Ultra Low Energy scattering of p on H atom

The simplest 3-body problem (almost)

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Summary

1. The physics

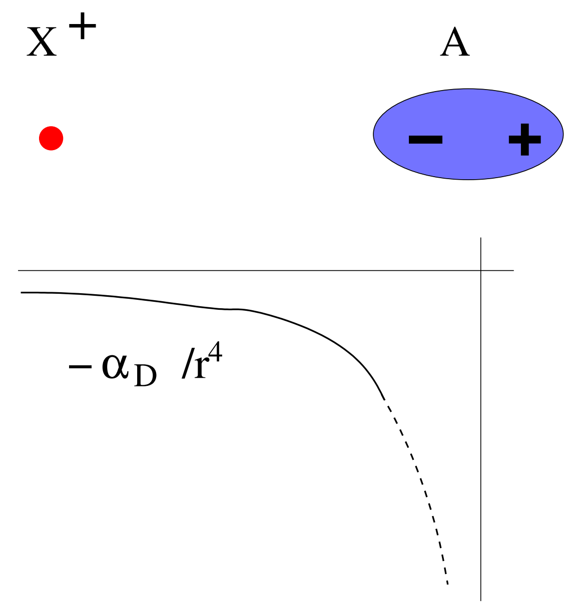
2. The numbers

3. Some remarks

THE PHYSICS

A charged particle X$^{+/-}$ approaching a neutral atom A, induces long range X-A attractive potential

$$V_D(x) \approx -\frac{\alpha_D}{x^4}$$



α_D = atomic dipole polarization polarizabilty (a.u.)

Exp. results [5]	
	α_d
H	4.5
He	1.37
Li	165.
N	7.6
Ne	2.5
Na	165.0
Ar	11.1

He, Ne frozen: V_{AA} interatomic « potentials » work well
Li, Na highly polarizable, V_{AA} fail ⇒ « 3-body » forces

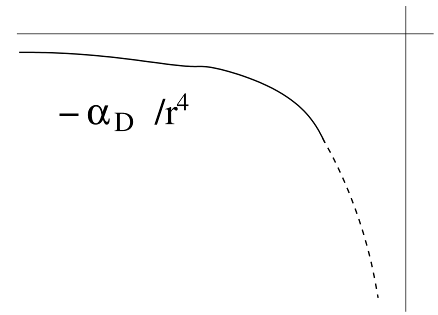
We will consider the simplest case : A=H and X=π^+,μ^+,K$^+$…p

THE PHYSICS

$V_D(x)$ is very weak (eV at 1A)

If X=e⁻ nothing interesting happens:

a_s=5.6 a.u. (2.96 Å) a_t=1.74 a.u (0.931 Å)



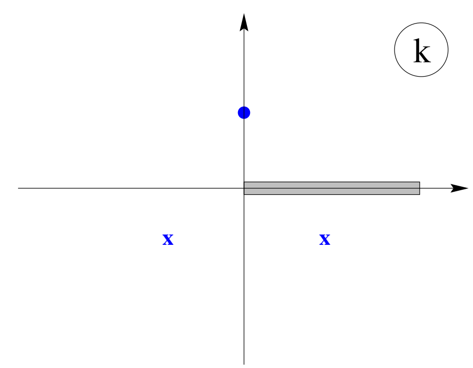
BUT

if X is heavy enough, the "effective X-A Hamiltonian"

$$H_{X^{\pm}A} \approx \frac{1}{M} + V_D$$

entails a rich spectrum of bound and resonant states

It happens with X=μ,π,K,…specially if X=p

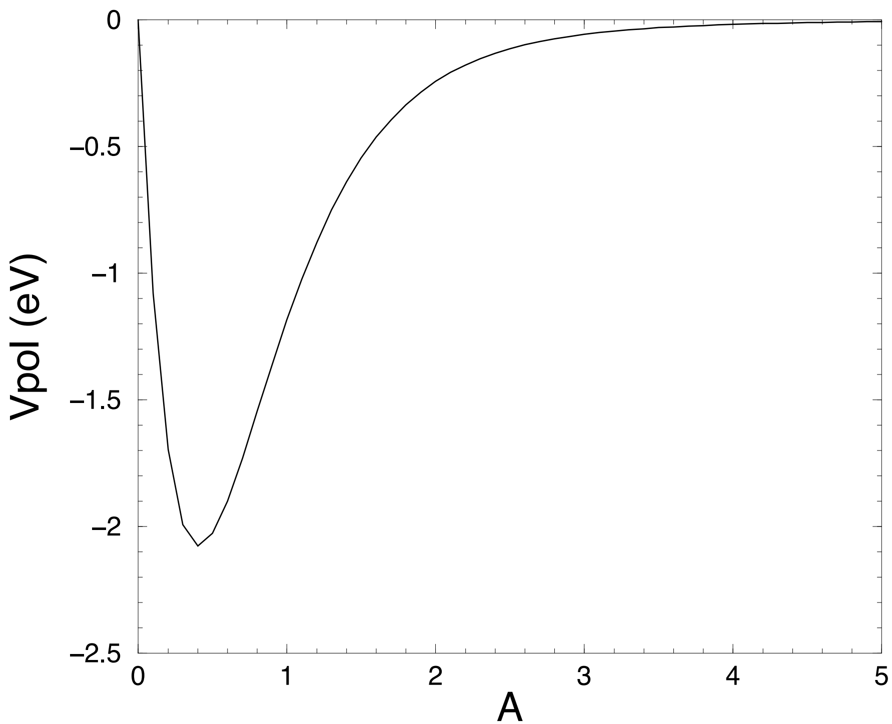


A two-body approach with « regularized V_D » gives all the physics

$$V(r) = -\frac{1}{2}\frac{\alpha(r)}{r^4} \qquad \alpha(r) \xrightarrow[r\to\infty]{} \alpha_D = \frac{9}{2}$$

e.g. Mott-Massey

$$\alpha(r) = \frac{9}{2} - \frac{2}{3}e^{-2r}\left(r^5 + \frac{9}{2}r^4 + 9r^3 + \frac{27}{2}r^2 + \frac{27}{2}r + \frac{27}{4}\right)$$

