FuPhy2024 : Future Nuclear and Hadronic Physics at the CERN-AD

Resonance states in antiprotonic helium

Jean Servais

Physique Nucléaire et Physique Quantique

Université libre de Bruxelles

(Brussels, Belgium)

Collaborator : J. Dohet-Eraly

April 2024

Background

The CERN AD & ELENA have opened the path to high-precision measurement on antimatter :

- exploring antimatter properties,
- probing CPT symmetry by searching tiny asymmetries in matter / antimatter properties.

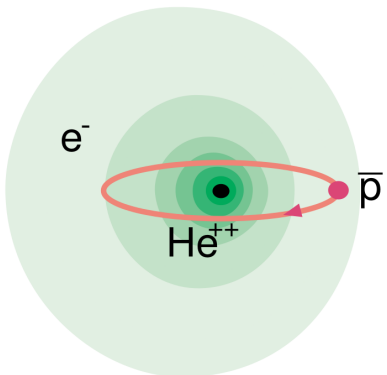
Some collaborations :

- AEgIS & GBAR : study of $\bar{g}$ on $\bar{\mathrm{H}}$,
- ALPHA : $\bar{\mathrm{H}}$ spectroscopy,
- BASE : antiproton magnetic moment,
- ASACUSA : experiments with **antiprotonic helium** ($\mathrm{He}^+\bar{p}$) to measure $m_{\bar{p}}/m_e$.

The ASACUSA experiments with $He^+\bar{p}$

Study of antiprotonic helium, a metastable three-body system made of He^{2+}, $\bar{p}$, and e^-, by **spectroscopic techniques**.

- 2011 : first high-precision measurement of $m_{\bar{p}}/m_e = 1836.1526736(23)$[1]
- 2016 : improvement of the previous value, $m_{\bar{p}}/m_e = 1836.1526734(15)$[2]. This value agrees with the ratio m_p/m_e, within the **experimental error bar**.
- 2020 : similar experiments with pionic helium $(He^+\pi^-)$[3], and prospects with other exotic atoms (He^+K^- or $H\bar{p}$).



Antiprotonic helium. Figure extracted from Yamazaki, T., *et al.* (2002). Physics Reports, 366, 183-329.

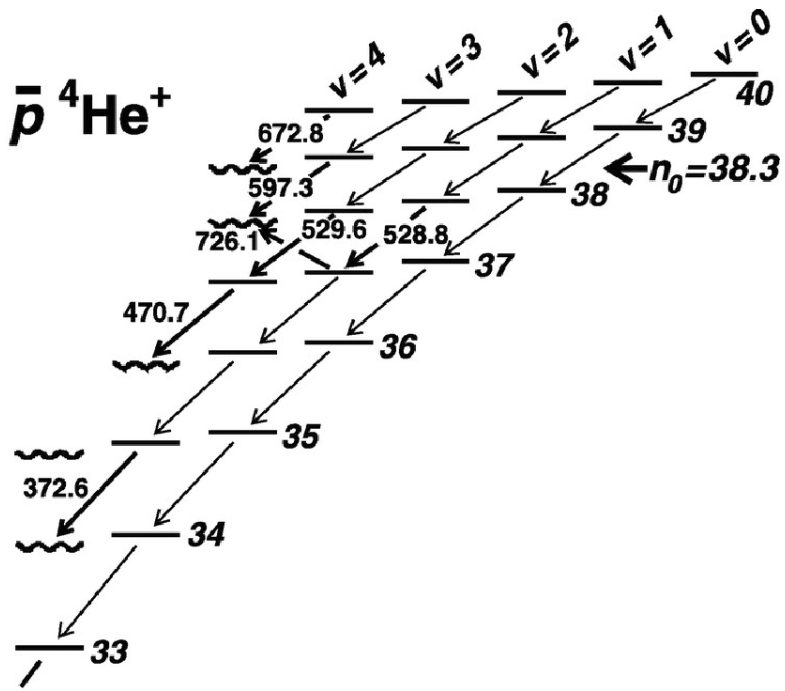
[1] Hori, M., *et al.* (2011). Nature, 475, 484-488.
[2] Hori, M., *et al.* (2016). Science, 354, 610-614.
[3] Hori, M., *et al.* (2020). Nature, 581, 37-41.

