Close-coupling approach to positron-atom scattering

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Antimatter-Matter Studies

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Introduction
Motivation

- The primary motivation is to provide accurate atomic collision data for science and industry:
  - Astrophysics
  - Fusion research
  - Lighting industry
  - Medical and materials applications
- Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials.
- Positron scattering is a prototype of all chemistry!

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- Prior to the 1990s theory and experiment generally did not agree for:
  - electron-hydrogen excitation or ionisation,
  - electron-helium excitation or ionisation,
  - single or double photoionisation of helium.
- Consequently, we have been developing the convergent close-coupling (CCC) theory for electron/positron/photon/(anti)proton collisions with atoms/ions/molecules that is applicable at all energies for the major excitation and ionisation processes.

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  - Two-body problems
  - Three-body problems
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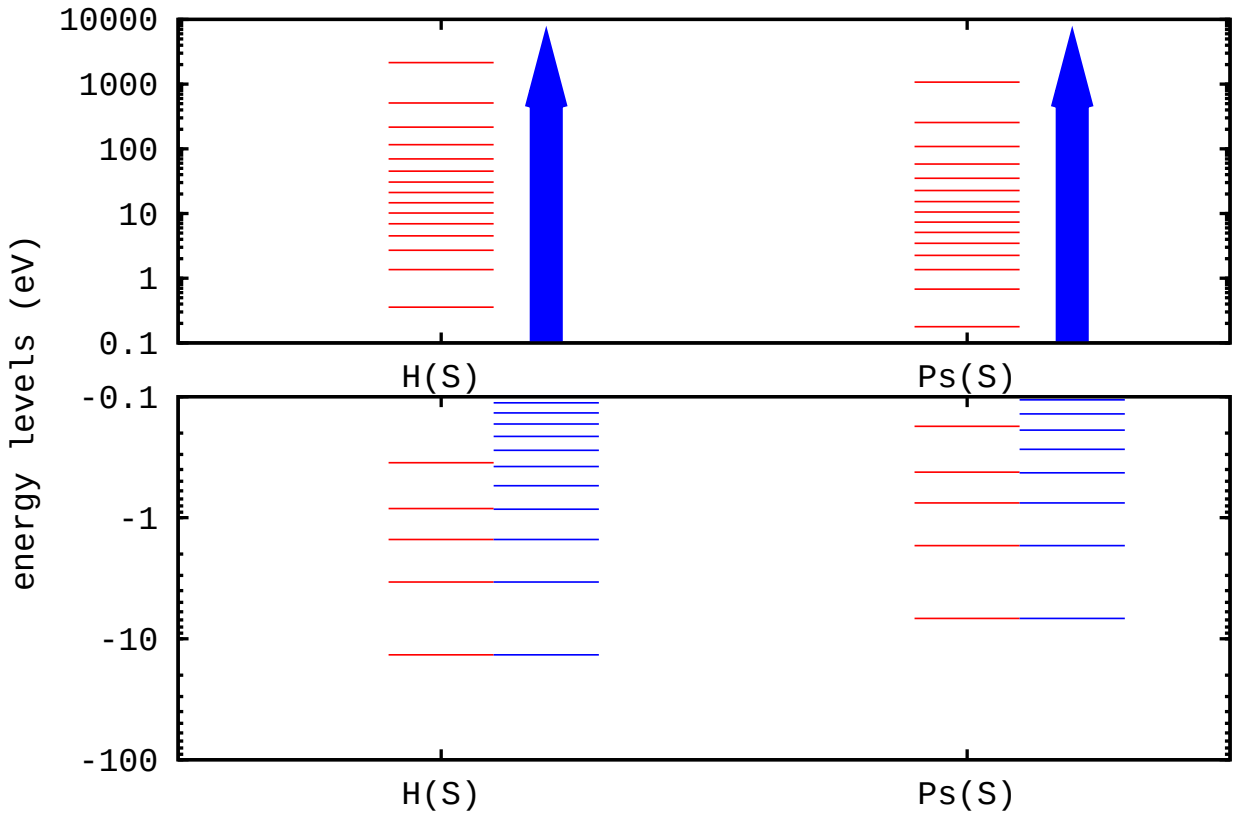
Nonrelativistic CCC theory