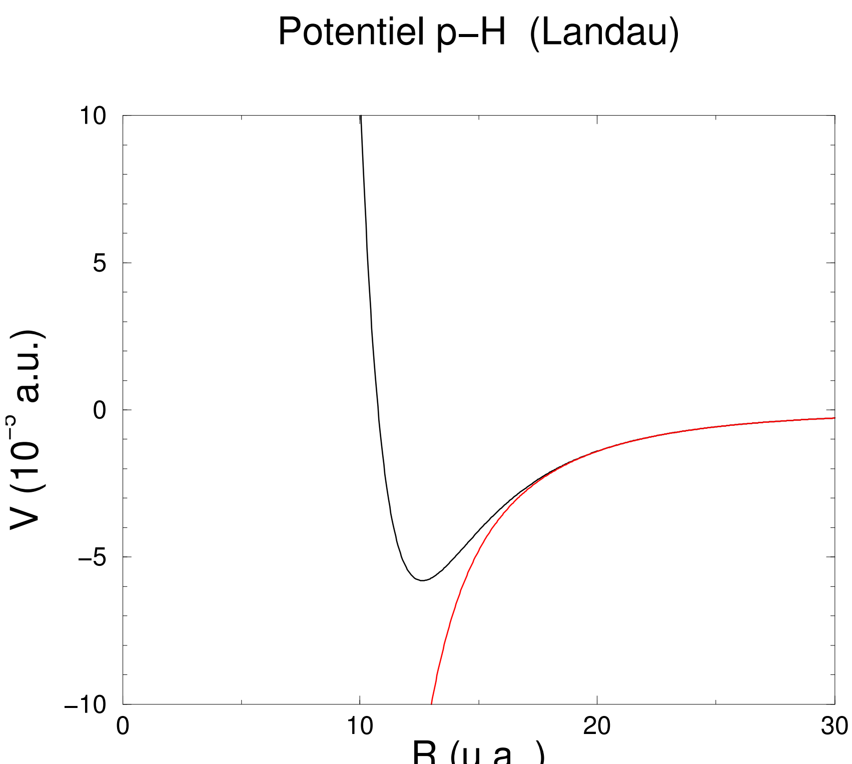


There exist more clever « regularizations »

e.g. Landau-Lifshitz proposed for S=1 (Σ_u) states (exercise § 81)

$$V_{LL}(x) = \frac{2x}{e^{x+1}} - \frac{\alpha_d}{2x^4} \qquad \Longrightarrow \qquad V^R_{LL}(x) = \begin{cases} V_{LL}(x) & \text{if} \quad x \geq x_c \\ V_{LL}(x_c) & \text{if} \quad x \leq x_c \end{cases}$$

with x=2.5



$X=\mu^+$

Rich spectrum of bound states

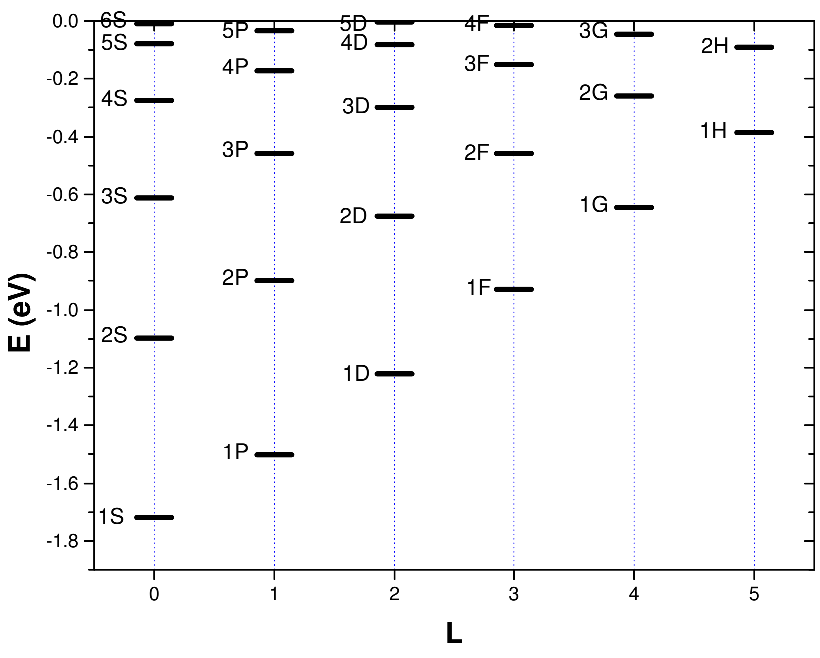
L=5,6,7 display **very narrow resonances**, visible in the total cross section (blue)

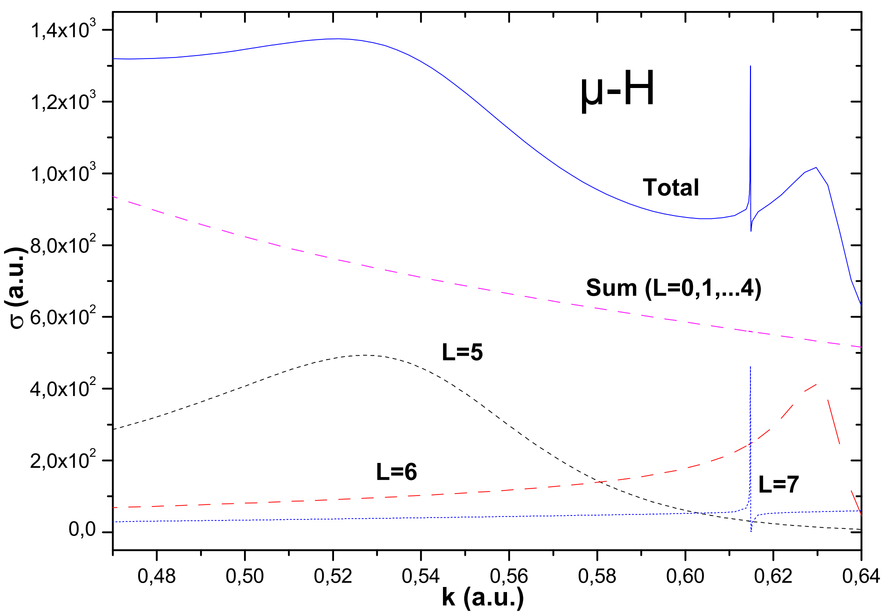
CSM calculations gives :

