Ab-initio calculations of reactions involving the 3-body system $(\bar{p}, e^+, e^-)$ between the $e^- + \bar{H}(n=2)$ and $e^- + \bar{H}(n=3)$ thresholds

Marianne DUFOUR
IPHC: Institut Pluridisciplinaire Hubert Curien

M. Valdes (PhD), R. Lazauskas (IPHC), P.A. Hervieux (IPCMS)

Motivations

- The aim of this work is to rigorously compute cross sections involving the 3-body system $(e^-, e^+, \bar{p})$ at low energy.
- Bring informations about antimatter behavior when only Coulomb interaction is present.
- Special interest for GBAR but also for other experiments involving antimatter (ATRAP, AEGIS).
- Highlight and study special resonant phenomena called Feshbach resonances and Gailitis-Damburg oscillations.

Plan

- The Gravitational Behavior of Antihydrogen at Rest (GBAR) project
- Generalities on the 3-body system $(e^-, e^+, \bar{p})$
- Origin of the resonant phenomena
- Theoretical framework - Faddeev-Merkuriev equations
- Results

M. Valdes, M. Dufour, R. Lazauskas, P.-A. Hervieux, *Ab-initio calculations of scattering cross sections of the 3-body system* $(\bar{p}, e^+, e^-)$ *between the* $e^- + \bar{H}(n=2)$ *and* $e^- + \bar{H}(n=3)$ *thresholds*, Phys. Rev. A **97**, 012709 (2018).

The GBAR project

- Experimental project supported by CERN (2012).
- International collaboration of 49 physicits from 14 different institutes.
- Equivalence principle verification : measure the free fall of ultracold $\bar{H}$ to study the behavior of antimatter in a gravitational field.
- $\bar{H}$ production controled by

$$\begin{aligned} \bar{p} + Ps &\rightarrow \bar{H} + e^- \\ \bar{H} + Ps &\rightarrow \bar{H}^+ + e^- \end{aligned}$$

The GBAR project

- Challenge for GBAR : to find the best conditions to enhance antihydrogen production
- Interesting to find resonances allowing an augmentation in the $\bar{H}$ production
- Few literature in theory and no experimental measurement at low energy
- Benchmark contribution of ab-initio methods interesting
- Here we focuss on the first reaction

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

The three-body system $(\bar{p}, e^+, e^-)$ Hamiltonian

- The Hamiltonian we work with reads

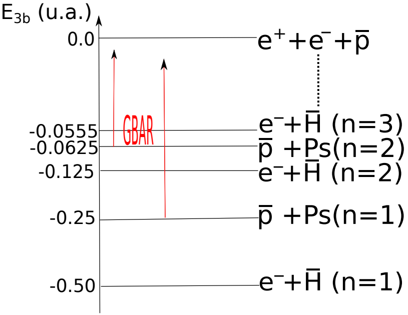
$$H^{lab} = \frac{\mathbf{p}_{\bar{p}}^2}{2m_{\bar{p}}} + \frac{\mathbf{p}_{e^+}^2}{2m_e} + \frac{\mathbf{p}_{e^-}^2}{2m_e} - \frac{\alpha\hbar c}{|\mathbf{r}_{e^+} - \mathbf{r}_{e^-}|} - \frac{\alpha\hbar c}{|\mathbf{r}_{\bar{p}} - \mathbf{r}_{e^+}|} + \frac{\alpha\hbar c}{|\mathbf{r}_{\bar{p}} - \mathbf{r}_{e^-}|}.$$

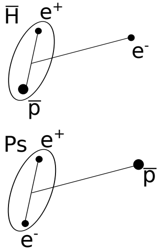
The 2-body interactions are represented by Coulomb potentials.