target structure and scattering

- Structure: using the complete Laguerre basis $\xi_{nl}^{(\lambda)}(r)$,
  - "one-electron" (H, Li, ..., Cs) states are:
    $\phi_{nl}^{(\lambda)}(r) = \sum_{n'} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r)$
  - "two-electron" (He, Be, ..., Hg) states are:
    $\phi_{nls}^{(\lambda)}(r_1, r_2) = \sum_{n',n''} C_{nls}^{n'n''} \xi_{n'l'}^{(\lambda)}(r_1) \xi_{n''l''}^{(\lambda)}(r_2)$.
  - Coefficients C are obtained by diagonalising the target (FCHF) Hamiltonian

$$\langle \phi_f^{(\lambda)} | H_{\rm T} | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}, \text{ with } \lim_{N\to\infty} \sum_{n=1}^{N} |\phi^{(\lambda)}\rangle\langle\phi^{(\lambda)}| = I$$

- Hydrogen and Ps S-state energies in CCC(20,20,0)



- Scattering:
  - Positron-atom wavefunction is expanded as
    - one-centre:

$$|\Psi_i^{(+)}\rangle \approx I_{\rm A}^{(N)} |\Psi_i^{(+)}\rangle$$

    - two-centre:

$$|\Psi_i^{(+)}\rangle \approx I_{\rm A}^{(N)} |\Psi_i^{(+)}\rangle + I_{\rm Ps}^{(N')} |\Psi_i^{(+)}\rangle$$

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

$$\langle \boldsymbol{k}_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} \boldsymbol{k}_i \rangle = \langle \boldsymbol{k}_f \phi_f^{(\lambda)} | V | \phi_i^{(\lambda)} \boldsymbol{k}_i \rangle + \sum_{n=1}^{N+N'} \sum\!\!\!\!\!\!\int d^3k \frac{\langle \boldsymbol{k}_f \phi_f^{(\lambda)} | V | \phi_n^{(\lambda)} \boldsymbol{k} \rangle \langle \boldsymbol{k} \phi_n^{(\lambda)} | T | \phi_i^{(\lambda)} \boldsymbol{k}_i \rangle}{E + i0 - \varepsilon_n^{(\lambda)} - \epsilon_k}.$$