A metastable hybrid atomic system

Antiprotonic helium is an exotic atom containing both matter and antimatter.
Process of **creation of this unstable long-lived atom** :

1. A fraction of antiprotons ($\sim 3\%$) replace one electron in the electronic cloud of He.
2. Capture in high-n, nearly circular states ($L_0 \sim n_0 - 1$), with

$$n_0 \sim \sqrt{\frac{m_{\mathrm{He}} m_{\bar{p}}}{(m_{\mathrm{He}} + m_{\bar{p}}) m_e}} \sim 38.$$



Antiprotonic helium quasibound spectrum. Figure exctracted from M. Hori, Can. Jour. Phys. 89.1 (2011)

A metastable hybrid atomic system

Antiprotonic helium is an exotic atom containing both matter and antimatter.
Process of **creation of this unstable long-lived atom** :

3. **Resonance** states (i.e. unstable but long-lived), with

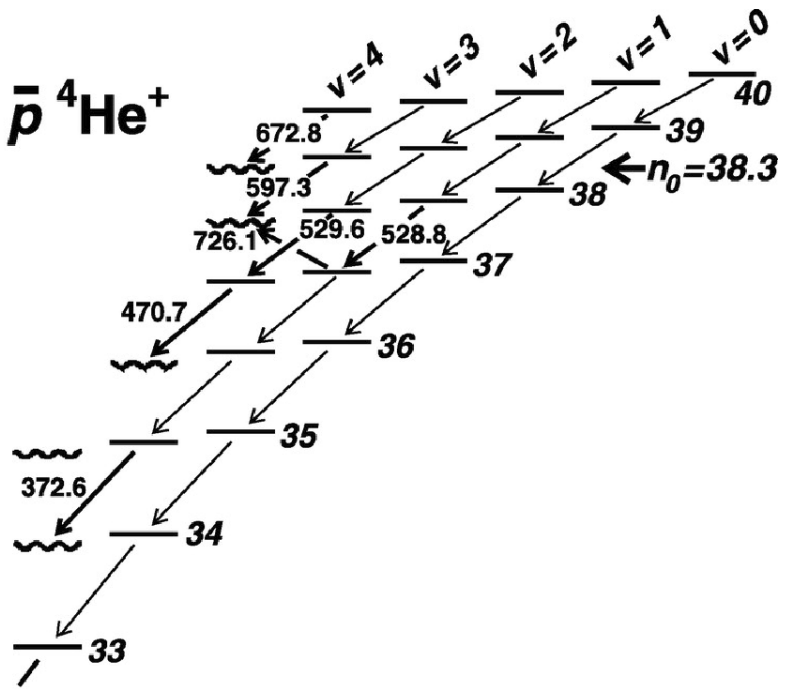
   $E_{\text{res}} = E_r - i\frac{\Gamma}{2}$ and $\tau_{\text{Auger}} \sim \hbar/\Gamma$.

   Resonances labeled by (L, υ).

4. Deexcitation mainly by two competing processes
   - Auger emission of e^-
   - Radiative transitions ($\rightarrow$ spectroscopy)

5. **Slow** cascade process

$\rightarrow$ long-lived atom suitable for experiments ($\sim \mu$s $\gg$ ps)



Antiprotonic helium resonance spectrum. Figure exctracted from M. Hori, Can. Jour. Phys. 89.1 (2011)

Theoretical description of exotic atoms

Given these high-precision measurements, as e.g.

$$1132609226.7(2.8)(2.5)(1.4)\ \text{MHz for the } (31,0) \rightarrow (30,0) \text{ transition,}$$

theoretical results are needed to infer the antiproton mass from spectroscopic data. This system has been studied very accurately **for a restricted number of states** ($L = 28 - 41$, $\upsilon = 0 - 5$), relevant from an experiment p.o.v., mostly by

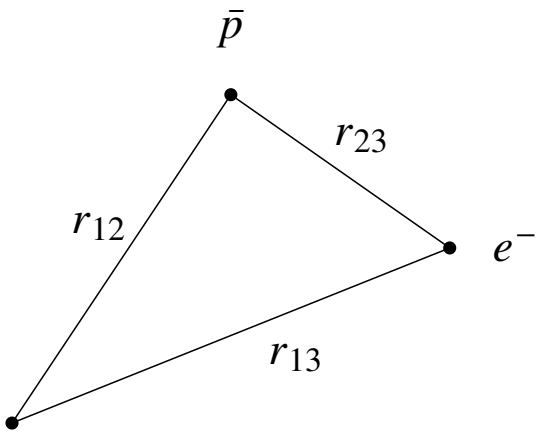
- Korobov and coworkers,
- the Kyushu group.

My research aims at

- studying **resonances in three-body atomic systems** (exotic or not), by means of a method as simple, fast, and accurate as possible,
- probing this method by performing **calculations on antiprotonic helium**, which has been studied very accurately (**appropriate benchmark system**),
- while enriching our knowledge of its resonance spectrum.