- The separation of the center of mass is rigorously performed by using appropriate sets of mass-scaled Jacobi coordinates

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

The three-particle system ($\bar{p}$, e^+, e^-) thresholds





- No bound state in the three-body system
- Bound states in the two-body systems $\bar{H}$ end Ps
- The figure represents schematically the lower thresholds

n: principal quantum number
$E_n^H = -\frac{m_p}{m_e+m_p}\frac{1}{n^2}$ Ryd, 1 Ryd = 13.6 eV, 1 a.u.= 2 Ryd
Degeneracy: $(n = 1 \ ; \ 1s), (n = 2 \ ; \ 2s, 2p), (n = 3 \ ; \ 3s, 3p, 3d), \ldots$

Consequences of the $n = 2$ degeneracy

- Charged particle in the field of an excited hydrogenlike atom generates a dipole potential which couples the degenerates states and leads to a long range effective potential, $\propto 1/y^2$, between the charged particle and the atom.
- One of the main technical difficulties of this work is to find the right expression of the asymptotic radial functions of the collision states.

Origin of resonant phenomena - Feshbach resonances

- Feshbach resonances are the consequence of the long range dipole potential between the degenerate states.
    - General study of the $V(y) = -\frac{\beta}{y^2}$ potential shows the existence of an infinity of bound states depending on the value of β.
    - According to this result and to the open channels, an infinity of very narrow resonances are expected below the degenerate thresholds.

Origin of resonant phenomena - Gailitis-Damburg oscillations

- The Gailitis-Damburg phenomenon is characterised by dense oscillations slightly above the degenerate thresholds.
- It has been predicted and interpreted by Gailitis and Damburg as the consequence of the Feshbach resonances.

Gailitis, Damburg, Soviet Physics JETP, vol 17, 5, (1963)

Gailitis, The influence of finite masses on the threshold behavior of scattering in a three charged particle system, J. Phys. B: At. Mol. Phys. 15 (1982) 3423-3440.

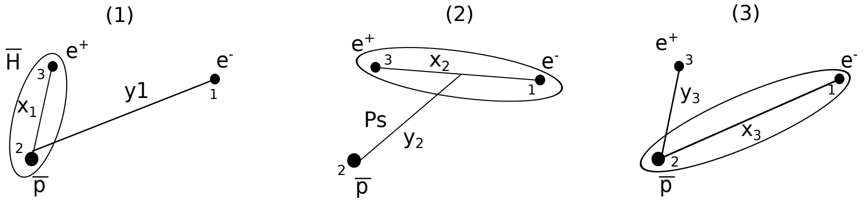
The Faddeev-Merkuriev equations (FME)

- The Faddeev-Merkuriev equations represent a mathematically rigorous ab-initio formulation of the scattering theory for 3 charged particle systems.
  In contrast to Schrödinger or Lippman-Schwinger equations, which fail to provide an unique solution for scattering problems involving different particle channels.

The Faddeev-Merkuriev equations (FME)

- In this framework the wave function is splited in 3 Faddeev-Merkuriev amplitudes,

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



The Faddeev-Merkuriev equations (FME)

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

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

- The Faddeev-Merkuriev equations read

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

The Faddeev-Merkuriev equations (FME)

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

$$F_i(\mathbf{x}_i, \mathbf{y}_i) = \sum_L F_i^L(\mathbf{x}_i, \mathbf{y}_i),$$

where L corresponds to the total orbital momentum,

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

$f^L_{i,\ell_x\ell_y}(x_i, y_i)$ = radial functions of the FM components

Calculation of collision states

• In order to incorporate proper boundary conditions, the radial function is separated into two parts

$$f_{i,\alpha}^{L}(x_i, y_i) \quad = \quad f_{i,\alpha}^{L,core}(x_i, y_i) + f_{i,\alpha}^{L,as}(x_i, y_i)$$

• $f_{i,\alpha}^{L,core}(x_i, y_i)$ = "core" part which describes the system in the region with 3-particle close to each other.
• $f_{i,\alpha}^{L,as}(x_i, y_i)$ = "asymptotic" part which contains the incoming and outcoming scattering waves and the K matrix elements (or the S scattering matrix elements $S = \frac{1+iK}{1-iK}$).