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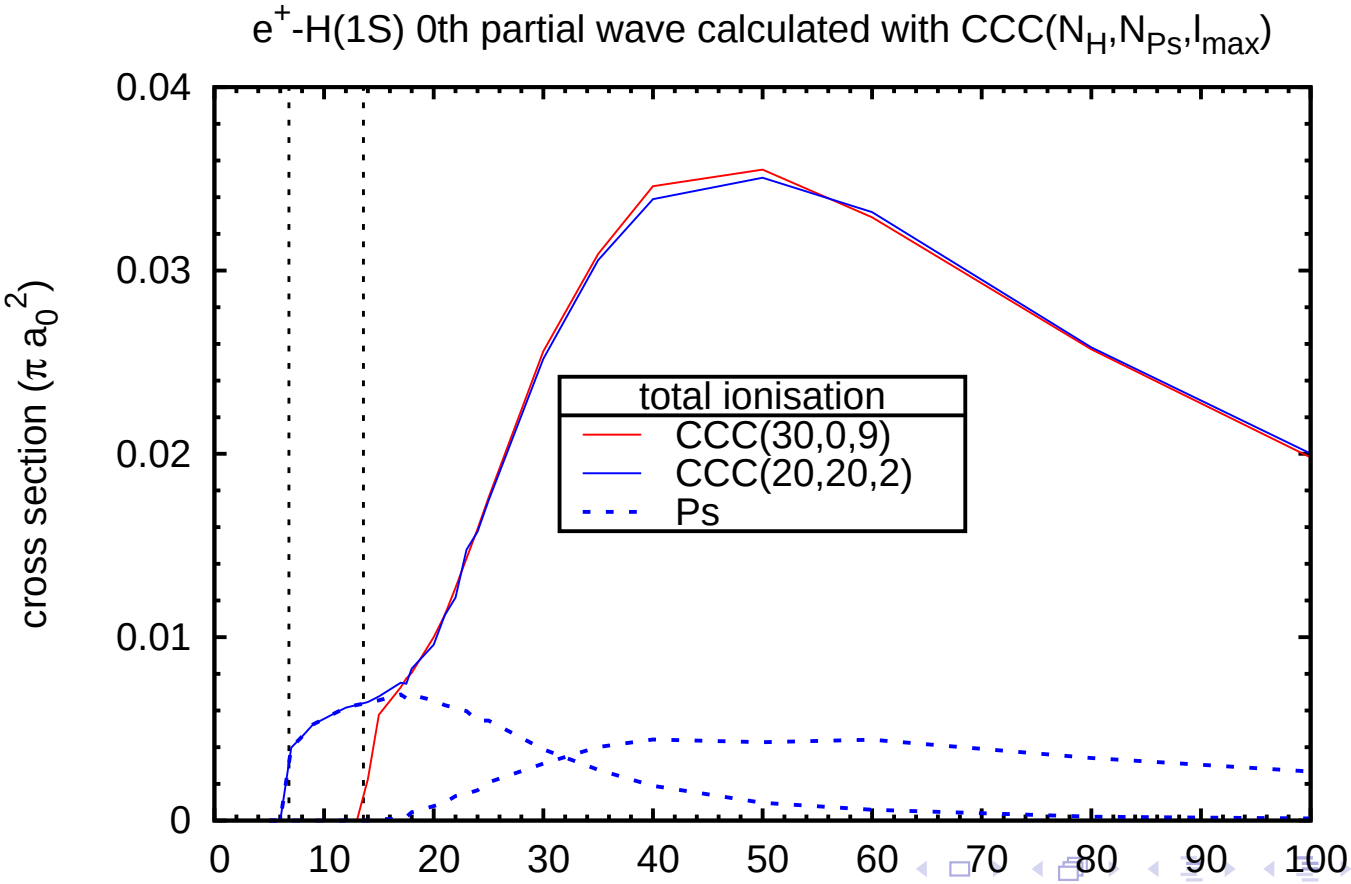
Positron-atom scattering results

validation

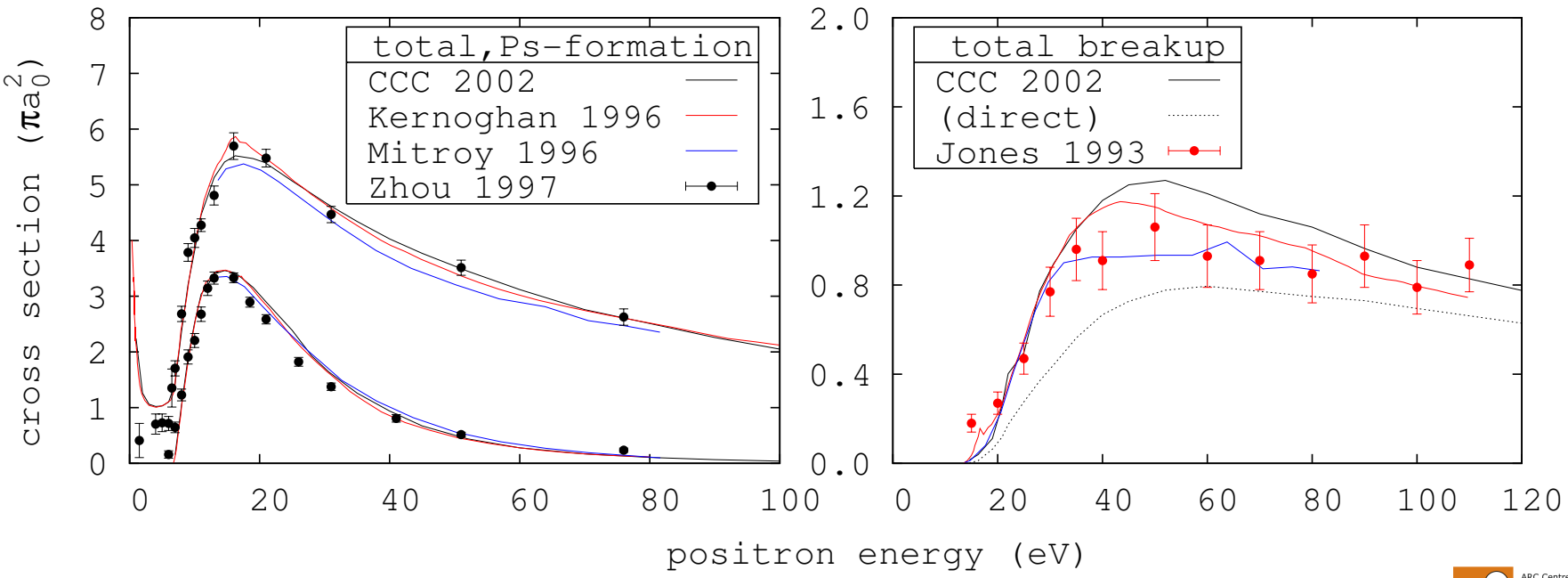
- positron-hydrogen: 2-center and 1-centre comparison