Preliminary theoretical description (E_r)

Three-body system



He^{2+}

$$E_{\text{res}} = E_r - i\frac{\Gamma}{2}$$

Internal coordinates

Perimetric coordinates $(x, y, z, \psi, \theta, \phi)$

$$\begin{cases} x &= r_{12} - r_{23} + r_{12} \\ y &= r_{12} + r_{23} - r_{13} \\ z &= -r_{12} + r_{23} + r_{13} \end{cases}$$

Wavefunction

$$\Psi^{\pi}_{c,LM} = \sum_{K=0}^{L} \mathcal{D}^{L\pi}_{MK}(\psi, \theta, \phi)\Phi_K(x, y, z)$$

Non-relativistic description

$$(T + V)\Psi^{\pi}_{c,LM} = E\ \Psi^{\pi}_{c,LM},$$

with $V = Z_1 Z_2/r_{12} + Z_2 Z_3/r_{23} + Z_1 Z_3/r_{13}$.

$\triangle$ Preliminary **simplified** description : apply a bound-state-like approach, and compute $E = E_r \in \mathbb{R}$.

Radial basis functions

Real wavefunction

$$\Psi^{\pi}_{c,LM} = \sum_{K=0}^{L} \mathcal{D}^{L\pi}_{MK}(\psi,\theta,\phi)\Phi_K(x,y,z)$$

The Lagrange-mesh method[1]

$$\Phi_K(x,y,z) = \sum_{ijk} C^K_{ijk} F^K_{ijk}(x,y,z)$$

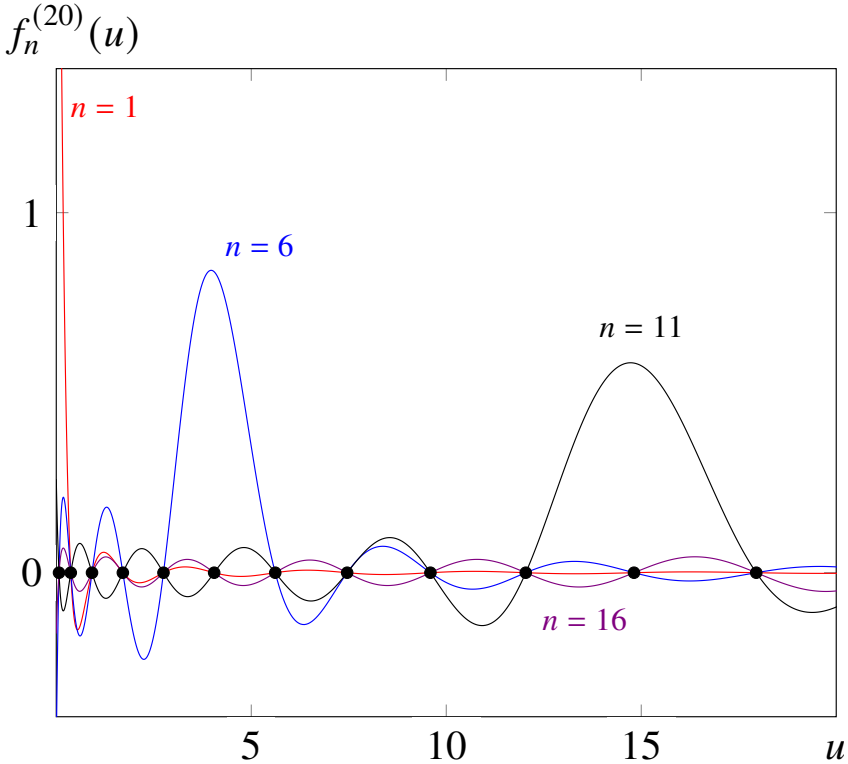
where

$$F^K_{ijk} \propto f_i^{(N_x)}\left(\frac{x}{h_x}\right) f_j^{(N_y)}\left(\frac{y}{h_y}\right) f_k^{(N_z)}\left(\frac{z}{h_z}\right),$$

Orthonormality at the Gauss approximation

$$\left\langle F_{ijk} \middle| F_{lmn} \right\rangle_G = \delta_{il}\delta_{jm}\delta_{kn}$$

+ diagonal potential matrix, sparse Hamiltonian matrix → **accuracy and ease**



The **Lagrange-Laguerre functions** $f_n(u)$ are proportional to the product of a Laguerre polynomial and an exponential.

[1] Baye, D. (2015). Physics reports, 565, 1-107.