Numerial Method - Lagrange-Mesh Method

The Lagrange-mesh method (D. Baye, Phys. Rep. 1, 565 (2015)) is used to describe the radial amplitudes core terms

$$f_{i,\alpha}^{L,core}(x_i, y_i) = \sum_{i_x, i_y}^{N_x, N_y} C_{\alpha_i, i_x, i_y} a_{i_x}(x_i) a_{i_y}(y_i)$$

where $a_{i_y}(y)$ is a Lagrange-Laguerre mesh function

$$a_{i_y}(y) = (-1)^{i_y} c_{i_y}^{1/2} \frac{L_{N_y}(y/\eta_y)}{y/\eta_y - y_{i_y}} y_{i_y}^{1/2} \left(\frac{y/\eta_y}{y_{i_y}} \right)^{1/2} e^{-y/2\eta_y}$$

where L_{N_y} is a Laguerre polynomial.

- C_{α_i, i_x, i_y} coefficients are determined by solving a linear problem.
- The K-matrix is obtained using the Wronskian theorem.

K-Matrix calculation

- Cross sections can be then calculated

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

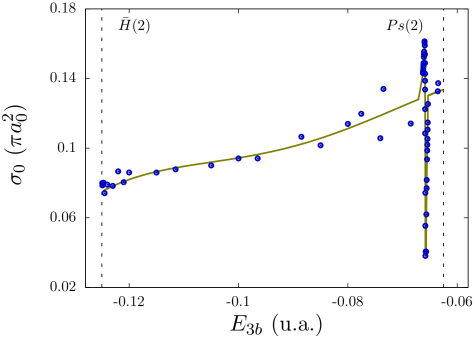
- a_0 is the Bohr radius.
- k_i is the relative momentum in the incoming channel.
- ℓ_i is the angular monentum of the two body system in the incoming channel.

Numerical aspects

- Linear algebra problem of 10^5 to 10^6 equations.
- Calculations are time-consuming.
- Numerical resolution is done on a supercomputer.
- Numbers of points used in the Lagrange-Laguerre grid are $45 \leq N_x \leq 75$ and $60 \leq N_y \leq 75$.
- Depending on the energy and the partial wave the time of the calculation can vary between 2-18 hours for one energy.
- On average there are about 30 different energies for each partial wave.
- Curves are added to guide the eye. They represent smoothing of the calculated values by a least square fit.

Results between the $e^- + \bar{H}(n=2)$ and $\bar{p} + Ps(n=2)$ thresholds

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



- Circles : our calculations, line: fit
- Calculations show a Feshbach resonance at $E_{3b} = -0.06583$ a.u., with a width of $\Gamma/2 \approx 8 \times 10^{-5}$ a.u.
- Deviations give an estimation of the accuracy

Comparison with complex scaling calculations

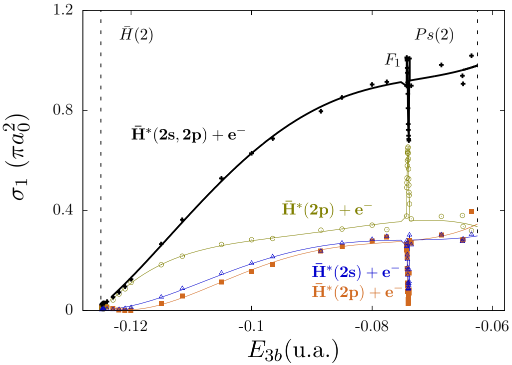
Threshold	Res(E_{res}) a.u.	$\Gamma/2$ a.u.
$Ps(n=2)$	-0.07513977	1.67290[-4]
-0.062500	-0.0658293	8.127[-5]
	-0.0633866	2.494[-5]
	- 0.06274	6.9[-6]

- Very good agreement with previous CSM calculations for the blue one
- We fail to reproduce the other resonances.
- Challenge to find the Feshbach resonances because of their closeness to the threshold and their extremely small width

M Umair and S Jonsell, J. Phys. B: At. Mol. Opt. Phys. 47 (2014) 225001

R Lazauskas, P-A Hervieux, M Dufour and M Valdes, J.Phys. B: At. Mol. Opt. Phys. 49 (2016) 094002

