Antiproton collisions with excited positronium

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In memory of Michael Brunger

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Motivation

The primary motivation is to provide accurate atomic and molecular collision data for science and industry:

- Astrophysics
- Fusion energy
- Nanolithography
- Medical imaging and therapy
- Antihydrogen formation
  - investigate origin of matter-antimatter asymmetry via spectroscopy
  - No theory for antimatter interaction with gravity
  - Calculate $e^+ + H(nl) \leftrightarrow Ps(n'l') + p^+$

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Convergent close-coupling theory

Target structure

Use complete Laguerre basis $\xi_{nl}^{(\lambda)}(r) \propto \exp(-\lambda r)$:

- "one-electron" (H, Ps, Li,. . . ,Cs, H_2^+)

$$\phi_{nl}^{(\lambda)}(r) = \sum_{n'=1}^{N_l} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r),$$

- "two-electron" (He, Be,. . . , Hg, Ne, . . . , Xe, H_2, H_2O)

$$\phi_{nls}^{(\lambda)}(r_1, r_2) = \sum_{n',n''} C_{nls}^{n'n''} \xi_{n'l'}^{(\lambda)}(r_1) \xi_{n''l''}^{(\lambda)}(r_2),$$

- Diagonalise the target (FCHF) Hamiltonian

$$\langle \phi_f^{(\lambda)} | H_{\mathrm{T}} | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}.$$

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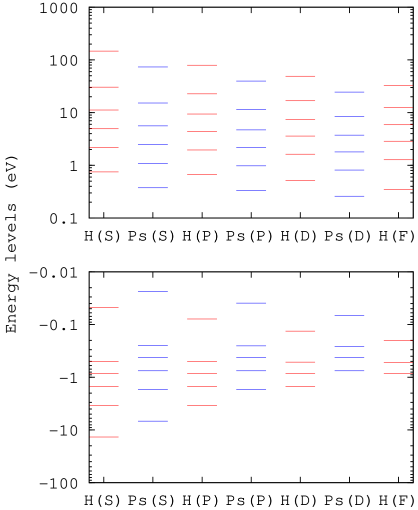
- H and Ps energies for $N_{\rm H}^{\ell} = N_{\rm Ps}^{\ell} = 12 - \ell$, for $\ell \leq 3$



two-center positron scattering

- Positron-target wavefunction is expanded as

$$|\Psi_i^{(+)}\rangle \approx \sum_{n=1}^{N_{\rm H}} |\phi_n^{\rm H} F_{ni}^{\rm H}\rangle + \sum_{n=1}^{N_{\rm Ps}} |\phi_n^{\rm Ps} F_{ni}^{\rm Ps}\rangle. \quad (1)$$

- Solve for $T_{fi} \equiv \langle \boldsymbol{k}_f \phi_f | V | \Psi_i^{(+)} \rangle$ at $E = \varepsilon_i + \epsilon_{k_i}$,

$$\langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle = \langle \boldsymbol{k}_f \phi_f | V | \phi_i \boldsymbol{k}_i \rangle + \sum_{n=1}^{N_{\rm H}+N_{\rm Ps}} \int d^3k \frac{\langle \boldsymbol{k}_f \phi_f | V | \phi_n \boldsymbol{k} \rangle \langle \boldsymbol{k} \phi_n | T | \phi_i \boldsymbol{k}_i \rangle}{E + i0 - \varepsilon_n - k^2/2}. \quad (2)$$

- Unitary (no double counting), but ill-conditioned.
- For $\bar{\rm H}$ formation set $\phi_i = \phi_{n'}^{\rm Ps}$ and $\phi_f = \phi_n^{\rm H}$.

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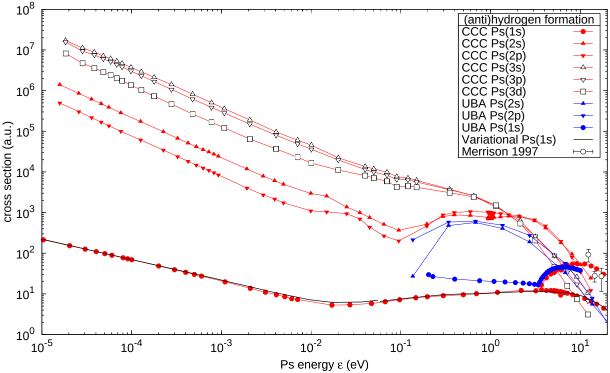
antihydrogen formation

- $\mathrm{Ps}(n \leq 3) + \bar{p} \leftrightarrow \bar{\mathrm{H}} + e^{-} \equiv \mathrm{H} + \mathrm{e}^{+}$



[Kadyrov *et al.* Phys. Rev. Lett. **114**, 183201 (2015)]

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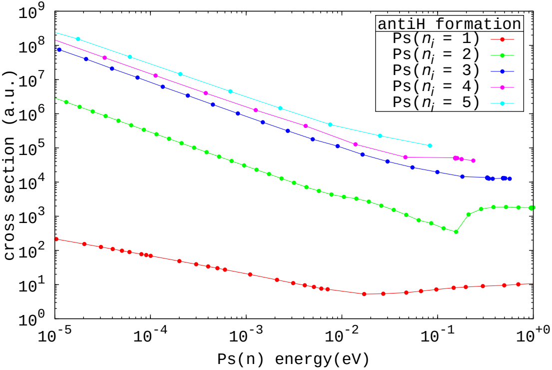
antihydrogen formation

- $\mathrm{Ps}(n \leq 5) + \bar{p} \rightarrow \bar{\mathrm{H}} + e^{-}$



[Kadyrov *et al.* Nature Comm. **8**, 1544 (2017)]

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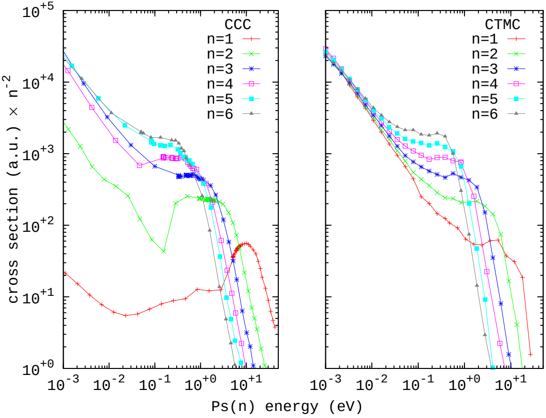
CCC comparison with CTMC

- $Ps(n \leq 6) + \bar{p} \leftrightarrow \bar{H} + e^{-}$: n^{-2} scaled cross sections



- Charlton *et al.* Phys. Rev. A **104** L060803 (2021)

Concluding remarks

- CCC valid at all energies for (anti)electrons, photons, (anti)protons scattering on quasi one- and two-electron atoms and molecules, as well as inert gases.
- Atomic CCC available: amosgateway.org,
- Data available: LXCAT, mccc-db.org, CCC-WWW.

To-do list

- Implementing general structure code of Zatsarinny
- X_2, H_2O and other molecular targets

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