Quasibound states: some valuable insights

Diagonalizing the Hamiltonian matrix, one obtains $E_r \in \mathbb{R}$,

$$E_{\text{res}} = E_r - i\frac{\Gamma}{2}.$$

- Quasibound real energies have been computed for a wide range of L, from 0 to 80 (see r.h.s. for $\upsilon = 0$).
- The number of stable digits on E_r is **very roughly** of the order of magnitude of $1/\Gamma$.

L	E_r	L	E_r
3	−183.862303	22	−6.090
4	−117.851910	23	−5.642
5	−81.99445	24	−5.2596
6	−60.37364	25	−4.90952
7	−46.3411	26	−4.60246
8	−36.7205	27	−4.330238
9	−29.8391	28	−4.0881916
10	−24.7480	29	−3.87240911
11	−20.876	30	−3.679774786
12	−17.863	31	−3.5076350311
13	−15.473	32	−3.35375786378
14	−13.546	33	−3.21624423252
15	−11.967	34	−3.09346690187
16	−10.662	35	−2.98402095424
17	−9.570	36	−2.88668239016
18	−8.645	37	−2.80037231540
19	−7.857	38	−2.72412479286
20	−7.180	39	−2.657056942961
21	−6.594	40	−2.598340648168

Quasibound real energies for ($L = 3-40,\ \upsilon = 0$)[1].

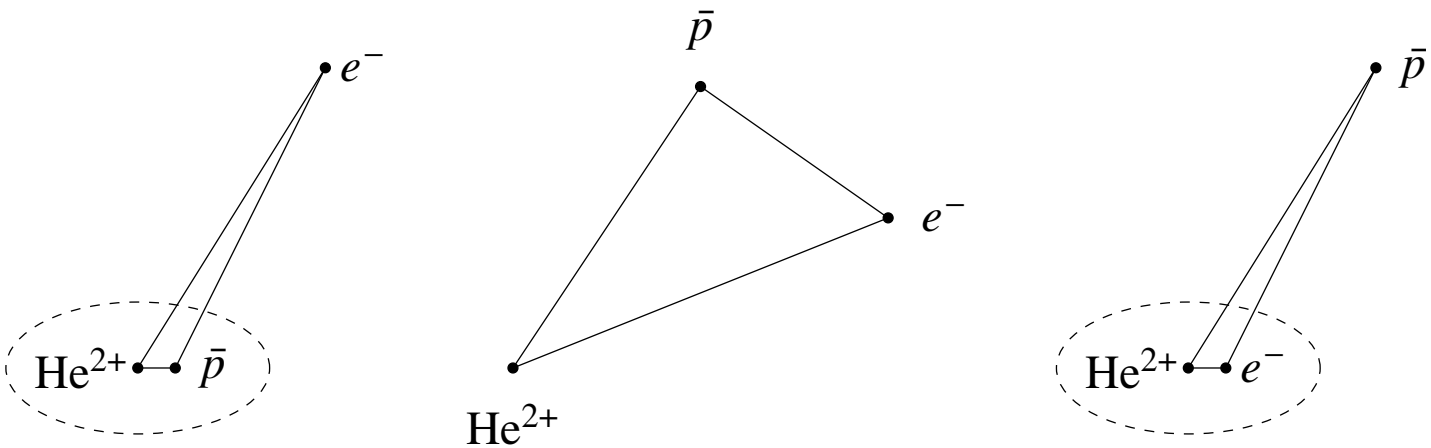
[1] Baye, D., Dohet-Eraly, J., and Schoofs, P. (2019). Physical Review A, 99, 022508.

Quasibound states: some valuable insights

In addition to E_r, the real wavefunction leads to

- the mean radii for the same angular momenta[1]
- relativistic corrections (discussed later in this talk)
- radiative-decay lifetimes (discussed later in this talk)

In addition, the hydrogenic picture appears for low and high L ($\rightarrow$ "atomcule"[2]).



$L \lesssim 20$ $\quad$ $21 \lesssim L \lesssim 45$ $\quad$ $46 \lesssim L$

[1] Baye, D., Dohet-Eraly, J., and Schoofs, P. (2019). Physical Review A, 99, 022508.

[2] Yamazaki, T., *et al.* (2002). Physics Reports, 366, 183-329.

Accessing resonance widths (E_r, Γ)

Generalities

A resonance $\equiv$ a pole of the $\mathcal{S}$ matrix.

The corresponding resonance wavefunction, also called a Siegert state, only contains outgoing components which **diverge at infinity**.