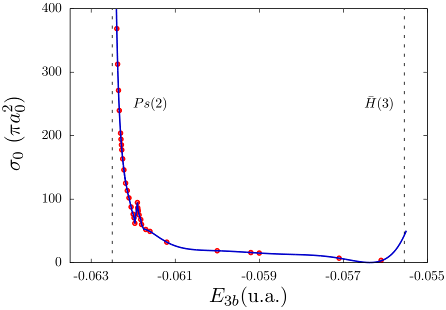
$L = 1$ partial cross section, $\bar{p} + Ps(n=1) \to e^- + \bar{H}(n=2)$



- Our calculations show another Feshbach resonance in the P partial wave at $E_{3b} = -0.0740719$ a.u. in agreement with M. Umair *et al.*

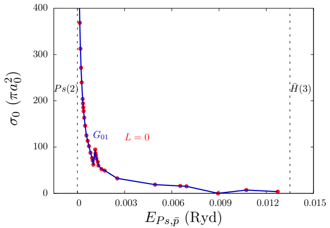
Results between the $\bar{p} + Ps(n = 2)$ and the $e^- + \bar{H}(n = 3)$ thresholds

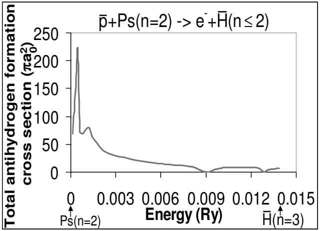
$L = 0$ partial cross section $\bar{p} + Ps(n = 2) \rightarrow e^{-} + \bar{H}(n \leq 2)$



- One Gailitis-Damburg oscillation at $E_{3b} = -0.06190$ a.u.
- Calculations show the signature of two Gailitis-Damburg oscillations.
- One is situated close to the threshold and does not lead to a resonant behavior of the cross section.

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





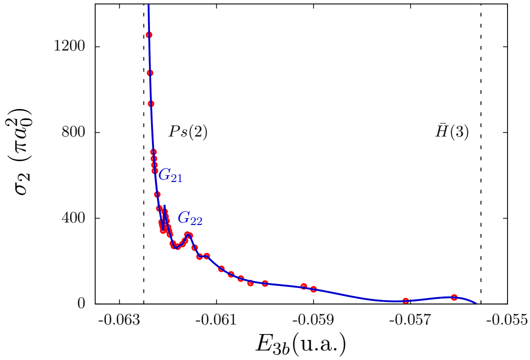
Hu *et al*, Phys. Rev. Lett **88**, 063401 (2002)

- Agreement with FM calculations of Hu *et al* for the observed Gailitis-Damburg oscillation but disagreement at the threshold
- Typical near-threshold behavior as $1/k^2$ in agreement with:

I.I. Fabrikant, A.W. Bray, A.S. Kadyrov, I. Bray, Phys. Rev. A bf 94, 012701 (2016)

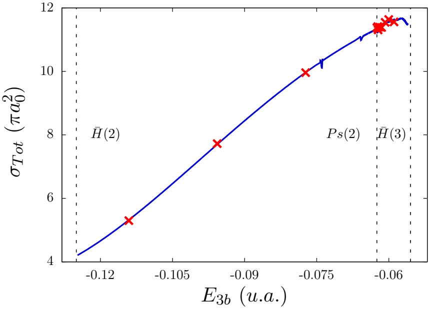
C.M. Rawlins, A.S. Kadyrov, A.T. Stelbovics, I. Bray, Phys. Rev. A bf 93, 012709 (2016)

$L = 2$ partial cross section $Ps(n=2) + \bar{p} \to \bar{H}(n \leq 2) + e^-$



- New results: two Gailitis-Damburg oscillations at $E_{3b} = -0.06222$ a.u. and at $E_{3b} = -0.06175$ a.u. can be observed in the D partial wave.

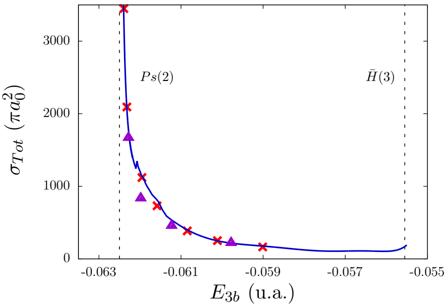
Total cross section
$\bar{p} + Ps(n=1) \rightarrow e^- + \bar{H}(n \leq 2)$ (GBAR)



- Line: our results by summing the partial cross sections up to $L = 7$
- The most important contributions come from the P, D and F partial waves at low energies and D, F and G partial waves at higher energies
- Good agreement with calculations done by A.S. Kadyrov *et al.* with the two-center convergent close-coupling method(red crosses).