$$E_5 = (7.9 - 1.4\ i\ )10^{-4}\ \text{(a.u.)}$$

$$E_6 = (1.1 - 0.25\ i\ )10^{-3}$$

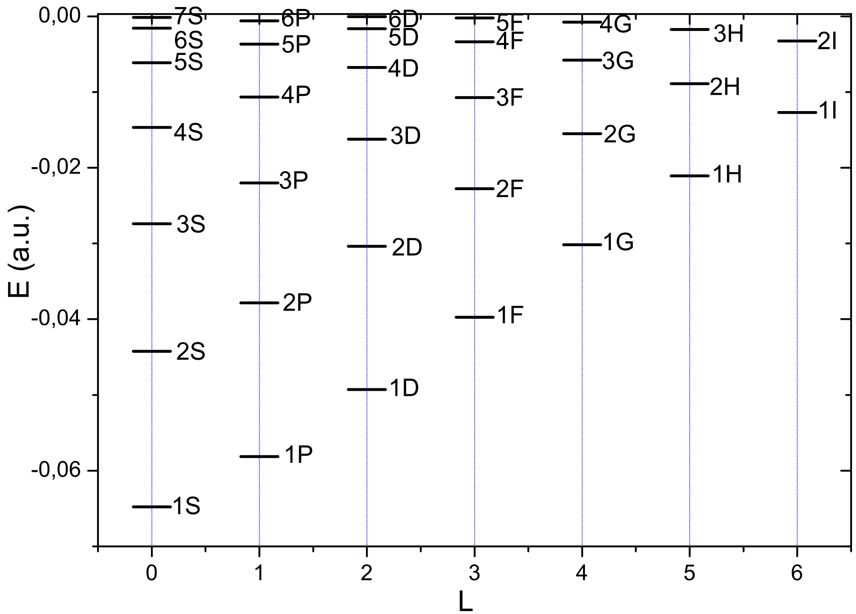
$$E_7 = 1.0 \times 10^{-3} - 1.3\ i\ \times 10^{-7}$$

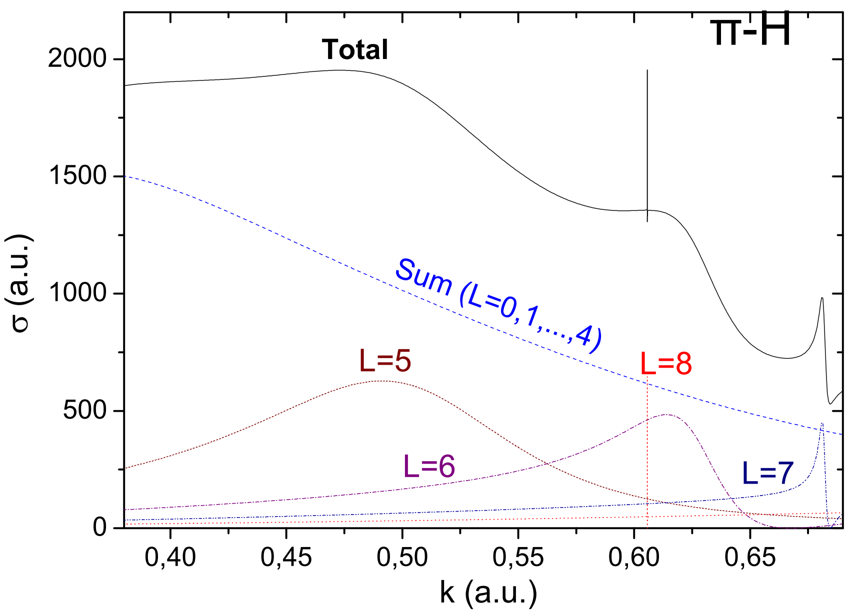




X=π^+

The same with π^+





Larger is m_X, richer is the spectrum

THE NUMBERS

Is the 2-body approach reliable ?

.... certainly not !

The dipole is not static !

It is not a two body problem… but an unpredictible 3-body one

Let’s do a good job and get an unambiguous answer: the privilege of Few-Body approach

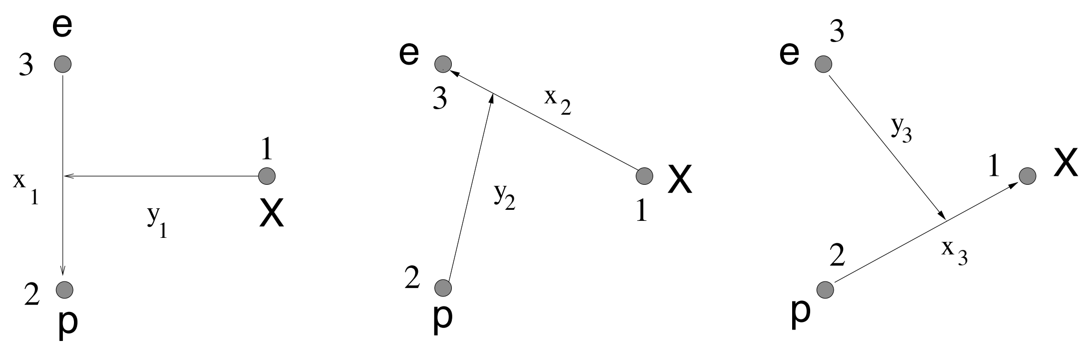
We solved the Faddeev-Merkutriev equations for the p,e,p three-body problem

No any “fantasy” in the Hamiltonian.

Only inputs : 1/r and m_e/m_p !!!

