Recent CCC progress in atomic and molecular collision theory

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Outline

1. Introduction
2. Convergent close-coupling theory
   - target structure and scattering
   - new approach to solving CCC equations
   - internal consistency
3. Recent applications of CCC
   - antihydrogen formation
   - positron and electron scattering on molecular hydrogen
   - heavy projectiles

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Motivation

Introduction

- The primary motivation is to provide accurate atomic and molecular collision data for science and industry
  - Astrophysics
  - Fusion research
  - Lighting industry
  - Neutral antimatter formation
  - Medical: cancer imaging and therapy
- Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials.

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Challenges

Introduction

Collisions between particles on the atomc scale are difficult to calculate:

- Governed by the Laws of Quantum Mechanics
- Charged particles interact at large distances
- Countably infinite discrete spectrum
- Uncountably infinite target continuum
- Can be multicentred (charge exchange, Ps-formation)

History: computational

Introduction

- Prior to the 1990s theory and experiment generally did not agree for:
  - electron-hydrogen excitation or ionization,
  - electron-helium excitation or (single) ionization,
  - single or double photoionization of helium.
- The convergent close-coupling (CCC) theory for electron, positron, photon, (anti)proton collisions with atoms or molecules is applicable at all energies for the major excitation and ionization processes.

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History: formal theory

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- Prior to 2008, no satisfactory mathematical formulation in the case of long-ranged (Coulomb) potentials for positive-energy scattering in
  - Two-body problems,
  - Three-body problems.
- Surface integral approach to scattering theory is valid for short- and long-ranged potentials:
  - Kadyrov *et al.* Phys. Rev. Lett., **101**, 230405 (2008),
  - Kadyrov *et al.* Annals of Physics, **324**, 1516 (2009),
  - Bray *et al.* Physics Reports, **520**, 135 (2012).

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Convergent close-coupling theory

target structure

For complete Laguerre basis $\xi_{nl}^{(\lambda)}(r)$, target states:

- "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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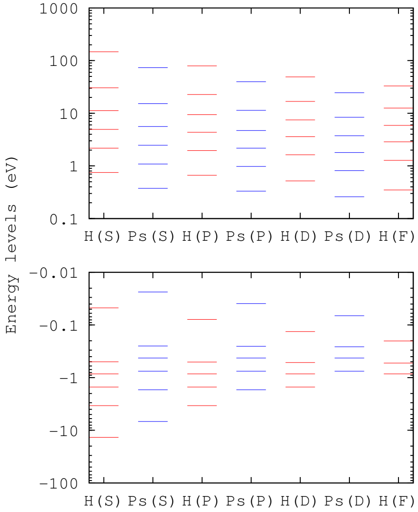
- e^+-H energies for $N_{\rm H}^\ell = N_{\rm Ps}^\ell = 12 - \ell$, for $\ell \le 3$



two-center positron scattering

- Positron-target wavefunction is expanded as

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

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

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

- ill-conditioned, but unitary (no double counting).

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new approach to solving CCC equations

- Use complete sets of states to isolate

$$G_n^L(r', r'') = \sum\!\!\!\!\!\!\int \mathrm{d}k \, \frac{f_L(kr')f_L(kr'')}{E + i0 - \epsilon_n - \varepsilon_k} = -\frac{\pi}{k_n} f_L(k_n r_<)\left(g_L(k_n r_>) + i\, f_L(k_n r_>)\right). \quad (3)$$

- Eq. (2) becomes [A. Bray *et al.* CPC **212** 55 (2017)]

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- Works for $k_f = 0$ for neutral and ionic targets.

