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Low-energy antiproton scattering

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LEAP 2018, Paris

Acknowledgements

- Prof Igor Bray
- Prof Mike Charlton (Swansea, UK)
- Prof Ilya Fabrikant (Nebraska, USA)
- Dr Ilkhom Abdurakhmanov
- Charlie Rawlins
- Jackson Bailey
- Shukhrat Alladustov
- Kym Massen-Hane
- Ozlem Erkilic
- Joshua Faulkner

This work is supported by Australian Research Council

Outline

- Convergent close-coupling (CCC) approach to $Ps + \bar{p} \rightarrow \bar{H} + e^-$
  - Quantum-mechanical single-centre CCC
  - Quantum-mechanical two-centre CCC (including rearrangement)
- CCC approach to $\bar{p}$ scattering on H and He
  - Semiclassical wave-packet CCC: WP-CCC
- Total and partial cross sections for $\bar{H}$ formation
- Total and differential cross sections for $\bar{p}$-impact ionisation of H and He

Why antiproton scattering?

- Several groups at CERN's Antiproton Decelerator facility plan to utilise reaction $Ps + \bar{p} \rightarrow \bar{H} + e^-$ to form antihydrogen
- The goal is to create $\bar{H}$ atoms in sufficient quantities to measure spectroscopic and gravitational properties of antimatter
  - AEgIS collaboration will produce an $\bar{H}$ beam for deflectometry studies by exciting Ps atoms to Rydberg states
  - ATRAP collaboration has already observed reaction $Ps + \bar{p} \rightarrow \bar{H} + e^-$ following the production of highly-excited Ps
  - GBAR collaboration intends to use $Ps + \bar{p} \rightarrow \bar{H} + e^-$ followed by $Ps + \bar{H} \rightarrow \bar{H}^+ + e^-$ to form $\bar{H}^+$
- FLAIR and FAIR facilities at GSI: $\bar{p}$ scattering on residual-gas atoms and molecules, like He and H_2
- ASACUSA, ELENA
- Antiproton therapy of cancer?

Modelling Ps-pbar scattering

- How to model

$$\mathrm{Ps}(n_i l_i) + \bar{\mathrm{p}} \rightarrow \bar{\mathrm{H}}(n_f l_f) + \mathrm{e}^-$$

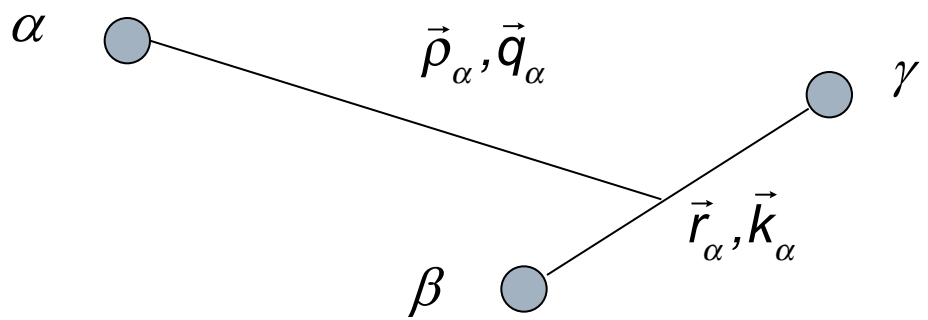
- Variational method: Humberston et al 1987, JPB 20, L25
- Very accurate but limited to Ps(1s)

- CDW: Comini and Hervieux 2013, NJP 15, 095022
- CDW works at a high energies

- CTMC: Krasnicky etal 2016, PRA 94, 022714
- Is classical treatment of Ps at low energies is valid?

CCC approach to 3-body problem

- Due to charge conjugation symmetry, reaction $\mathrm{Ps} + \bar{\mathrm{p}} \rightarrow \bar{\mathrm{H}} + \mathrm{e}^-$ is equivalent to reaction $\mathrm{Ps} + \mathrm{p} \rightarrow \mathrm{H} + \mathrm{e}^+$
- The latter is the inverse process to Ps formation $\mathrm{e}^+ + \mathrm{H} \rightarrow \mathrm{Ps} + \mathrm{p}$



$$\mathrm{e}^- + \mathrm{H}(1s) \rightarrow \Psi^+_\alpha \rightarrow \begin{cases} \mathrm{e}^- + \mathrm{H}(nl) \\ \mathrm{e}^- + \mathrm{e}^- + \mathrm{p} \end{cases}$$

Pseudostate expansion

- The total wave function is a solution to the Schrödinger equation (SE)

$$\left(E-H\right)\Psi_{\alpha}^{+}=0 \quad \text{with outgoing-wave boundary condition}$$

- Expand the w.f. in a pseudostate basis

$$\Psi_{\alpha}^{+}=\sum_{n=1}^{\infty}f_{n}\varphi_{n}+\int d\varepsilon f_{\varepsilon}\psi_{\varepsilon}\approx\sum_{n=1}^{N}f_{n}\phi_{n}$$