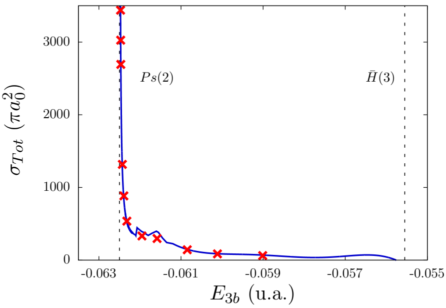
A. S. Kadyrov, C. M. Rawlins, A. T. Stelbovics, and I. Bray., Phys. Rev. Lett. **114** 183201 (2015)

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



- Line: our results by summing the partial cross sections up to $L=7$
- The most important contributions: D, F and H partial waves.
- Red crosses from A.S. Kadyrov *et al*, purple triangles from C.Y. Hu *et al*
- The oscillating structure of the D wave remains noticeable.

Total cross section $Ps(2p) + \bar{p} \rightarrow \bar{H}(n \leq 2) + e^-$ (GBAR)



- The most important contributions: D, F and H partial waves.
- Red crosses from A.S. Kadyrov *et al.*

Summary

- Our calculations show two Feshbach resonances and (five) Gailitis-Damburg oscillations.
- In relation with GBAR
  - Absence of a significant resonance of interest for the GBAR experiment.
  - More complete mapping of cross sections between the $e^- + \bar{H}(n = 2)$ and $e^- + \bar{H}(n = 3)$ thresholds.

Thank you for your attention.

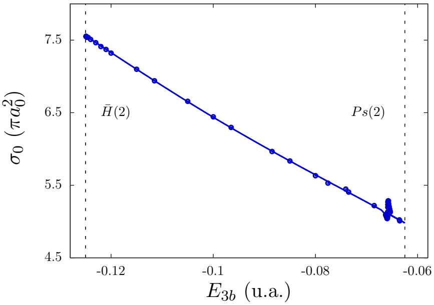
Consequences of the $n=2$ degeneracy

$L \geq 1$, natural parity, asymptotic region

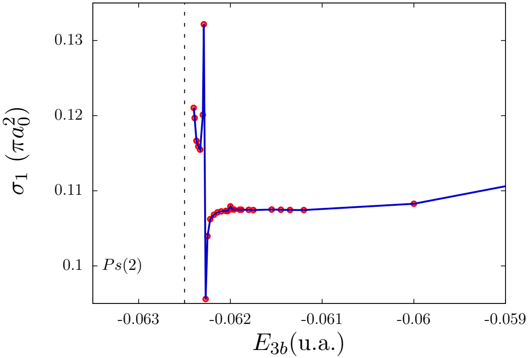
$$\begin{pmatrix} -\frac{d^2}{dy_i^2} + \frac{L(L+1)}{y_i^2} - k_i^2 & \frac{\tilde{V}_{12}}{y_i^2} & \frac{\tilde{V}_{13}}{y_i^2} \\ \frac{\tilde{V}_{21}}{y_i^2} & -\frac{d^2}{dy_i^2} + \frac{L(L-1)}{y_i^2} + \frac{\tilde{V}_{22}}{y_i^3} - k_i^2 & \frac{\tilde{V}_{23}}{y_i^3} \\ \frac{\tilde{V}_{31}}{y_i^2} & \frac{\tilde{V}_{32}}{y_i^3} & -\frac{d^2}{dy_i^2} + \frac{(L+1)(L+2)}{y_i^2} + \frac{\tilde{V}_{33}}{y_i^3} - k_i^2 \end{pmatrix} [g] = 0,$$

- One of the main technical difficulties of this work is to find the right expression of the asymptotic radial functions.
- In the asymptotic region the coupling between the channels associated to different thresholds tends to zero, but it is no the case for the coupling between channels associated to the same threshold