In few words, solve $(E - H_0)\Psi = V\Psi \qquad V = V_1 + V_2 + V_3$

by assuming $\Psi = \Psi_1 + \Psi_2 + \Psi_3$



$\Psi_1 \equiv \Psi_{X-(pe)}$ $\Psi_2 \equiv \Psi_{p-(eX)}$ $\Psi_3 \equiv \Psi_{e-(pX)}$

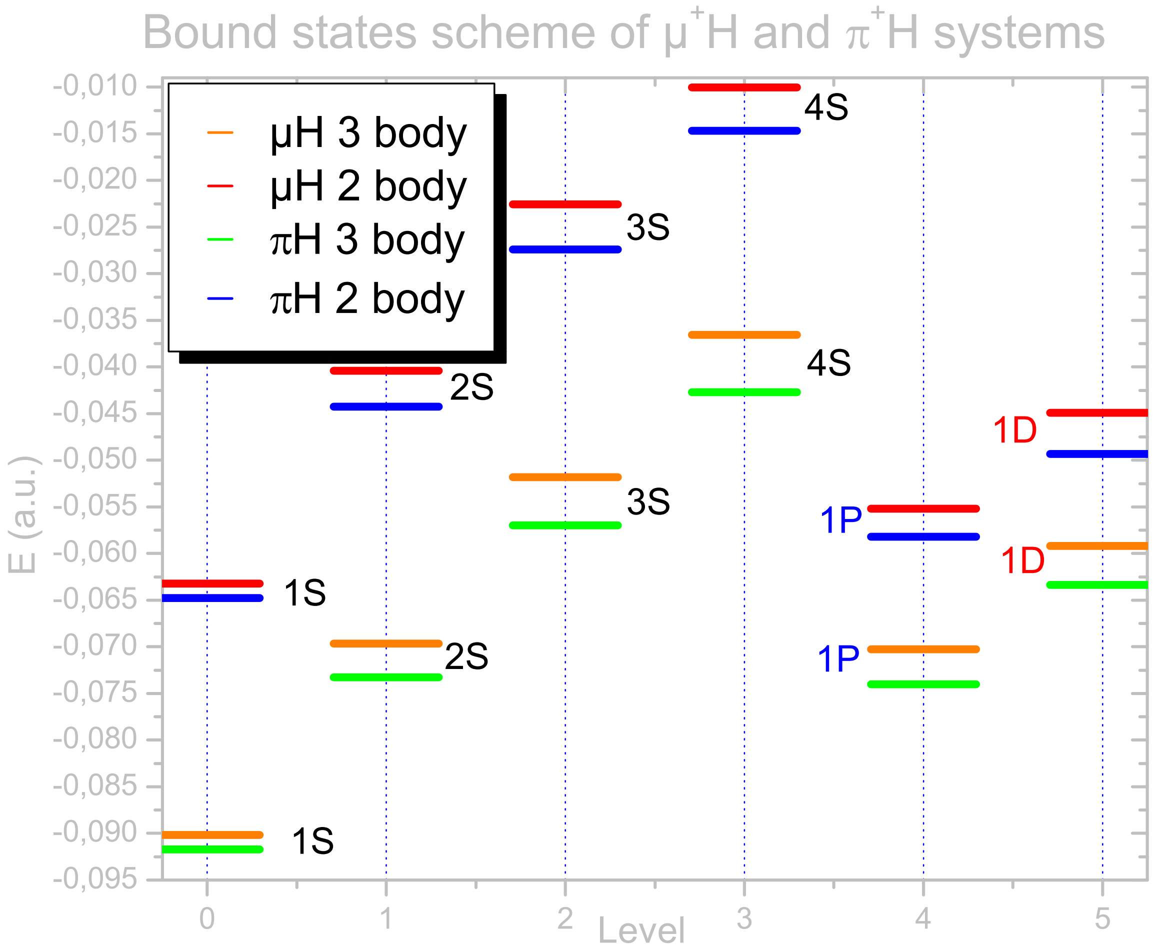
which fulfill

$$
\begin{aligned}
(E - H_0 - V_1)\Psi_1 &= V_1(\Psi_2 + \Psi_3) \\
(E - H_0 - V_2)\Psi_2 &= V_2(\Psi_3 + \Psi_1) \\
(E - H_0 - V_3)\Psi_3 &= V_3(\Psi_1 + \Psi_2)
\end{aligned}
$$

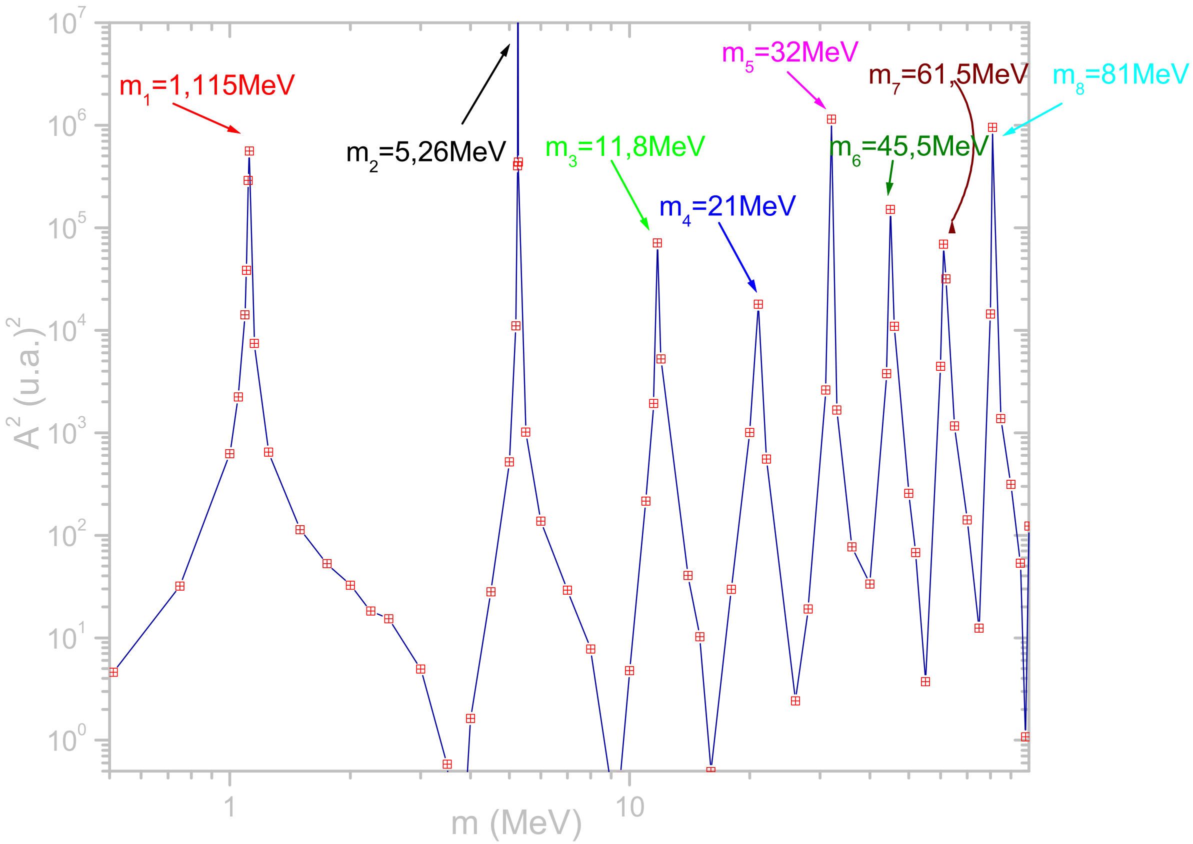
with proper assymptotic boundary conditions