Positron-atom scattering results

positron-hydrogen

- positron-hydrogen (2-center CCC)



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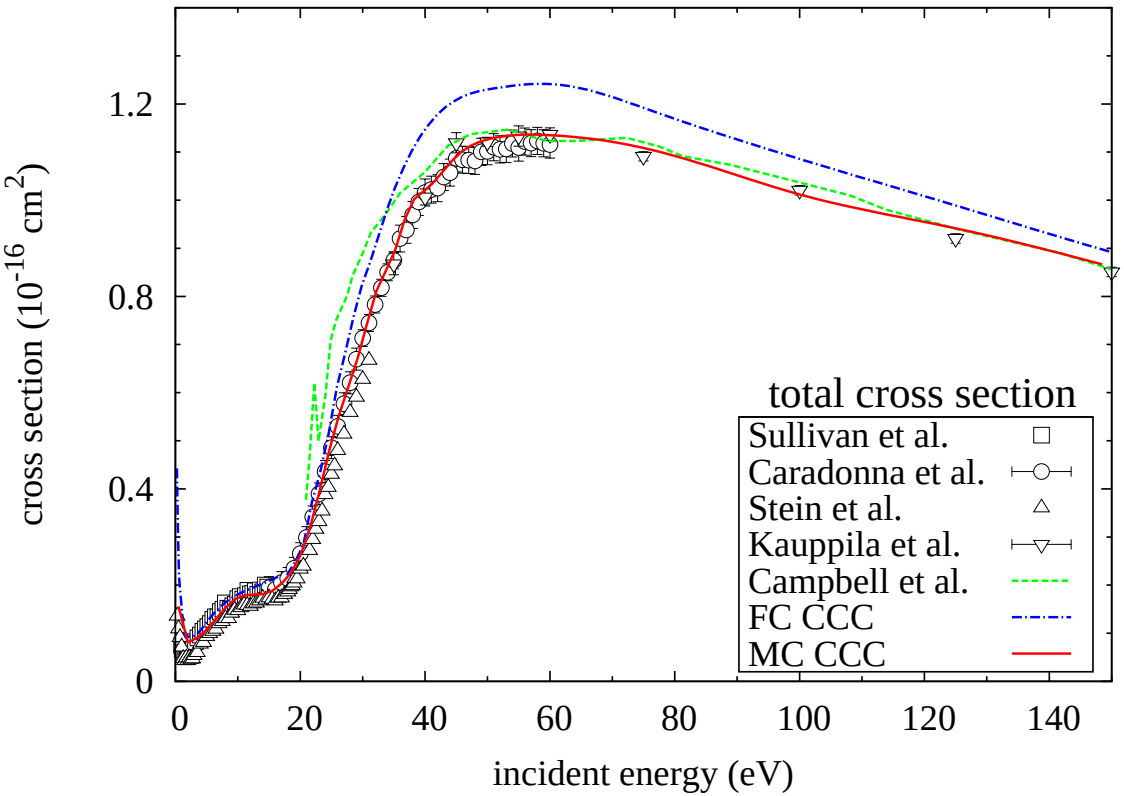
Positron-atom scattering results

positron-helium

- positron-helium (2-centre CCC)