S-wave partial cross section
$\bar{p} + Ps(n=1) \rightarrow \bar{p} + Ps(n=1)$



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



- New results: one Gailitis-Damburg oscillations can be observed in the P partial wave

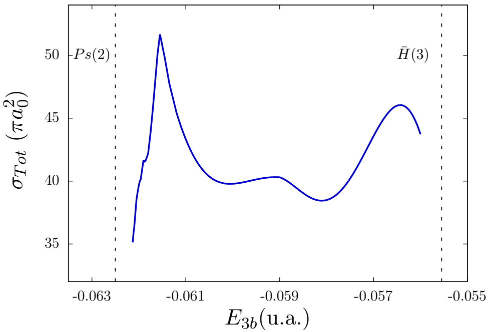
Perspectives

- To continue the calculation above the $e^- + \bar{H}(n = 3)$ threshold.
- Study the $(e^-, e^+, e^+, \bar{p})$ four-body system to calculate cross sections of the second GBAR reaction,

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

- the code can be easily adapted to other three body systems (μ^-, p, e^+), (e^-, e^-, e^+), (p, p, e^-), etc, where Feshbach resonances and Gailitis-Damburg oscillations are also predicted.

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



Total cross section of $Ps(n \leq 2)$ production with $\bar{H}(n=2) + e^-$. Higher contribution coming from $L = 2(D)$, $L = 3(F)$ and $L = 5(H)$ partial waves.

The Merkuriev separation of the potential

$$\begin{aligned} V_i^{(s)}(x_i, y_i) &= V_i(x_i) f^{(M)}(x_i, y_i), \\ V_i^{(l)}(x_i, y_i) &= V_i(x_i)(1 - f^{(M)}(x_i, y_i)). \end{aligned}$$

$f^{(M)}$ 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

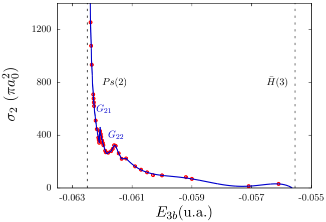
2) $Ps(n=1)+\bar{p}$ partial cross section between i and j

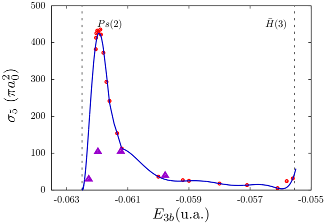
3) $\bar{H}(n=2)+e^-$

E_{cm}	work	σ_{11}	σ_{13}	σ_{12}
-0.115 u.a.	[5]	0.0900	0.001156	0.00572
	[7]	0.0951	0.001004	0.00558
	This work.	0.0964	0.000891	0.00570
-0.10 u.a.	[5]	0.096	0.001514	0.00585
	[7]	0.1010	0.001641	0.00563
	This work.	0.1015	0.001675	0.00574

[5] C.-Y. Hu, Phys. Rev. A 59, 4813 (1999)
[7]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.

$\tilde{S}$ determination

chose to look for regular solutions under the form

$$G^- - \tilde{S}G^+,$$

in an analogy with the one channel case we stipulate

$$\begin{aligned} G^+ &= A\tilde{J} + B\tilde{N} \\ G^- &= A^\dagger\tilde{J} + B^\dagger\tilde{N}, \end{aligned}$$

replacing this expression into the first,

$$\tilde{S} = B^\dagger B^{-1}$$

$\tilde{S}$ determination

actually we use

$$\tilde{V} = f^{cut} V$$

$\tilde{V}$ potential with the good asymptotic behavior but tends to zero near the origin. in this cas we can use

$$\begin{aligned} G^{+}(y_a) &= A\tilde{J}(y_a) + B\tilde{N}(y_a) \\ \frac{dG^{+}}{dy}(y_a) &= A\frac{d\tilde{J}}{dy}(y_a) + B\frac{d\tilde{N}}{dy}(y_a) \end{aligned}$$

y_a interconnection point, G^{+} determined solutions, $\tilde{N}$ and $\tilde{J}$, Bessel functions.

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