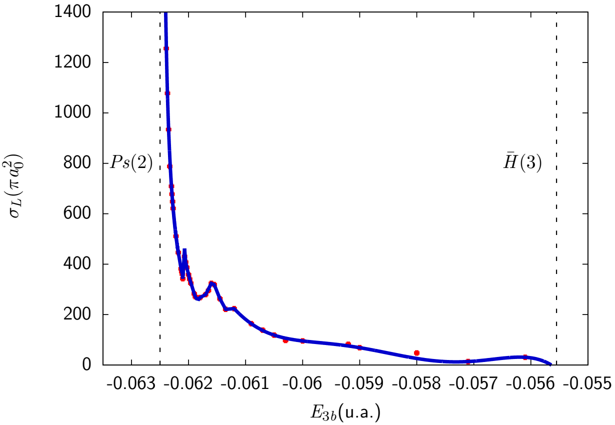


Chi-yu Hu *et al* [6]
$\sigma_{55} \rightarrow$ elastic $Ps(2s)$
$\sigma_{66} \rightarrow$ elastic $Ps(2p)$

- Gailitis oscillation in the elastic $Ps(n = 2) + \bar{p}$ reaction near the $Ps(n = 2)$ threshold for the S-wave.

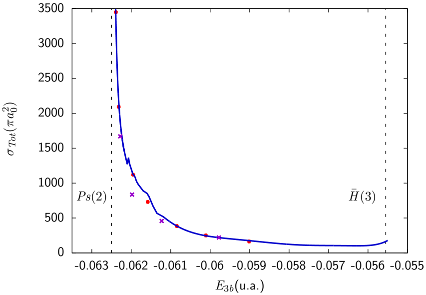
[6]Low-energy anti-hydrogen formation differential crosssections from $Ps(n = 2)$via the modified Faddeev equations Chi-Yu Hu and David Caballero, J. Phys. B: At. Mol. Opt. Phys. 35 (2002) 3879–3886

$L = 2$ partial cross section
$Ps(n=2) + \bar{p} \rightarrow \bar{H}(1s, 2s, 2p) + e^-$



- New result, a Gailitis oscillation in the D partial wave.

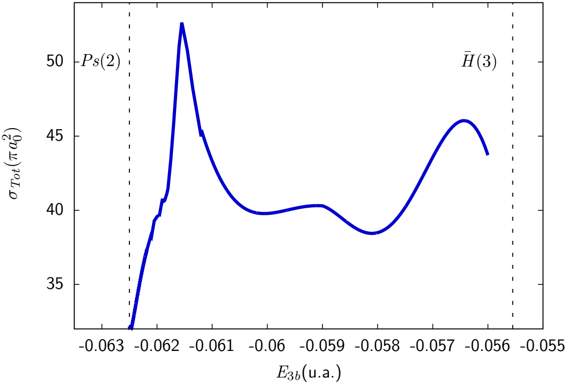
Total cross section
$Ps(n=2) + \bar{p} \rightarrow \bar{H}(1s, 2s, 2p) + e^-$



We have calculated the total cross section with a maximum total angular momentum $L_{max} = 7$. The bigger contribution comes from the $L = 2(D)$, $L = 1(P)$ and $L = 5(H)$ partial waves.
read dots A.S. Kadyrov *et al.*, purple dots C.Y. Hu *et al.* [6].

[6]Low-energy anti-hydrogen formation differential crosssections from $Ps(n=2)$via the modified Faddeev equations Chi-Yu Hu and David Caballero, J. Phys. B: At. Mol. Opt. Phys. 35 (2002) 3879–3886

Total cross section $\bar{H}(2s,2p) + e^- \rightarrow Ps(1s,2s,2p) + \bar{p}$



Total cross section of $Ps(1s,2s,2p)$ production with $\bar{H}(2s,2p) + e^-$.

Higher contribution coming from $L = 2(D)$, $L = 3(F)$ and $L = 5(H)$ partial waves.

Summary

- Highlight of the cross section resonant behaviour through,
  - Feschbach resonances
  - Gailitis oscillations, possibility to furtherly confirm these oscillations experimentally.
- In relation to the GBAR experiment,
  - More complete mapping of low energy cross sections.
  - Absence of a significant resonance of interest for the GBAR experiment.

Thank you for your attention.

The merkuriev separation of the potential.

$$V_i^{(s)}(x_i, y_i) = V_i(x_i) f^{(M)}(x_i, y_i),$$
$$V_i^{(l)}(x_i, y_i) = V_i(x_i)(1 - f^{(M)}(x_i, y_i)).$$

$f^{(M)}$ is a cut-off function which goes to zero when $x_i \quad y_i \to \infty$ and goes to one when $x_i << y_i \to \infty$.

$$f^{(M)}(x, y) = 2(1 + exp\{\frac{(x/x_0)^\mu}{y/y_0 + 1}\})^{-1}$$

where $\mu > 2$ and x_0 and y_0 must be of the size of the system.

Results

Comparison with previous results obtained for the S wave.

1) $\bar{H}(n=1)+e^-$ $\sigma_{ij}(E_{cm})$ en πa_0^2

2) $Ps(n=1)+\bar{p}$ partial cross section between i and j

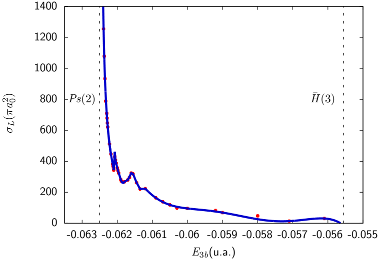
3) $\bar{H}(n=2)+e^-$

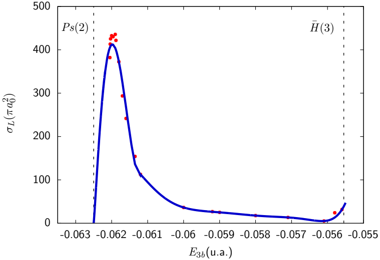
E_{cm}	work	σ_{11}	σ_{13}	σ_{12}
-0.115 u.a.	[4]	0.0900	0.001156	0.00572
	[5]	0.0951	0.001004	0.00558
	This work.	0.0964	0.000891	0.00570
-0.10 u.a.	[4]	0.096	0.001514	0.00585
	[5]	0.1010	0.001641	0.00563
	This work.	0.1015	0.001675	0.00574

[4] C.-Y. Hu, Phys. Rev. A 59, 4813 (1999)

[5]Three-potential formalism for the three-body scattering problem with attractive Coulomb interactions (2008) Z. Papp , C-.Y. Hu , Z. T. Hlousek , B. Konya and S. L. Yakovlev.

Partial cross section behaviors





$$\sigma^L \propto \frac{1}{k_i^2} \left| < \psi_{Tot}^{(\beta)} \mid V_{ij} - V_{ij}^{as} \mid \psi_\alpha^{in} > \right|^2$$

- $L \leq 4$ existence an attractive interaction $\sigma^L \propto k_i^{-2}$
- $L \geq 5$ only repulsive interactions $\sigma^L \propto k_i^{2\ell-1}$

where ℓ is a L dpendent real value obtained through the pontential interaction.

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