Evaluating the Auger width $\Gamma \leftrightarrow$ **calculations in the complex plane** ($E_{\text{res}} \in \mathbb{C}$).
In this work, two approaches have been adopted :

1. the **complex-scaling method**, which rotates the wavefunction in the complex plane, to make it convergent at infinity ($\rightarrow$ bound-state-like techniques are applicable)
2. the **Kohn variational principle**, which includes explicitly the asymptotic wavefunctions describing the scattering

$$\mathrm{He}^{2+}\bar{p} + e^- \rightarrow \mathrm{He}^{2+}\bar{p} + e^-$$

in the total wavefunction, in order to determine the scattering properties of the state (e.g. phase shift, $\mathcal{S}$ matrix)

Complex scaling method

Principle

Scaling of the radial coordinates

$$r_{lm} \rightarrow r_{lm} e^{i\theta}$$

in the real wavefunction $\Psi^{\pi}_{c,LM}$ in perimetric coordinates.

Energies are rotated by an angle 2θ in the complex plane. Bound and **resonance energies are stable**,

$$\frac{\partial E_{\text{res}}}{\partial \theta} = \left\langle \Psi^{\pi}_{c,LM}(\theta) \middle| \frac{\partial H}{\partial \theta} \middle| \Psi^{\pi}_{c,LM}(\theta) \right\rangle \approx 0,$$

while scattering states rotate.

L	E	E_r	Γ
2	-326.477424	-326.477423	$< 10^{-6}$
3	-183.862303	-183.862303	2×10^{-6}
4	-117.851910	-117.851909	8×10^{-6}
5	-81.99445	-81.994465	2.5×10^{-5}
6	-60.37364	-60.373637	6.1×10^{-5}
7	-46.3411	-46.341003	1.3×10^{-4}
8	-36.7205	-36.720433	2.3×10^{-4}
9	-29.8391	-29.839104	4.0×10^{-4}
10	-24.7480	-24.74797	6.3×10^{-4}
11	-20.876	-20.87608	9.6×10^{-4}
12	-17.863	-17.86326	1.4×10^{-3}
13	-15.473	-15.47318	1.9×10^{-3}
14	-13.546	-13.5456	2.6×10^{-3}
15	-11.967	-11.9687	3.4×10^{-3}
16	-10.662	-10.6626	4.3×10^{-3}
17	-9.570	-9.5691	5.4×10^{-3}
18	-8.645	-8.6448	6.5×10^{-3}
19	-7.857	-7.8568	7.8×10^{-3}
20	-7.180	-7.1800	9.2×10^{-3}
21	-6.594	-6.5951	1.1×10^{-2}

Extracted from Baye, D., *et al.* (2019). Physical Review A, 99, 022508.

Complex scaling method

The complex scaling and Lagrange-mesh methods

- succeeded in computing resonance energies and widths for $3 \leq L \leq 21$ ($\upsilon = 0$),
- failed to obtain states with higher L, relevant from an experiment p.o.v. ($l_{e^-} > 1$).

However,

- some authors succeeded to describe these resonances by means of the complex scaling, using a more complicated wavefunction[1,2],
- combining the Lagrange-mesh and complex-scaling methods proved to be highly efficient in bielectronic atoms such as Ps^- or He[3,4].

$\rightarrow$ the rotated wavefunction in perimetric coordinates is **unsuited to describe the present system** (different scales)
$\rightarrow$ a **variational scattering approach** is adopted in the following.

---

[1] Kino, Y., Kamimura, M., and Kudo, H. (1998). Nuclear Physics A, 631, 649-652.
[2] Korobov, V. I. (2014). Physical Review A, 89, 014501.
[3] Dohet-Eraly, J. and Servais, J. (2022). Journal of Physics B 55, 245001.
[4] Servais, J. and Dohet-Eraly, J. (2023). Journal of Physics B 56, 075001.