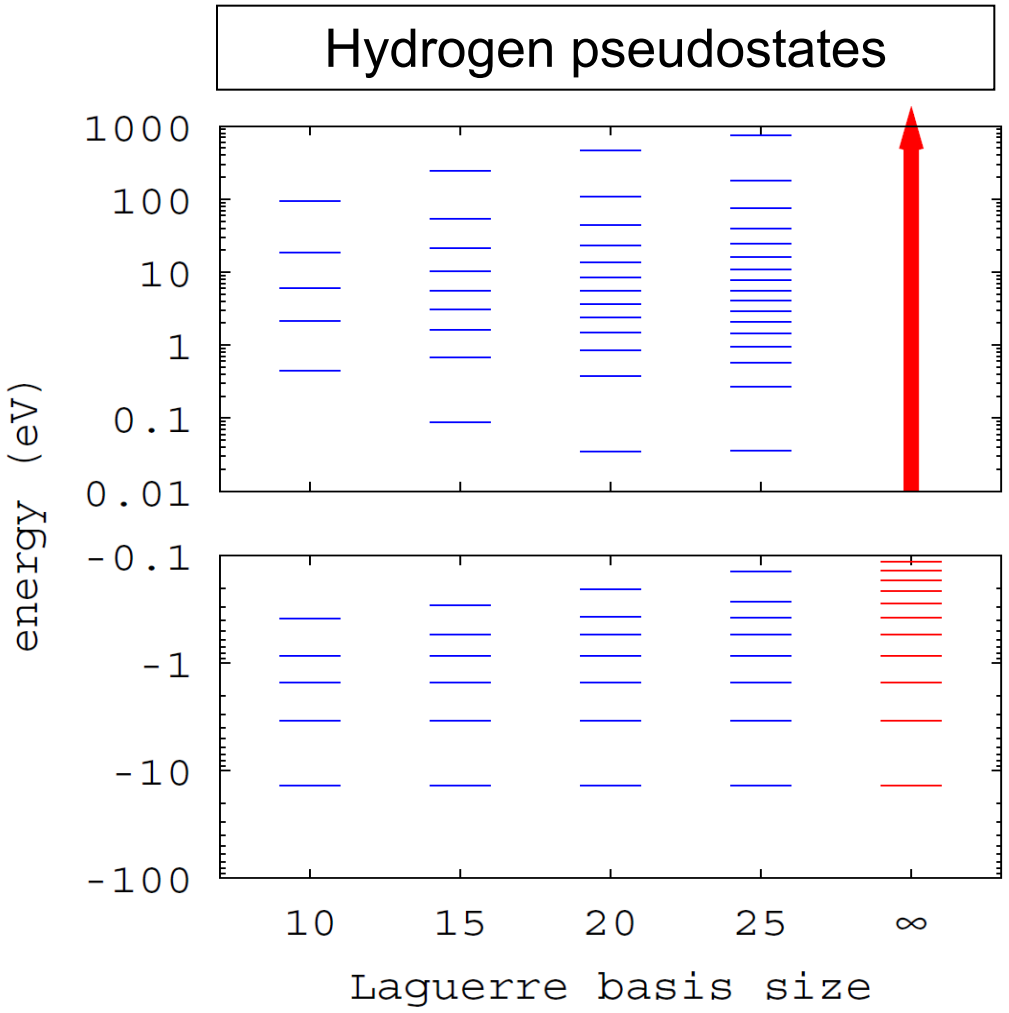
- How do we generate pseudostates?

$$\left\langle \phi_{f}\left|H_{T}\right|\phi_{i}\right\rangle =\varepsilon_{f}\delta_{fi}$$

- A linear combination of *N* Laguerre functions

CCC method: pseudostates

- This gives a set of negative- and positive-energy states which we call pseudostates
- With increasing *N* the negative-energy pseudostates converge to true discrete eigenstates of H
- Positive energy states provide a discretization of the continuum
- Alternative method: wave packets or bins



CCC equations

- Pseudostate expansion

$$0 = \left(E - H\right)\left|\Psi_i^+\right\rangle \approx \left(E - H\right)\sum_{n=1}^{N} f_n \left|\phi_n\right\rangle$$

- For any given N we require that

$$0 = \left(E - H\right)\sum_{n=1}^{N} f_n \left|\phi_n\right\rangle$$

- The Bubnov-Galerkin principle (generalisation of the Ritz theorem):

$$\left\langle \phi_m \right| \left(E - H\right)\sum_{n=1}^{N} f_n \left|\phi_n\right\rangle = 0, \qquad m = 1,\ldots,N$$

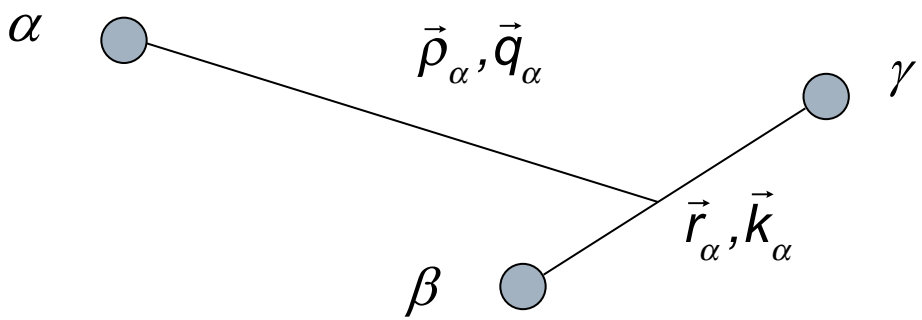
- Transform into a set of NxN momentum-space integral equations