Modified by S.P. Merkuriev, to avoid long range coupling among equations

Numbers, now totally reliable, are different than in 2-body
… but physics is the same



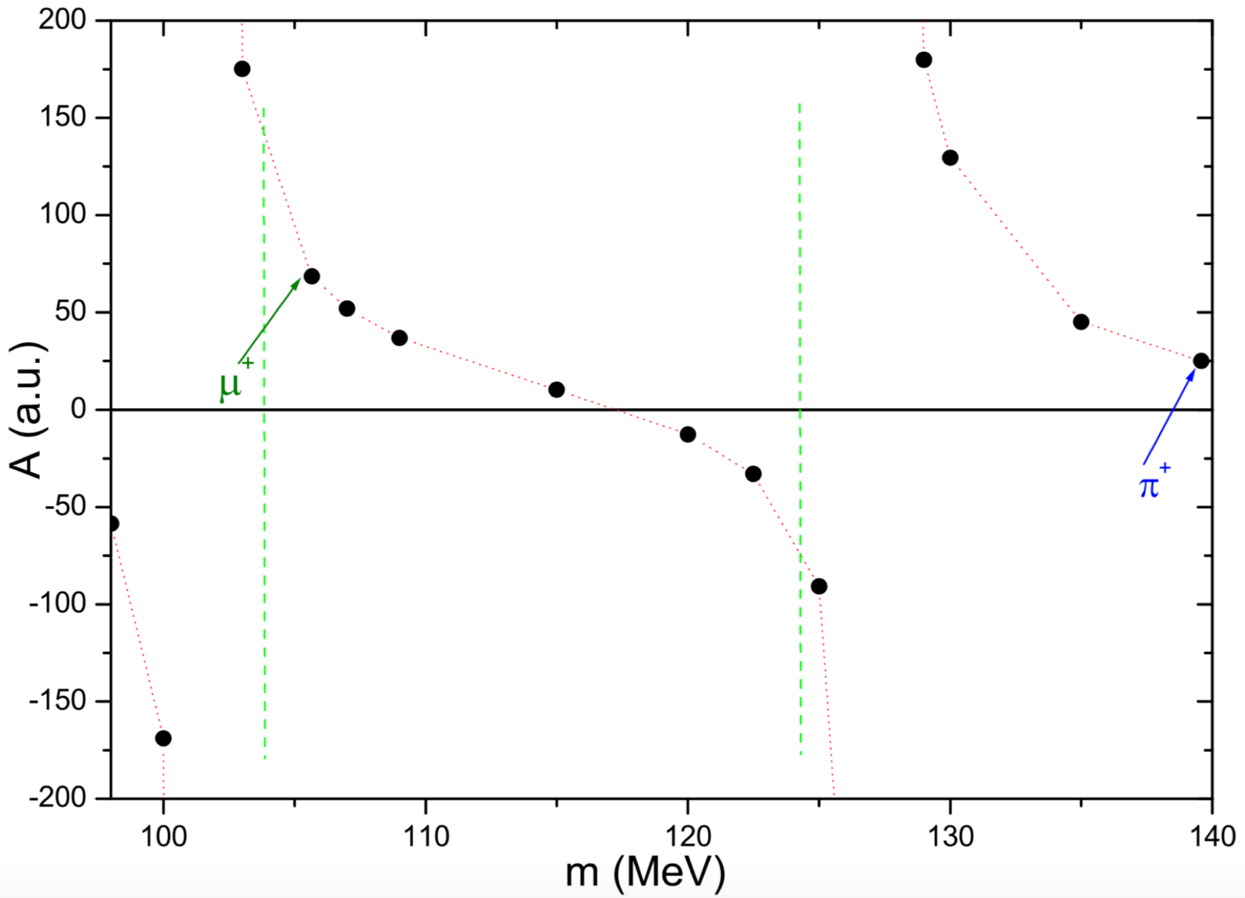
Scattering lengths as a function of m_X



Each peak denotes the appearance of a (L=0) X-H bound state

Interesting things start at 1.115 MeV (2.18 m_e)….but no particles there

Predictions for scattering lengths of physical interest



$$a_{\pi^+H} = 24.4 \text{ et } a_{\mu^+H} = 69.1 \text{ (u.a.)}$$

The very particular case X=p

Total wf must be antisymmetric with respect to **p↔p** exchange.