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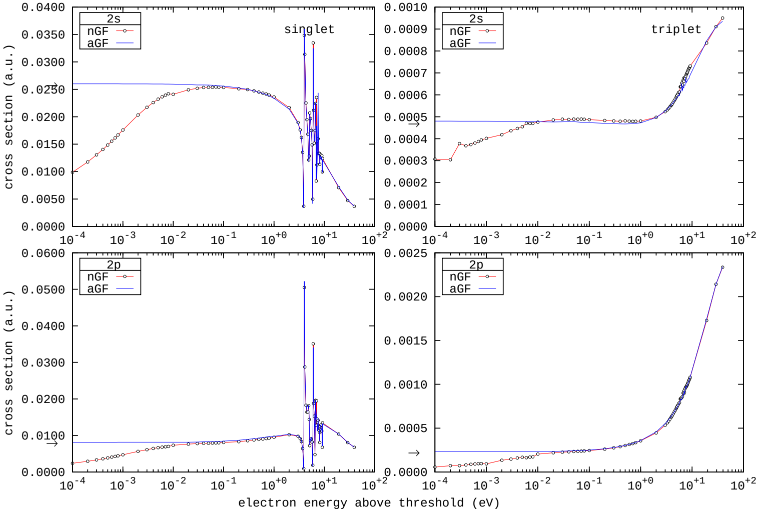
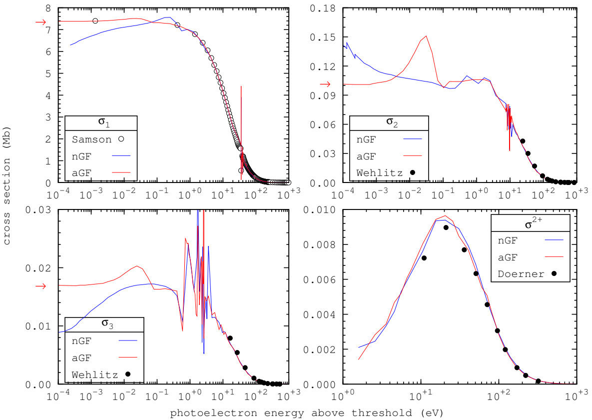
e-He^+ 2s and 2p excitation



Helium single and double photoionisation



[A. Bray, A. Kheifets, I. Bray, PRA **95**, 053405 (2017)]
[A. Kheifets, A. Bray, I. Bray, PRL **117**, 143202 (2016)]

internal consistency

- In positron scattering there are two centres:
  1. target: discrete and continuous spectrum
  2. positronium: discrete and continuous spectrum
- One-centre complete expansion:
  - Ps-formation is within ionization $\sigma^{(1)}_{\rm ion}$: e-loss
  - boundary condition problem in the extended Ore gap
- Two-centre complete expansion:
  - explicit Ps-formation $\sigma^{(2)}_{\rm Ps}$ and breakup $\sigma^{(2)}_{\rm brk}$: e-loss
  - ill-conditioned, but no double counting
- Internal consistency:
  - above ionization threshold: $\sigma^{(1)}_{\rm ion} = \sigma^{(2)}_{\rm Ps} + \sigma^{(2)}_{\rm brk}$
  - below Ps-formation threshold: $\sigma^{(1)}_{ii} = \sigma^{(2)}_{ii}$