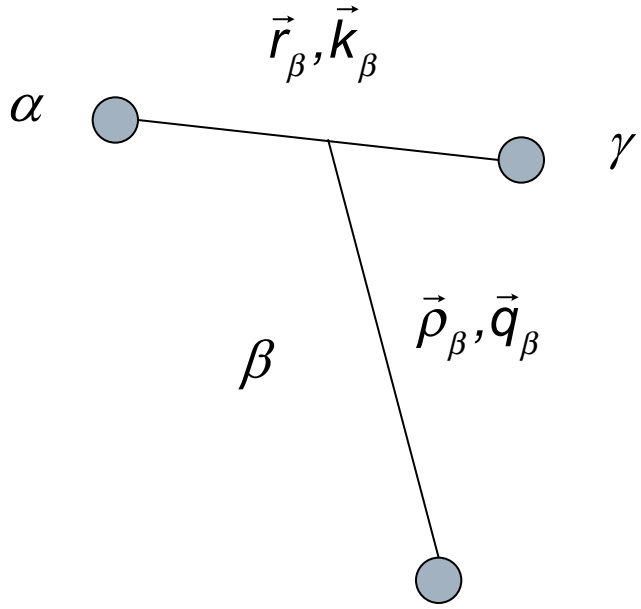
CCC method in a nutshell

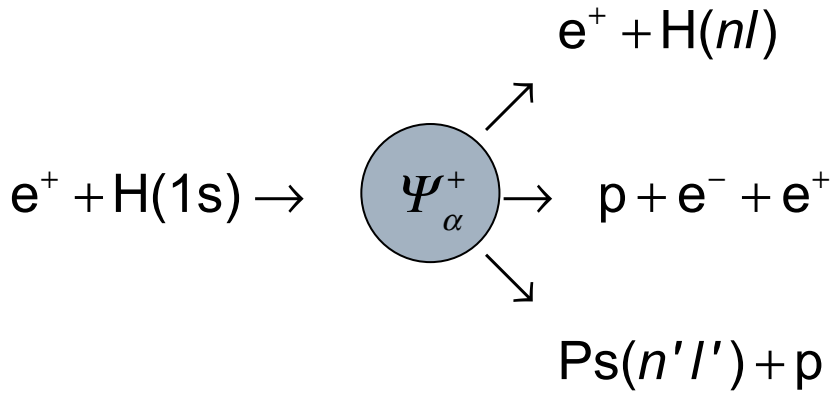
$$\left\langle \vec{q}_f,\phi_f \middle| T \middle| \phi_i,\vec{q}_i \right\rangle = \left\langle \vec{q}_f,\phi_f \middle| V \middle| \phi_i,\vec{q}_i \right\rangle + \sum_{r=1}^{N} \int d\vec{q} \frac{\left\langle \vec{q}_f,\phi_f \middle| V \middle| \phi_r,\vec{q} \right\rangle \left\langle \vec{q},\phi_r \middle| T \middle| \phi_i,\vec{q}_i \right\rangle}{E - \varepsilon_r - q^2 / 2\mu_r + i0}$$

- Solved in partial waves
- Total breakup cross section is obtained by summing the cross sections for excitation of the positive-energy pseudostates
- Convergence in cross sections is obtained by increasing *N*
- e^- scattering on H, He, He-like targets, alkalis, inert gases, H_2^+, H_2
- Topical Review: Bray *et al*. 2017, JPB 50, 202001

CCC with rearrangement







2-centre CCC: associated difficulties

- The total w.f. is expanded using two independent bases, one for each centre:

$$\Psi_{\alpha}^{+} \approx \sum_{n=1}^{N} f_n \phi_n^{H} + \sum_{m=1}^{M} g_n \phi_m^{Ps}$$

Atomic basis is obtained by diagonalising the H atom Hamiltonian with *N* states

Ps basis is obtained by diagonalising the Ps Hamiltonian with *M* states

- This brings three difficulties into play. The combined basis is
  - Non-orthogonal ⇒ numerical instabilities
  - Over-complete ⇒ double counting?

  } problem is ill-conditioned

- 3rd difficulty: Ps-formation matrix elements are significantly more complicated

2-centre CCC equations

- Again require our expansion to satisfy the SE

$$0 \approx \left(E - H\right)\left(\sum_{n=1}^{N} f_n \left|\phi_n^H\right\rangle + \sum_{m=1}^{M} g_n \left|\phi_m^{Ps}\right\rangle\right)$$

- Project this on each pseudostate (Bubnov-Galerkin principle)

$$\begin{cases} \left\langle \phi_{n'}^H \middle| \left(E - H\right) \sum_{n=1}^{N} f_n \left|\phi_n^H\right\rangle + \left\langle \phi_{n'}^H \middle| \left(E - H\right) \sum_{m=1}^{M} g_n \left|\phi_m^{Ps}\right\rangle = 0 & n' = 1,\ldots,N \\ \left\langle \phi_{m'}^{Ps} \middle| \left(E - H\right) \sum_{n=1}^{N} f_n \left|\phi_n^H\right\rangle + \left\langle \phi_{m'}^{Ps} \middle| \left(E - H\right) \sum_{m=1}^{M} g_n \left|\phi_m^{Ps}\right\rangle = 0 & m' = 1,\ldots,M \end{cases}$$