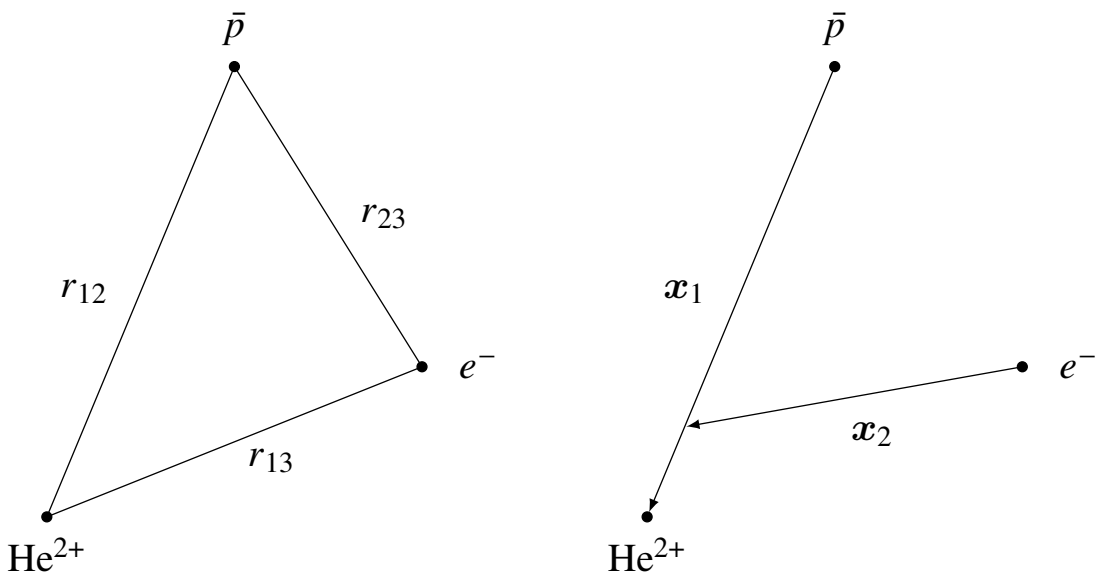
Kohn Variational principle

The principle is to include explicitly wavefunctions describing **the asymptotic state related to the scattering**

$$\mathrm{He}^{2+}\bar{p} + e^- \rightarrow \mathrm{He}^{2+}\bar{p} + e^-.$$

The real wavefunction $\Psi^{\pi}_{c,LM}$ is complemented with asymptotic functions Ω depending on the Jacobi coordinates $(\boldsymbol{x}_1, \boldsymbol{x}_2)$,

$$\Psi = \Psi^{\pi}_{c,LM}(x, y, z, \psi, \vartheta, \phi) + \tilde{\mathcal{S}}\Omega^{O}(\boldsymbol{x}_1, \boldsymbol{x}_2) + \Omega^{I}(\boldsymbol{x}_1, \boldsymbol{x}_2).$$



Kohn Variational principle

The total wavefunction then reads,

$$\Psi = \Psi^{\pi}_{c,LM}(x, y, z, \psi, \vartheta, \phi) + \tilde{\mathcal{S}}\Omega^{O}(\boldsymbol{x}_1, \boldsymbol{x}_2) + \Omega^{I}(\boldsymbol{x}_1, \boldsymbol{x}_2).$$

Complex Kohn variational principle[1]:

$$\mathcal{S}(E) = \tilde{\mathcal{S}} + i \left\langle \Psi | H - E | \Psi \right\rangle ,$$

where $\tilde{\mathcal{S}}$ is obtained by varying the coefficients of the total wavefunction Ψ.

As **a resonance corresponds to a pole of the $\mathcal{S}$ matrix**,

$$\mathcal{S}\left(E_r - i\Gamma/2\right) \longrightarrow \infty,$$

the resonance parameters can be obtained by extrapolating the $\mathcal{S}$ matrix in the complex plane, from the real-energy axis[2].

[1] Miller, W. H., and Jansen op de Haar, B. M. (1987). The Journal of chemical physics, 86, 6213-6220.

[2] Rakityansky, S. A., *et al.* (2007). Journal of Physics A, 40, 14857.