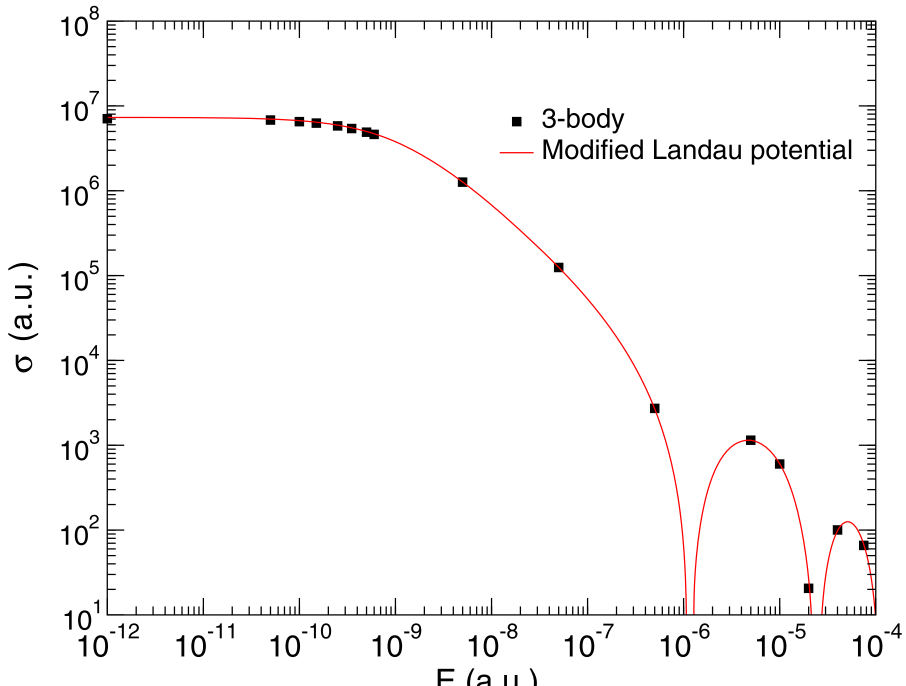
If $\mathbf{S_{pp}=0}$, the spatial part is **symmetric** **(state 1sσ_g** , molecular notation)

If $\mathbf{S_{pp}=1}$, the spatial part is **antisymmetric** **(state 2p σ_u ,** molecular notation)

For $\mathbf{S_{pp}=0}$ we found **a_0=-29.3 a.u** **R. Lazauskas, J. Carbonell, Few-Body Syst 31 (2002)125**

For $\mathbf{S_{pp}=1}$ we found **a_1=750 a.u.**

and the corresponding huge cross section **(all that is L=0)** !!!



A very slow proton approaching an H atom « feels » a monster

See horizontal scale !!!

The very particular case X=p

By computing the **L=0** pH phase shifts and the (modified) low energy parameters

$$k\cot\delta(k) = -\frac{1}{a} + \frac{\pi\alpha_D}{3a_0^2}\,k + \frac{4\alpha_D}{3a_0}\,k^2\log k + o(k^2)$$

we showed that it corresponds to a **H_2^+** **S_{pp}=1** bound state(*) with **B=1.1 x 10^{-9}** a.u.

R. Lazauskas, J. Carbonell, Few-Body Syst 31 (2002)125

- Never found before !

- To our knowledge, **the weakest bound ever found :** smaller than ^{4}He dimer

- It happens in the (almost) simplest system: no any parameter !

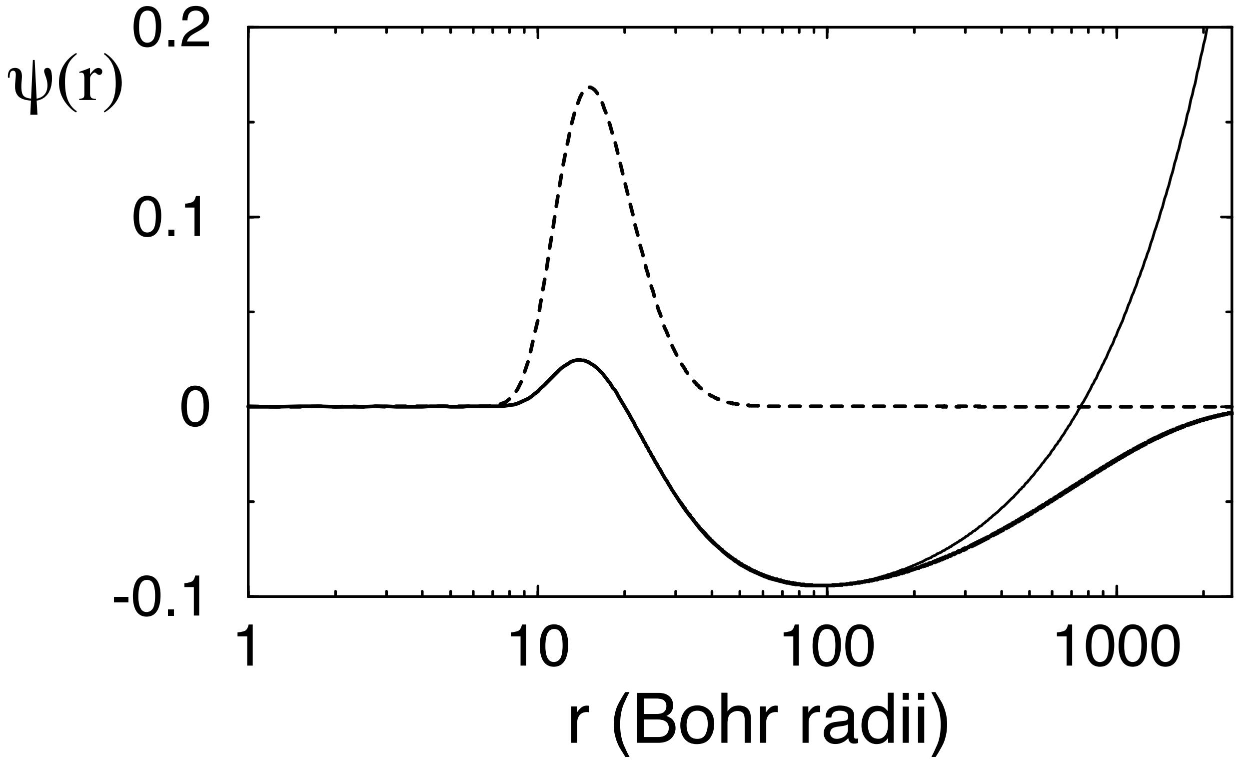
(*) It's the 1st excited: the ground state (already known) has **B=1.56 10^{-5}** a.u.