- This is a set of (N+M)x(N+M) integro-differential equations

2-centre CCC method in a nutshell

- Transform into a set of (N+M)x(N+M) momentum-space integral eqs

$$\left\langle \vec{q}_f,\phi_f \left| T \right| \phi_i,\vec{q}_i \right\rangle = \left\langle \vec{q}_f,\phi_f \left| V \right| \phi_i,\vec{q}_i \right\rangle + \sum_{r=1}^{N+M} \int d\vec{q} \frac{\left\langle \vec{q}_f,\phi_f \left| V \right| \phi_r,\vec{q} \right\rangle \left\langle \vec{q},\phi_r \left| T \right| \phi_i,\vec{q}_i \right\rangle}{E-\varepsilon_r - q^2/2\mu_r + i0}$$

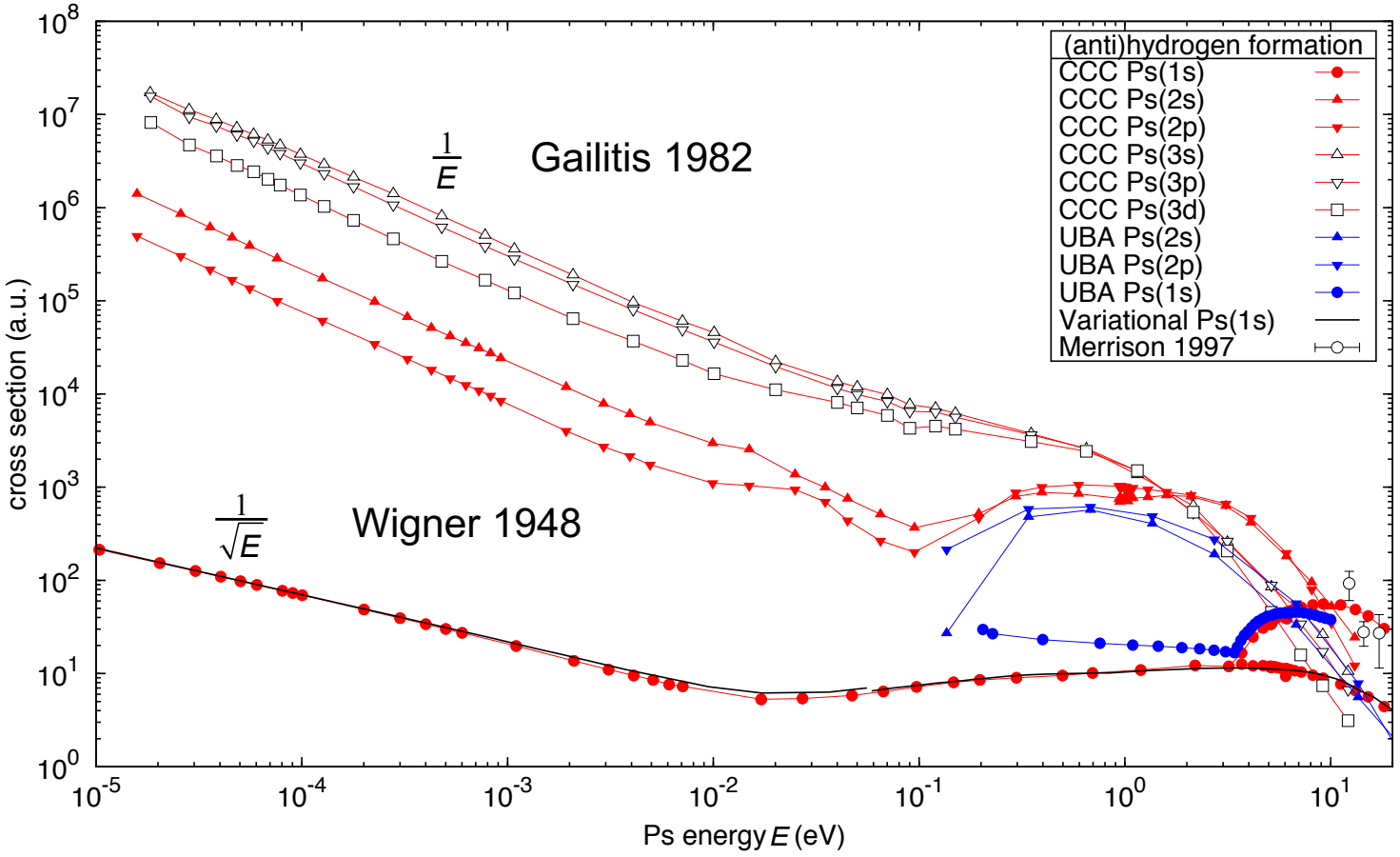
Now $\phi = \left\{ \phi^H, \phi^{Ps} \right\}$

- All direct and rearrangement matrix elements coupled
- Ps formation in continuum is included
- Total breakup cross section is obtained by summing the cross sections for excitation of the positive-energy pseudostates of both H and Ps
- Convergence in cross sections is obtained by increasing N and M

- e^+ scattering on H, He, Mg, alkalis, H_2
- Topical Review: Kadyrov & Bray 2016, JPB 50, 202001