Resonance parameters for $v = 0$

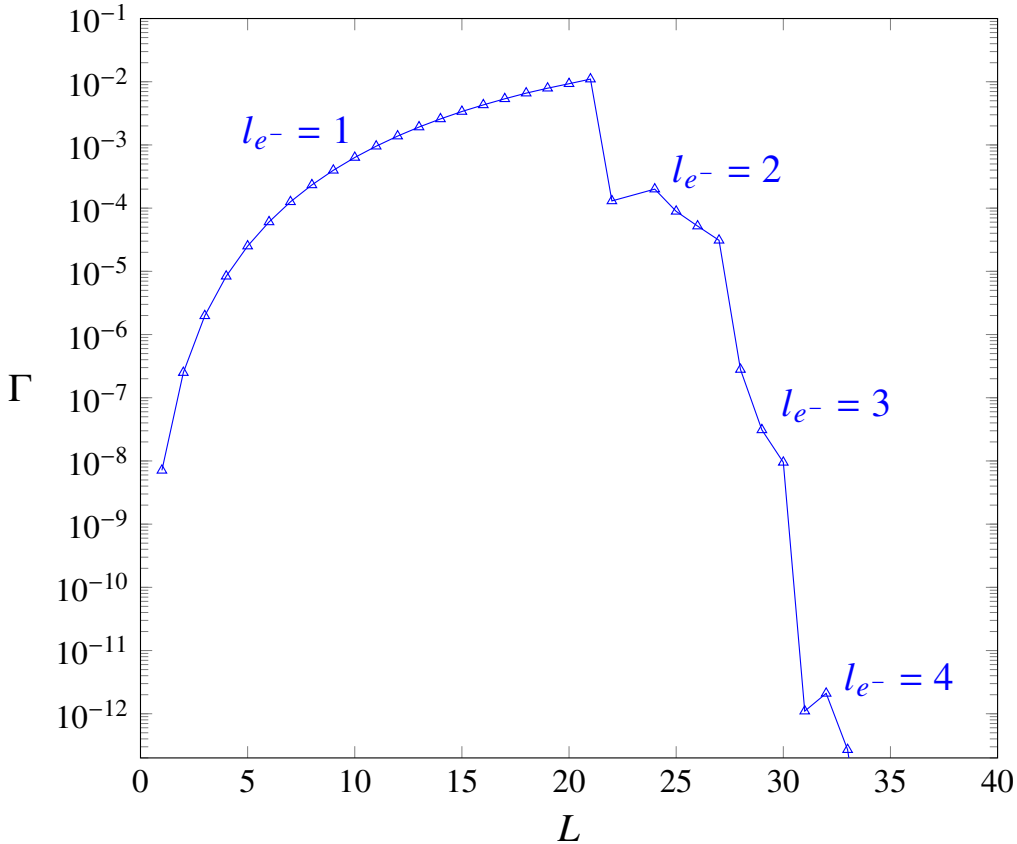
L	l_{e-}	E_r	Γ	E_r	Γ
		Current method		Complex scaling + LMM	
1	1	$-733.949\,246\,2$	7.1×10^{-9}	/	/
2	1	$-326.477\,424$	2.5×10^{-7}	$-326.477\,424$	/
3	1	$-183.862\,303$	1.98×10^{-6}	$-183.862\,303$	2×10^{-6}
4	1	$-117.851\,909$	8.36×10^{-6}	$-117.851\,909$	8×10^{-6}

L	l_{e-}	E_r	Γ	E_r	Γ
		Current method		Korobov[1]	
30	3	$-3.679\,774\,787\,7$	9.5×10^{-9}	$-3.679\,774\,787\,657\,6$	9.5204×10^{-9}
31	4	$-3.507\,635\,038\,98$	1.1×10^{-12}	$-3.507\,635\,038\,971\,01$	1.1×10^{-12}
32	4	$-3.353\,757\,870\,84$	2.1×10^{-12}	$-3.353\,757\,870\,833\,40$	2.14×10^{-12}
33	4	$-3.216\,244\,239\,07$	2.8×10^{-13}	$-3.216\,244\,239\,070\,02$	2.8×10^{-13}

Converged nonrelativistic resonance energies and widths for antiprotonic helium ($v = 0$). Korobov performed **complex-scaling calculations** with a higher number of nonlinear parameters, in sextuple-precision arithmetic ($\sim$ 48-digits numbers), hence achieving a higher accuracy.

[1] Korobov, V. I. (2008). Physical Review A, 77, 042506.

Widths for $v = 0$



- **The higher the momentum carried by the electron l_{e-}, the lower the Auger width**: the width decreases by several orders of magnitude when l_{e-} increases by one unit
- Auger emission is strongly hindered in **states with low** Γ, hence they **are suited for spectroscopic measurements**

Widths for $L = 32$

L	υ	l_{e^-}		E_r	Γ
32	0	4	Current	$-3.353\,757\,870\,84$	2.1×10^{-12}
			Korobov[1]	$-3.353\,757\,870\,833\,40$	2.14×10^{-12}
32	1	3	Current	$-3.227\,676\,379\,7$	5.45×10^{-9}
			Korobov[1]	$-3.227\,676\,379\,629\,4$	5.4474×10^{-9}
32	2	3	Current	$-3.116\,679\,796$	1.398×10^{-7}
			Korobov[1]	$-3.116\,679\,795\,873$	1.3947×10^{-7}

Resonance energies and Auger widths for $L = 32$, for rovibrational bands $\upsilon = 0 - 2$.

The Auger widths tend to increase as the rovibrationnal number increases.

[1] Korobov, V. I. (2008). Physical Review A, 77, 042506.