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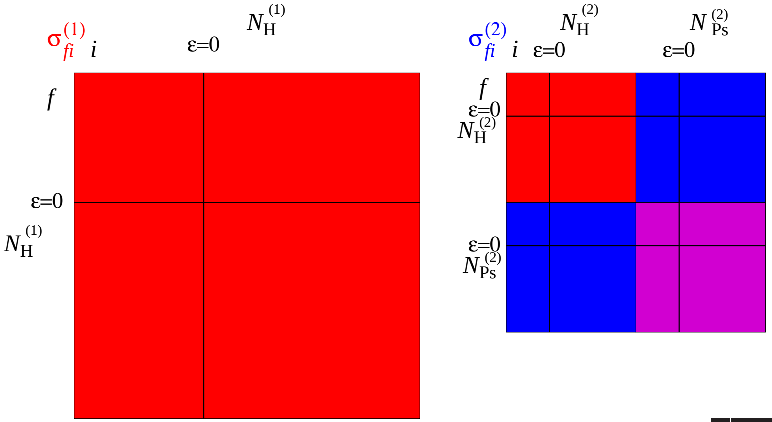
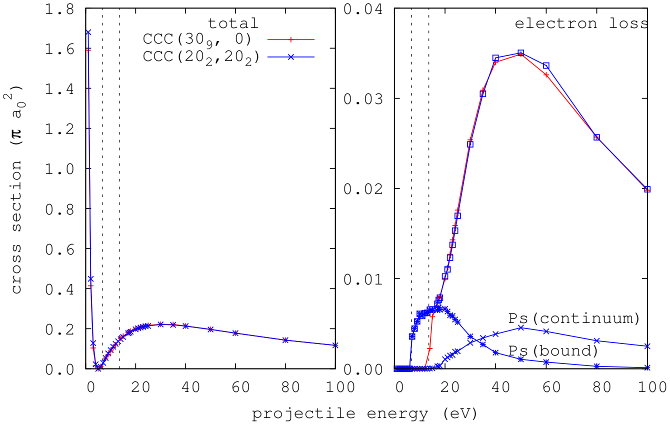
- one- and two-centre positron-hydrogen calculations



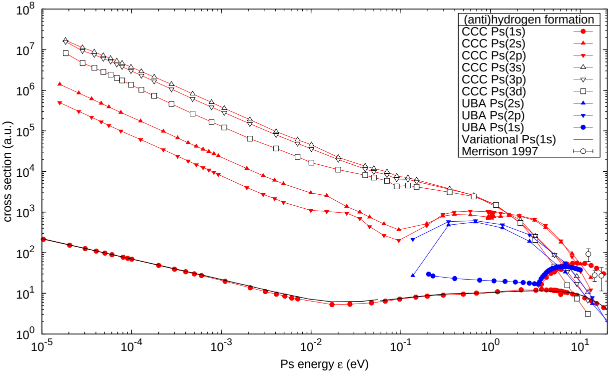
- e^+-H(1s) calculated with CCC($N^{\rm H}_{l_{\max}}$, $N^{\rm Ps}_{l_{\max}}$) for $L = 0$



[Bailey *et al.* Phys. Rev. A **91**, 012712 (2015)]

antihydrogen formation

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



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

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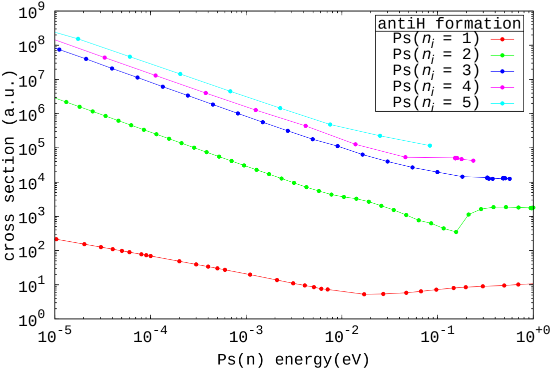
antihydrogen formation

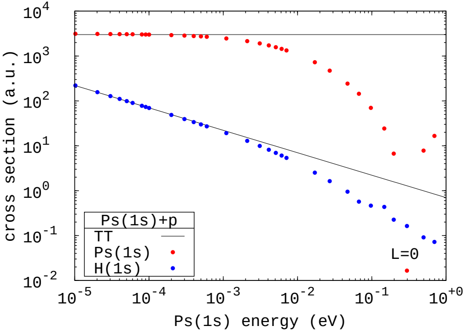
- $\mathrm{Ps}(n \leq 5) + \bar{p} \rightarrow \bar{\mathrm{H}} + e^{-}$