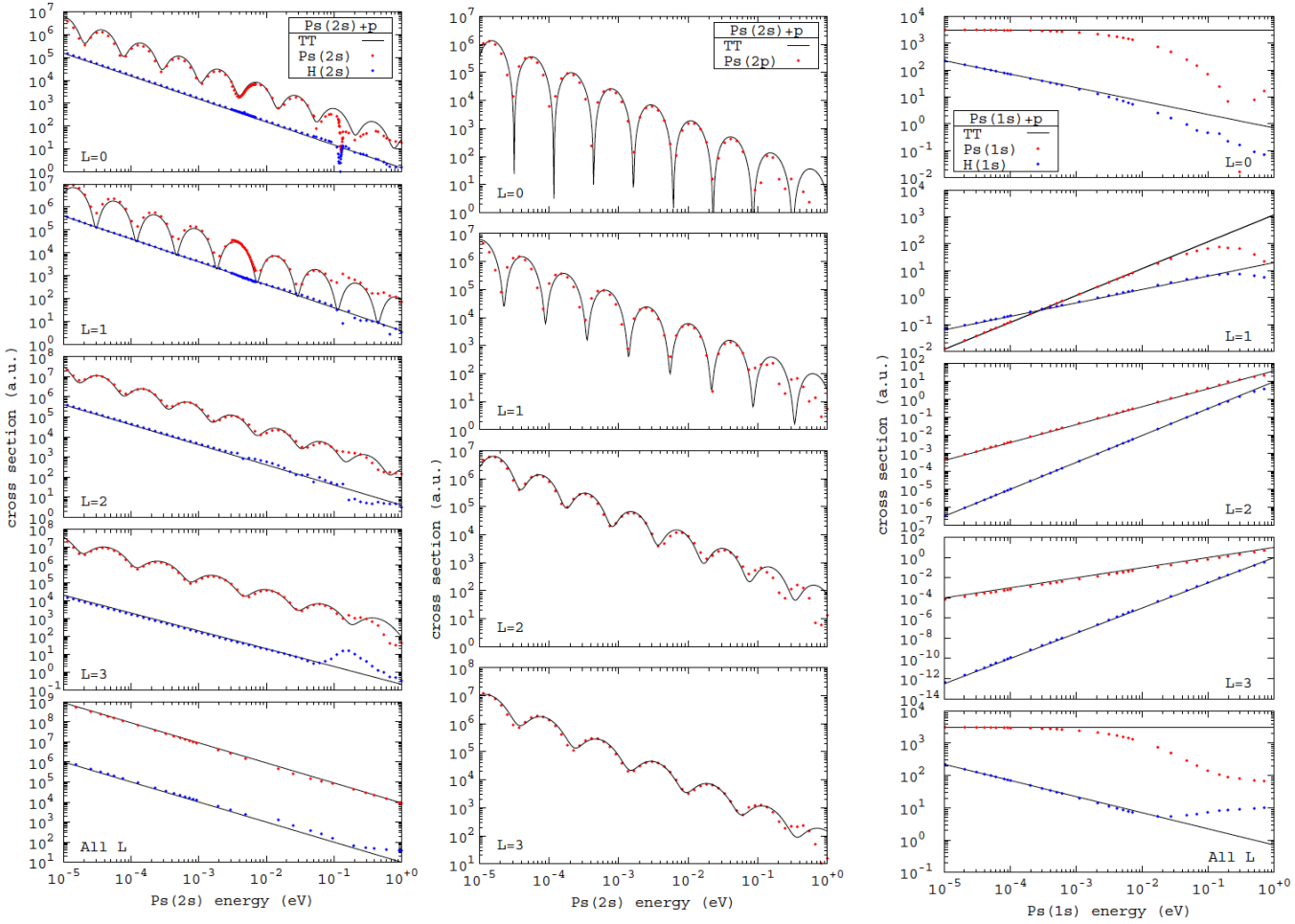
Antihydrogen formation in Ps($n_i l_i$) + $\bar{p}$