Conclusion regarding the nonrelativistic description

In this work, the Lagrange-mesh method (LMM) has been combined to

- the complex scaling method $\rightarrow \times$ (lack of flexibility)
- an explicit scattering approach $\rightarrow \checkmark$
  - simplicity of the LMM is mostly preserved
  - accurate results (Γ up to $\sim 10^{-13}$)

Overall, efficient method that competes well with more complicated ones[1].

However, this **nonrelativistic picture** is limited if comparison to experiments is needed.

[1] Note that resonances in H^- have been described accurately using this method, see arXiv : 2404.04191.

Other properties and corrections

Radiative transitions

The real wavefunction $\Psi^{\pi}_{c,LM}$ can be used to compute several quantities.

1. The quasibound wavefunction is used for computing $E1$ transitions[1],

$$\Gamma^{E1}_{i\to f} = \frac{4}{3}\alpha^3 (E_i - E_f)^3 \frac{1}{2L_i+1} \sum_{M_i M_f \mu} \left| \left\langle \Psi^{\pi_i}_{c,L_i M_i} \middle| O^{(1)}_{\mu} \middle| \Psi^{\pi_f}_{c,L_f M_f} \right\rangle \right|^2$$

   with $O^{(1)}_{\mu}$ a function of the Wigner-D matrices and of the perimetric coordinates.

The radiative lifetime is defined as

$$\tau_{E1} = \hbar \left(\sum_{\forall \text{ permitted } f} \Gamma^{E1}_{i\to f} \right)^{-1} .$$

It can be compared to the Auger lifetime $\tau_{\text{Auger}} \sim \hbar/\Gamma$.

[1] Pilón, H. O., and Baye, D. (2013). Physical Review A, 88(3), 032502.

Radiative transitions

L	l_{e^-}	E_r	Γ_{E1}
30	3	$-3.679\,774\,779$	1.28×10^{-11}
31	4	$-3.507\,635\,034$	1.602×10^{-11}
32	4	$-3.353\,757\,864$	1.795×10^{-11}
33	4	$-3.216\,244\,232$	1.885×10^{-11}
34	5	$-3.093\,466\,902$	1.898×10^{-11}

Nonrelativistic resonance energies and radiative widths for antiprotonic helium ($L \to L-1$), in the lowest rovibrational band $\upsilon = 0$.

Relativistic corrections

The real wavefunction $\Psi^{\pi}_{c,LM}$ can also be used to compute relativistic corrections.

2. The leading-order relativistic corrections is derived from the Breit-Pauli Hamiltonian,

$$H_e = -\alpha^2 \left\{ \frac{\boldsymbol{p}^4}{8} - \frac{\pi}{2} \left[Z_3 Z_1 \delta(\boldsymbol{r}_{13}) + Z_3 Z_2 \delta(\boldsymbol{r}_{23}) \right] \right\}.$$

The correction is evaluated perturbatively by computing the mean value of these operators.

Relativistic corrections

L	v	Γ	$\langle \boldsymbol{p}_2^4 \rangle$	$\langle \delta_{13} \rangle$	$\langle \delta_{23} \rangle$
32	0	2.1×10^{-12}	30.718 21	1.066 497	0.104 457 7
Korobov[1]		2.120×10^{-12}	30.718 284	1.066 498 3	0.104 458 28
33	0	2.7×10^{-13}	33.304 85	1.144 395 7	0.095 613 5
Korobov[1]		2.76×10^{-13}	33.304 865	1.144 396 3	0.095 613 57
33	1	5.3×10^{-12}	37.278 74	1.263 515	0.083 869 6
Korobov[1]		5.33×10^{-12}	37.278 814	1.263 524 0	0.083 870 45
34	0	–	36.069 94	1.227 561	0.086 593 3
Korobov[1]		–	36.069 959	1.227 561 4	0.086 593 37

The obtained accuracy on the corrections is of **at least 5 significant digits**. The results are more accurate as Γ decreases, as the bound-state-like description becomes more appropriate.

[1] Korobov, V. I. (2014). Physical Review A, 89(1), 014501.

Conclusion and prospects

Conclusion

- **Simple, fast and accurate numerical method** for describing theoretically antiprotonic helium and computing the resonance parameters for a wide range of the total angular momentum,
- Validated by very accurate results found in literature, still **powerful despite its high simplicity** (one open-channel, sparse Hamiltonian matrix, double-precision arithmetic), obtaining widths smaller than 10^{-12}

Prospects

- **Improving the accuracy** provided by the method (e.g. going beyond double-precision arithmetic, implementing higher-order relativistic corrections)
- Evaluating radiative transitions and relativistic corrections with the *total* wavefunction Ψ, containing the complex asymptotic functions
- **Explore other exotic three-body atoms**: pionic helium, kaonic helium