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

antihydrogen formation and elastic scattering

- $\mathrm{Ps(1s)}+\bar{p} \rightarrow \begin{cases} \bar{\mathrm{H}}(1\mathrm{s}) + e^- \\ \mathrm{Ps}(1\mathrm{s}) + \bar{p} \end{cases}$



[Fabrikant *et al.* Phys. Rev. A **94**, 012701 (2016)]

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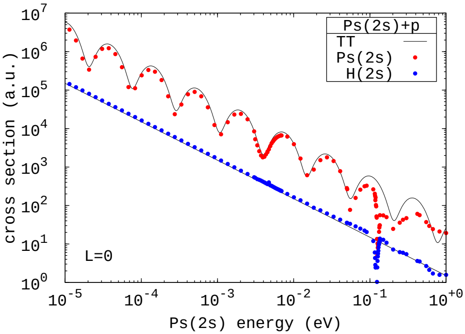
antihydrogen formation and elastic scattering

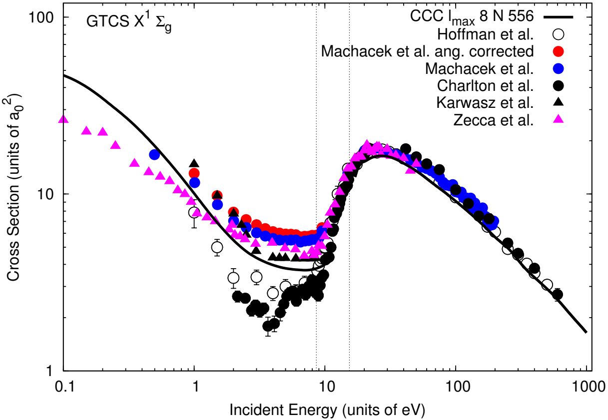
- $\mathrm{Ps(2s)} + \bar{p} \rightarrow \begin{cases} \bar{\mathrm{H}}(2\mathrm{s}) + e^{-} \\ \mathrm{Ps}(2\mathrm{s}) + \bar{p} \end{cases}$



[Fabrikant *et al.* Phys. Rev. A **94**, 012701 (2016)]

positron scattering on molecular hydrogen

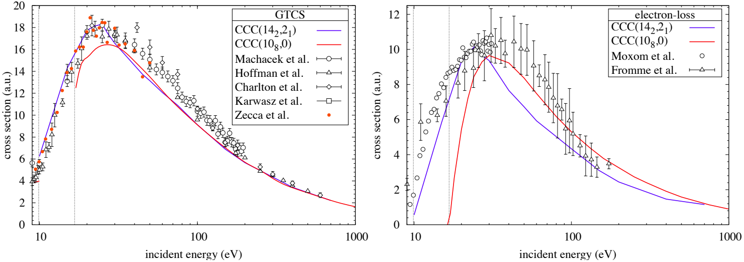
- e^+-H_2 collisions: total cross section



[Zammit *et al.* Phys. Rev. A **87**, 020701 (2013)]

positron scattering on molecular hydrogen

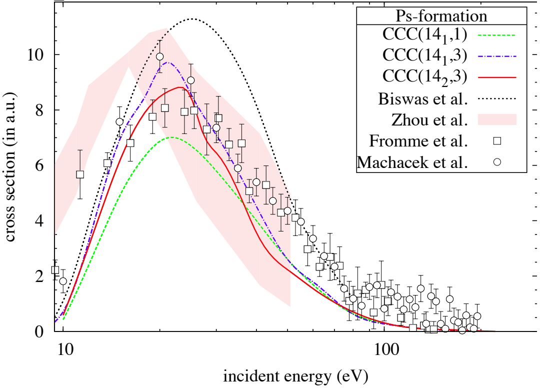
- e^+-H_2 collisions: internal consistency