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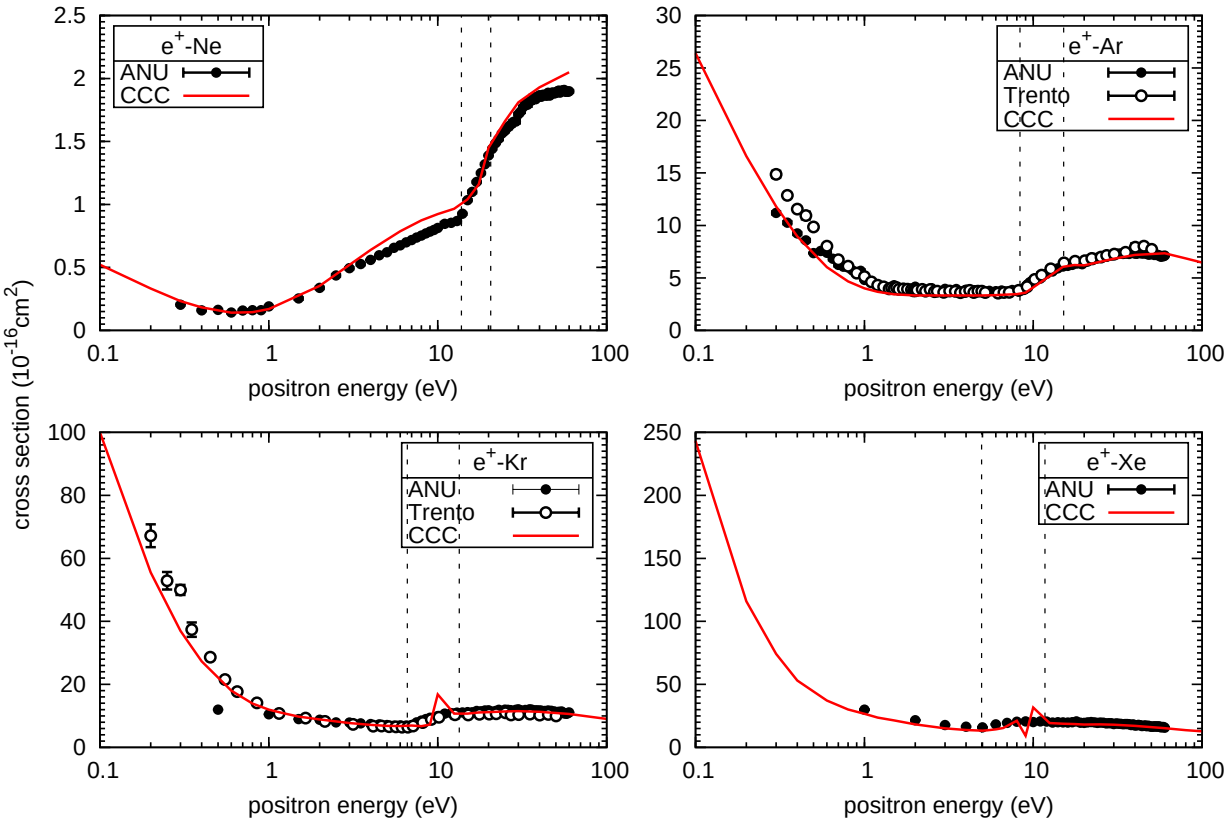
Positron-atom scattering results

positron-inert gases

- positron-inert gases (1-centre CCC)



Concluding remarks

- Close-coupling uses L^2 states for atomic and Ps states.Validated via internal consistency.
- 1-centre close-coupling valid below Ps-formation, and above ionization thresholds
  - implemented for H, He, Li, Be, . . . , Ne, Ar, Kr, Xe.
- 2-centre close-coupling valid on the full energy range
  - implemented for H, He, Li, Na, . . .
- Presently we are extending CCC to
  - 2-centre positron collisions with quasi two-electron targets and inert gases
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  - more complicated targets, such as molecules.

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