Very low energies relevant to $\bar{H}$ experiments at CERN: $n_i \leq 3$



Kadyrov et al. 2015, PRL 114, 183201

Ps(nl) + $\bar{p}$ scattering



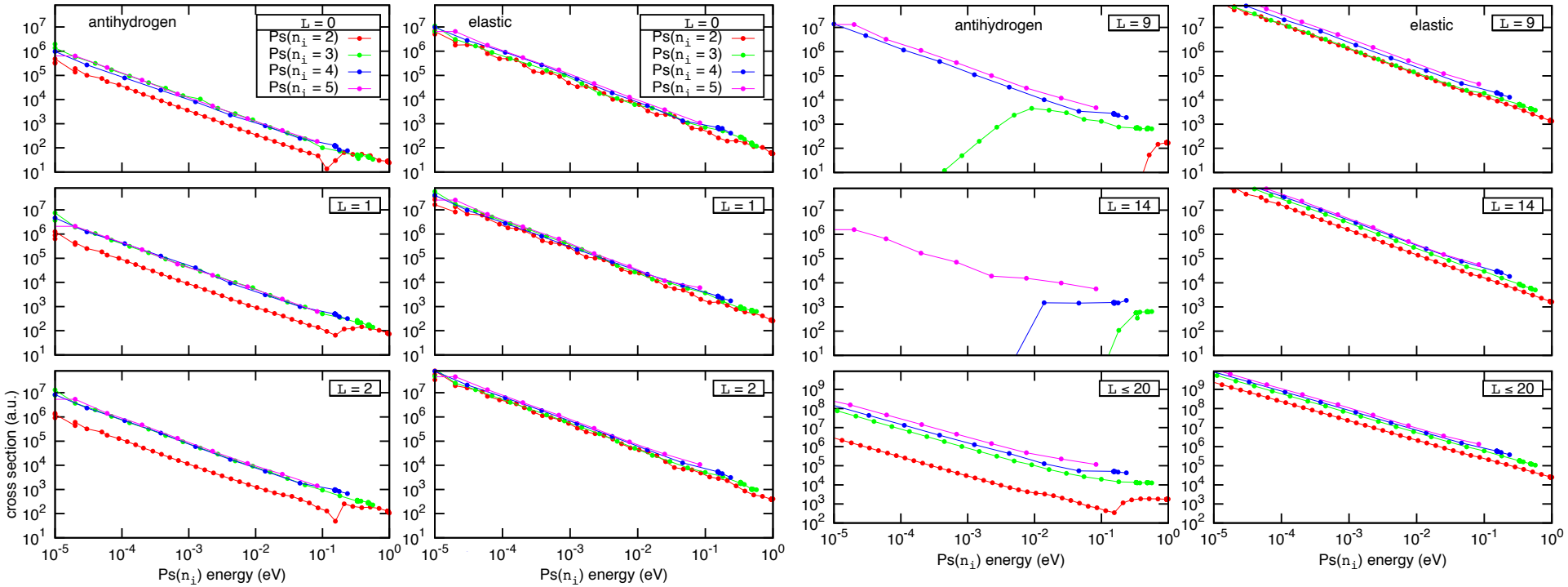
Fabrikant et al. 2016, PRA 94, 012701

Extension of CCC to n_i = 4 and 5

- Krasnicky et al 2016, PRA 94, 022714:
  - $\bar{H}$ -formation cross section σ is scaled as n_i^4
  - the 1/E dependence according to the CCC for n_i = 3

- Recently we extended the CCC to n_i = 5
- We established that the dramatic increase in the cross section for $\bar{H}$ formation, when n_i is increased from 1 to 2 and from 2 to 3, was absent for the higher values of n_i.
- In the Ps kinetic energy region where the data for all n_i behave as 1/E
  - there is a factor of 3 between the cross section for n_i = 5 when compared to n_i = 3.
  - the factor of 30 increase between n_i = 2 and 3, and
  - a few orders of magnitude enhancement in the formation of $\bar{H}$ when Ps in an n_i = 2 state over the ground state.

Quantum suppression



- Due to quantum-mechanical effects, the growth of the $\bar{H}$- formation cross section with n_i is much slower than in the classical calculations
- This arises primarily due to the limited number of partial waves contributing to the process.

Quantum suppression

- For moderate values of n_i we predict $\sigma \sim n_i^2 / E$ scaling
- The threshold theory analysis confirms this trend

- Conclusion: quantum effects strongly suppress the increase of $\bar{H}$ formation cross section, in contrast to expectations from classical approaches

- If this trend persists at high n_i , then the implications for current experimental efforts, which aim to exploit efficient $\bar{H}$ formation from excited-state Ps, could be important.
- For instance
  - Ps(18) → σ(CTMC)/σ(CCC) = 324
  - Ps(32) → σ(CTMC)/σ(CCC) = 1024

- Details: Kadyrov et al 2017, Nature Commun. 8, 1544

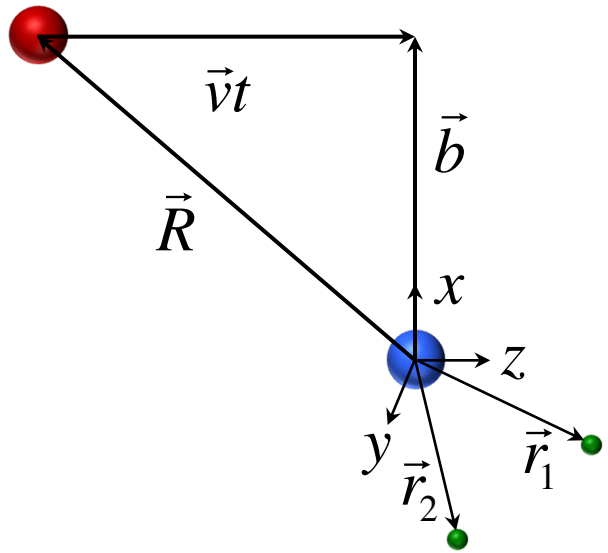
CCC approach to pbar-atom collisions

A lab frame: the origin at the target, z-axis $\parallel \vec{v}$ and x-axis $\parallel \vec{b}$

Projectile position $\vec{R}(t) = \vec{b} + \vec{Z} = \vec{b} + \vec{v}t$

The w.f. is a solution to SC TDSE

$$i\frac{\partial \Psi(\vec{r},t)}{\partial t} = (H_T + V_P)\Psi(\vec{r},t)$$



Expand Ψ in terms of pseudostates of H_T

$$\Psi(\vec{r},t) = \sum_{\alpha} a_\alpha(t)\exp(-i\varepsilon_\alpha t)\phi_\alpha(\vec{r})$$

$\vec{r} = \{\vec{r}_1, \vec{r}_2, ...\}$ is a collective coordinate of all electrons

CCC approach to pbar-atom collisions

Then we get

$$i\dot{a}_\alpha(t) = \sum_\beta \exp[i(\varepsilon_\alpha - \varepsilon_\beta)t] a_\beta(t) D_{\alpha\beta}$$