[Utamuratov *et al.* Phys. Rev. A **92**, 032707 (2015)]

positron scattering on molecular hydrogen

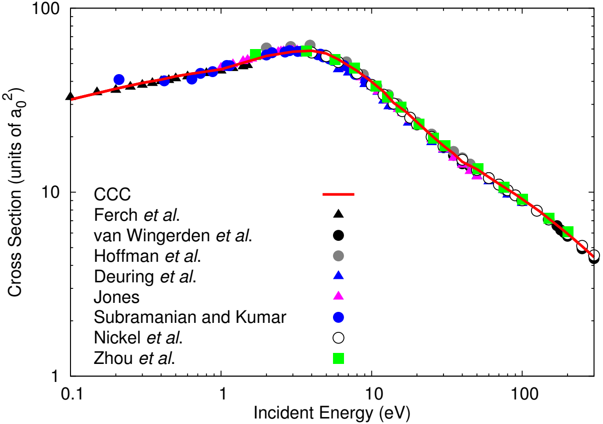
- e^+-H_2 collisions: Ps-formation



[Utamuratov *et al.* Phys. Rev. A **92**, 032707 (2015)]

electron scattering on molecular hydrogen

- e^{-}-H_2 collisions: total cross section



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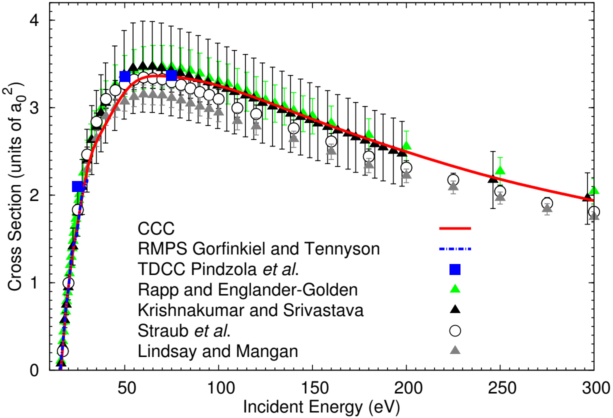
[Zammit *et al.* Phys. Rev. Lett. **116**, 233201 (2016)]

electron scattering on molecular hydrogen

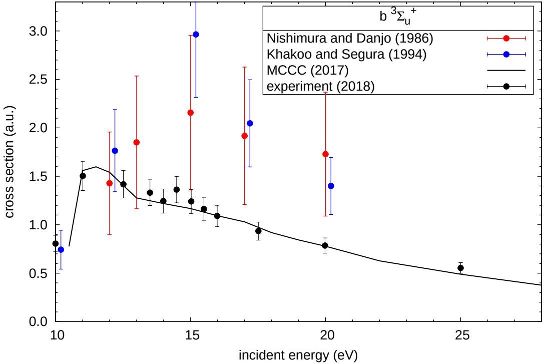
- e^{-}-H_2 collisions: total ionization



[Zammit *et al.* Phys. Rev. Lett. **116**, 233201 (2016)]

electron scattering on molecular hydrogen

- e^--H_2 collisions: $b^3\Sigma_u^+$ excitation



[Zawadski *et al.* PRA **98**, 050702R (2018)]

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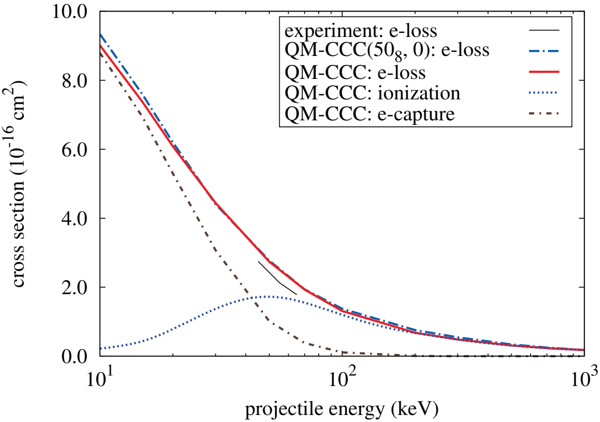
proton scattering on hydrogen