The very particular case X=p

Direct bound state calculation were performed one year later using variational methods

J. Carbonell, R. Lazauskas, D. Delande, L. Hilico, S.Kilic, Europhys Lett 64 (2003) 316

And totally confirming our results **$B=1.085045 \times 10^{-9}$** a.u.



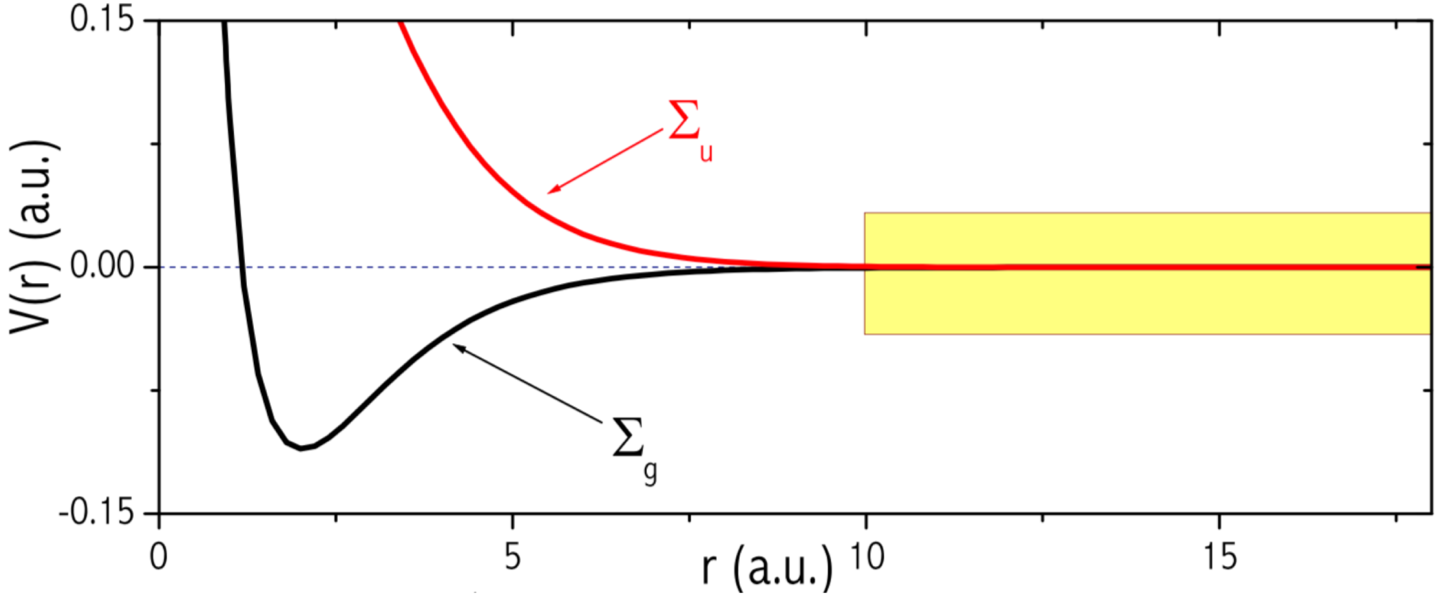
Ground and first excited S=1 state compared to pH scattering wf

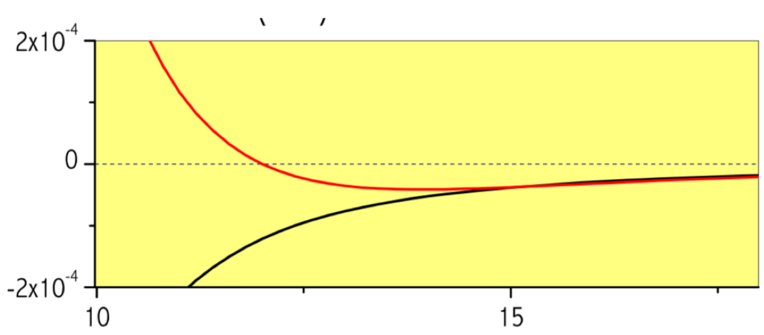
Born-Openheimer view of H_2^+

For S=0, V(Σu) is quite attractive with 20 bound states (v=1,2,…20)

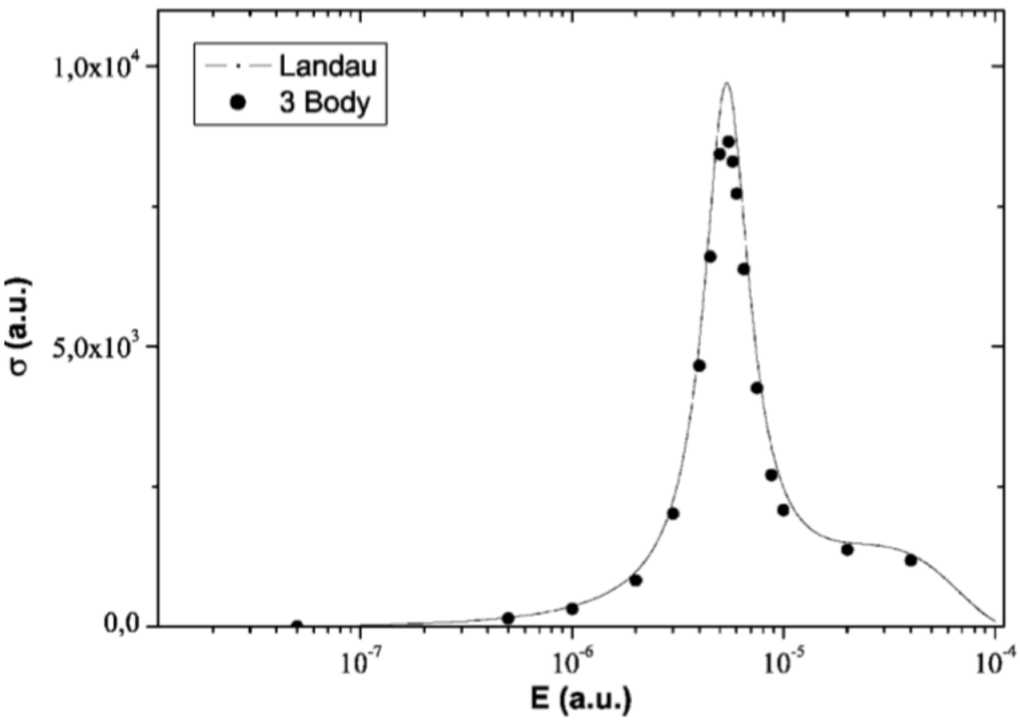
Pauli PhD (Sommerfeld) : « show » H_2^+ cannot exist !