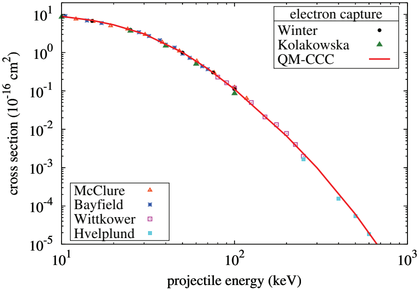
- p^+-H collisions: internal consistency

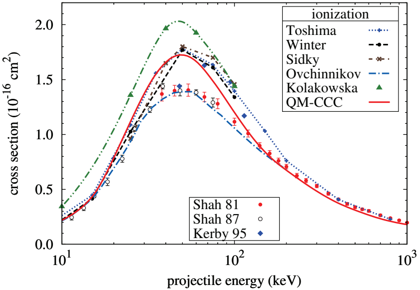


[Abdurakhmanov *et al.* J. Phys. B **49**, 115203 (2016)]

proton scattering on hydrogen

- p^+-H collisions: capture and ionization





[Abdurakhmanov *et al.* J. Phys. B **49**, 115203 (2016)]

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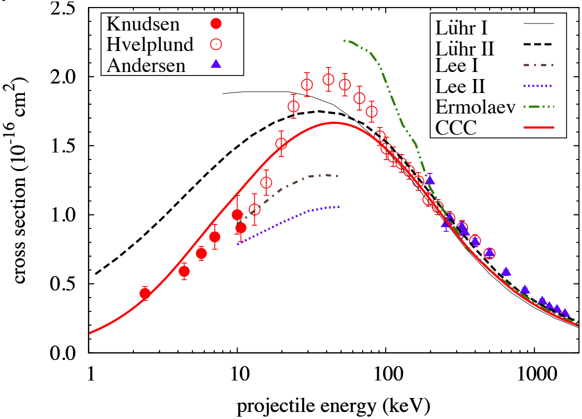
antiproton scattering on molecular hydrogen

- $\bar{p}$-H_2 collisions: total ionization



[Abdurakhmanov *et al.* PRL **111**, 173201 (2013)]

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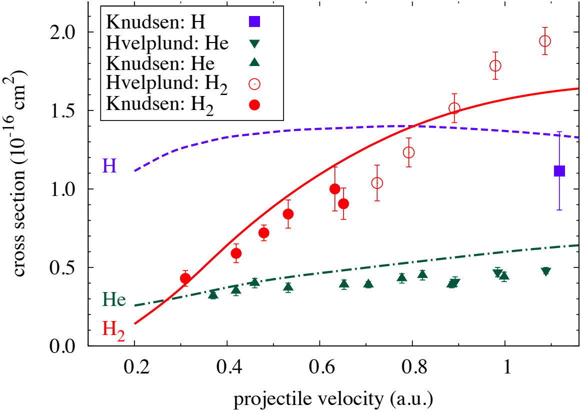
antiproton scattering on molecular hydrogen

- $\bar{p}$-H_2 collisions: comparison with H and He



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Concluding remarks

- CCC method has been implemented for scattering of electrons, positrons, photons, protons and antiprotons on quasi one- and two-electron targets, as well as inert gases.
- Two-center problems have self-consistency checks

To-do list

- Ps-H, Ps-He^+, Ps-H_2^+
- Ps-Ne^+, and other inert gas ions
- H-He^+, H-H_2^+, H-Ne^+, and other inert gas ions
- X_2, H_2O and other molecular targets

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- Two-center problems have self-consistency checks

To-do list

- Ps-H, Ps-He^+, Ps-H_2^+
- Ps-Ne^+, and other inert gas ions
- H-He^+, H-H_2^+, H-Ne^+, and other inert gas ions
- X_2, H_2O and other molecular targets

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