For S=1, V(Σg) is repulsive, but has tiny attractive pocket at r=15





There are also interesting p-H (S=1) resonances



Relativistic corrections were computed …and are small

J. Carbonell, R. Lazauskas, D. Delande, L. Hilico, S.Kilic, Europhys Lett 64(2003)316
J. Carbonell, R. Lazauskas, V.I. Korobov, J. Phys. B: At. Mol. Opt. Phys. 37(2004)2997 **

Casimir-Polder retardation effects
at V(100 a.u) is 10^{-15} and $\Delta B/B=10^{-6}$

$$V(R) = -\frac{\alpha_d}{2R^4}\left(1 - \frac{11\alpha}{2\pi}\frac{m_e}{m_p}\frac{1}{R}\right)$$

Corrections due to Breit-Pauli Hamiltonian

$$\delta E^{(2)}_{\rm rc} = \alpha^2\left\langle -\frac{\mathbf{p}_e^4}{8m_e^3} + \frac{4\pi}{8m_e^2}\left[\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)\right]\right\rangle$$

$$\delta E^{(2)}_{\rm tr-ph} = \frac{\alpha^2}{2M_p}\left\langle \frac{\mathbf{p}_e\mathbf{p}_1}{r_1} + \frac{\mathbf{r}_1(\mathbf{r}_1\mathbf{p}_e)\mathbf{p}_1}{r_1^3} + (1\leftrightarrow 2)\right\rangle - \frac{\alpha^2}{2M_p^2}\left\langle \frac{\mathbf{p}_1\mathbf{p}_2}{R} + \frac{\mathbf{R}(\mathbf{R}\mathbf{p}_1)\mathbf{p}_2}{R^3}\right\rangle.$$

$$\delta E_{\rm nuc} = \frac{2\pi(R_p/a_0)^2}{3}\langle\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)\rangle,$$

Radiative and higher order corrections

$$\delta E^{(3)} = \alpha^3\sum_{i=1,2}\left[\frac{4}{3}\left(-\ln\alpha^2 - \beta(L,v) + \frac{5}{6} - \frac{1}{5}\right)\langle\delta(\mathbf{r}_i)\rangle + \frac{2}{3M_p}\left(-\ln\alpha - 4\beta(L,v) + \frac{31}{3}\right)\langle\delta(\mathbf{r}_i)\rangle - \frac{14}{3M_p}Q(r_i)\right]$$

$$\beta(L,v) = \frac{\langle\mathbf{p}_e(H_0-E_0)\ln((H_0-E_0)/R_\infty)\,\mathbf{p}_e\rangle}{4\pi\,\langle\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)\rangle}$$

$$Q(r) = \lim_{\rho\to 0}\left\langle\frac{\Theta(r-\rho)}{4\pi r^3} + (\ln\rho + \gamma_E)\delta(\mathbf{r})\right\rangle$$

All that for …almost nothing !

Table 3. Relativistic and QED corrections to the $2p\sigma_u(v = 1)$ state of the hydrogen molecular ion H_2^+.

ΔE_{nr}	$-1.085\,045\,252(1) \times 10^{-9}$
ΔE_{α^2}	$0.003\,298\,5(4) \times 10^{-9}$
ΔE_{α^3}	$-0.000\,470\,02(1) \times 10^{-9}$
ΔE_{α^4}	$-0.000\,003\,29 \times 10^{-9}$
E_B	$1.082\,219\,8(4) \times 10^{-9}$

Instead of $B=1.085045 \times 10^{-9}$

SOME REMARKS

This nice adventure inspired me some "thoughts"
I leave them to you as a way of conclusion

I. Simple approaches are helpful to feel things, but have no any predictive power

II. Exact solutions, even for the simplest three-body problem, contain **unexpected**, **fascinating** - and **reliable** - surprises … still quite unknown to AMO community

III. The existence of this **S_{pp}=1** excited state of **H_2^+** with **B=1.09 10^{-9}** is not only a curiosity of nature, but dominates the low energy scattering of p's by H atoms

Hard to believe that such gigantic cross section would have no any consequence

- huge enhancement in the **H_2^+** production cross sections

IV. Experimental observation would be more than welcome !

- Hard in direct spattering pH (cf. Prof. R. Doerner, last week)
- The predicted state is coupled radiatively to L=1 S=0 states.

  elect-dipole transition between these levels should be observable in 6GHz range

« Why it is bound ? »

Of course no any need for it, but we are facing an incredible object !!!

The problem presented is just the simplest of a long series of « simple » problems

Of particular interest are those related to the anti-hydrogen production at CERN AD

p-Positronium charge exchange $\bar{p} + Ps \rightarrow \bar{H} + e^-$ **(I)**

3-body recombination $\bar{p} + e^+ + e^- \rightarrow \bar{H} + e^+$

$\bar{H}^+$ production $\bar{H} + Ps \rightarrow \bar{H}^+ + e^-$ **(II)**

Astonishly, GBAR uses **(I)** and (**II**) to get $\bar{\mathrm{H}}$ after e^+ ejection

In (I)

- What is the optimal $\bar{\mathrm{p}}$ energy ?
What states are populated and with what crosss ection
- Is it interesting to use Ps* targets ?

In (II)

- What are the optimal states, both for $\bar{\mathrm{H}}$ and Ps ?

Wait for R. Lazauskas talk