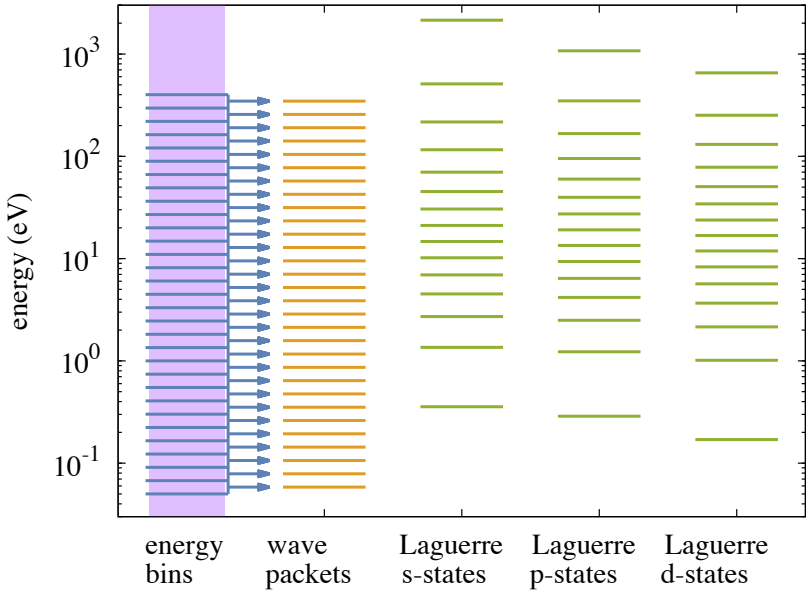
$$D_{\alpha\beta} = \left\langle \phi_\alpha \left| -\frac{1}{R(t)} + \sum_i \frac{1}{|\vec{R}(t) - \vec{r}_i|} \right| \phi_\beta \right\rangle$$

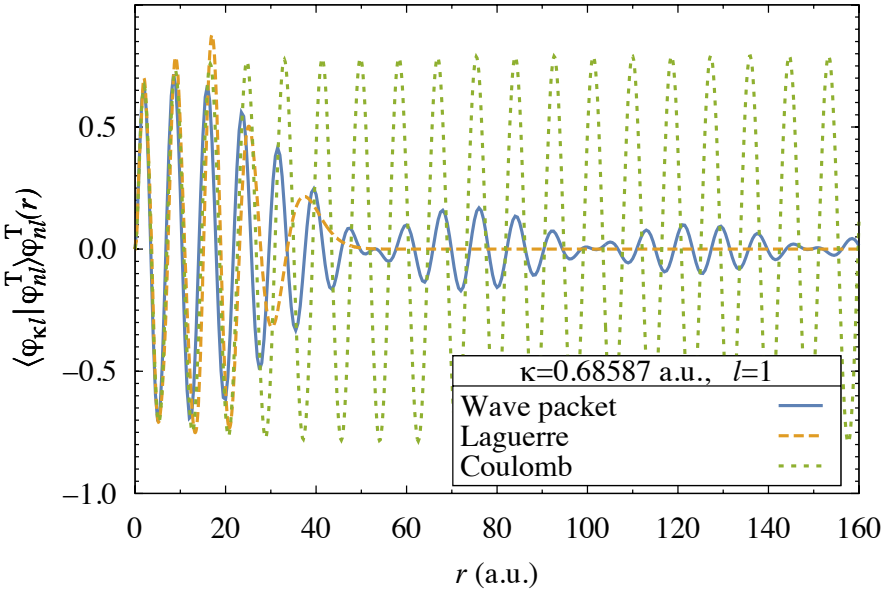
In matrix form $i\dot{\mathbf{a}} = \mathbf{D}\mathbf{a}$

Pseudostates $\left\langle \phi_\beta \left| H_T \right| \phi_\alpha \right\rangle = \delta_{\beta\alpha}\varepsilon_\alpha$

- Pseudostates are generated using an alternative method: wave packets or bins

Wave-packet continuum discretisation





- $\phi_{il}^{WP}(r) = \dfrac{1}{\sqrt{w_i}} \int_{k_{i-1}}^{k_i} dk \varphi_{kl}(r)$

  Coulomb function

$$\left\langle \phi_{jl}^{WP} \middle| H_T \middle| \phi_{il}^{WP} \right\rangle = \delta_{ji}\varepsilon_i$$

- Advantages of WP: there are 3

$$\left\langle \psi_{\vec{k}} \middle| \phi_f \right\rangle = \sqrt{\tfrac{2}{\pi}}(-i)^l e^{i\sigma_l} b_{nl}(k) Y_{lm}(\hat{k})$$

$$b_{nl}(k) = \int_0^\infty dr \varphi_{kl}(r)\ \varphi_n^{WP}(r) = \frac{1}{\sqrt{w_n}}$$

Abdurakhmanov et al. 2016, PRA 94, 022703

Ionisation amplitude

$$T^{post} \neq \left\langle \vec{q}_f, \vec{k} \middle| V \middle| \Psi_i^+ \right\rangle$$

- Surface-integral formulation of scattering theory

  Kadyrov *et al.* 2008, PRL 101, 230405

  Kadyrov *et al. 2009*, AP 324, 1516:

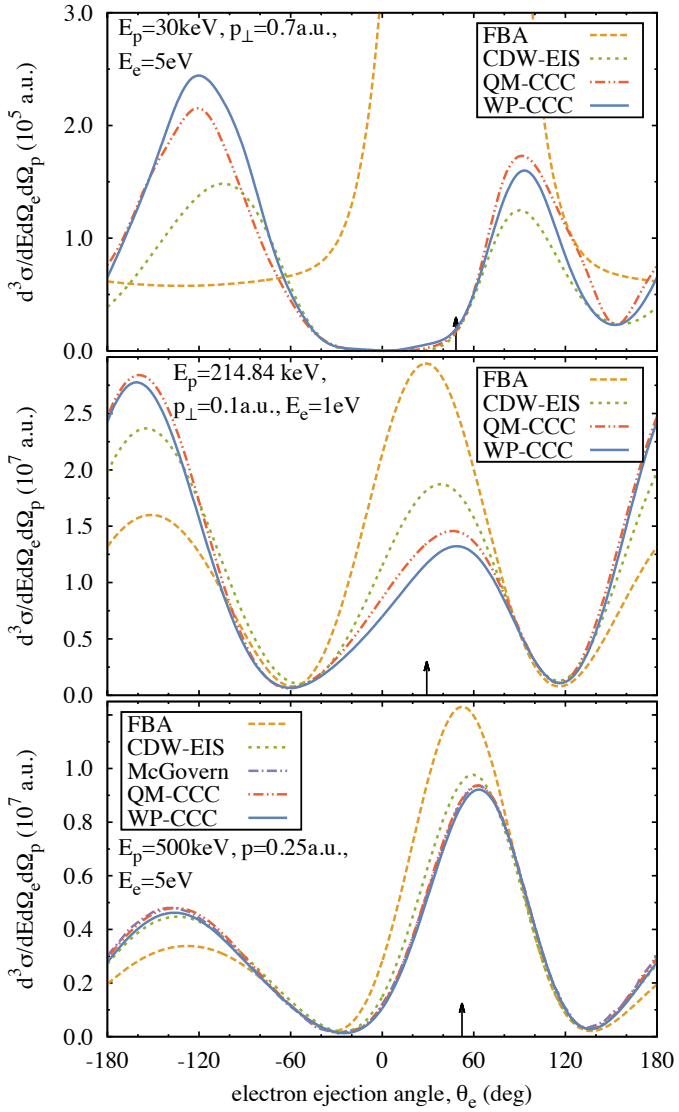
$$T^{post} = \left\langle \Phi_0^- \middle| \overleftarrow{H} - E \middle| \Psi_i^+ \right\rangle$$

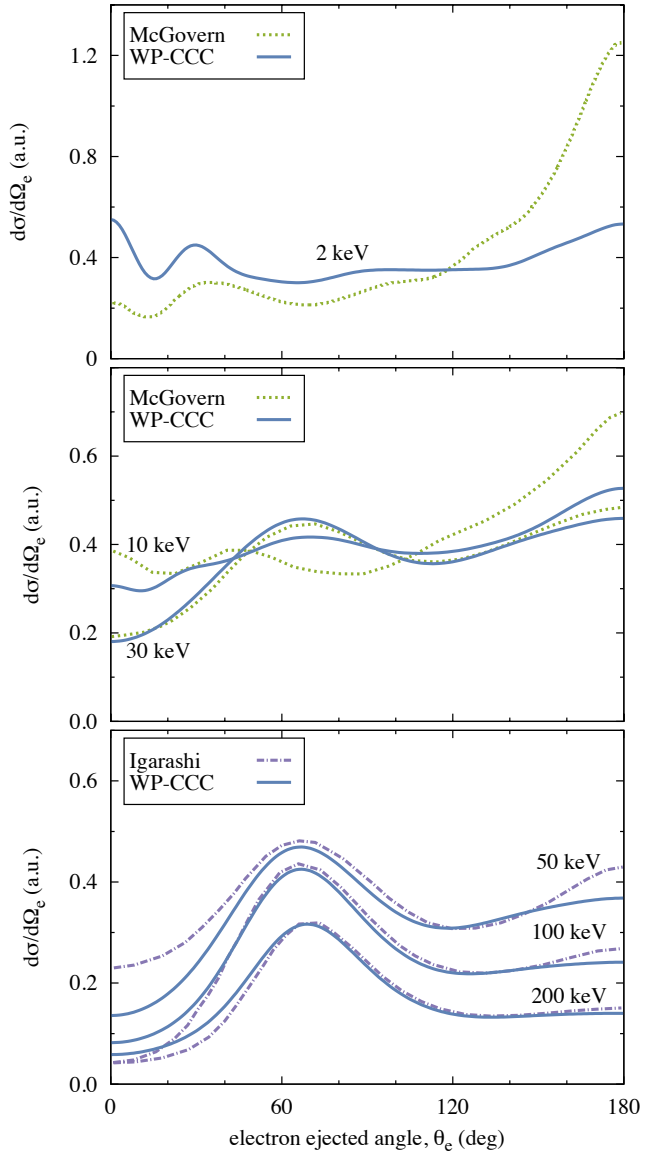
$$\approx \left\langle \Phi_0^- \middle| I_N \left(\overleftarrow{H} - E \right) I_N \middle| \Psi_i^+ \right\rangle$$

$$= \left\langle \vec{q}_f, \psi_{\vec{k}} \middle| I_N \left(\overleftarrow{H} - E \right) \middle| \Psi_i^{N+} \right\rangle \equiv \sum_{n=1}^{N} \left\langle \psi_{\vec{k}} \middle| \phi_n \right\rangle \left\langle \phi_n, \vec{q}_f \middle| \overleftarrow{H} - E \middle| \Psi_i^{N+} \right\rangle$$

$$= \left\langle \psi_{\vec{k}} \middle| \phi_f \right\rangle \tilde{T}_{fi} \qquad \text{for} \quad k^2 / 2 = \varepsilon_f$$

Wave-packet CCC: $\bar{p}$ + H(1s) ionisation





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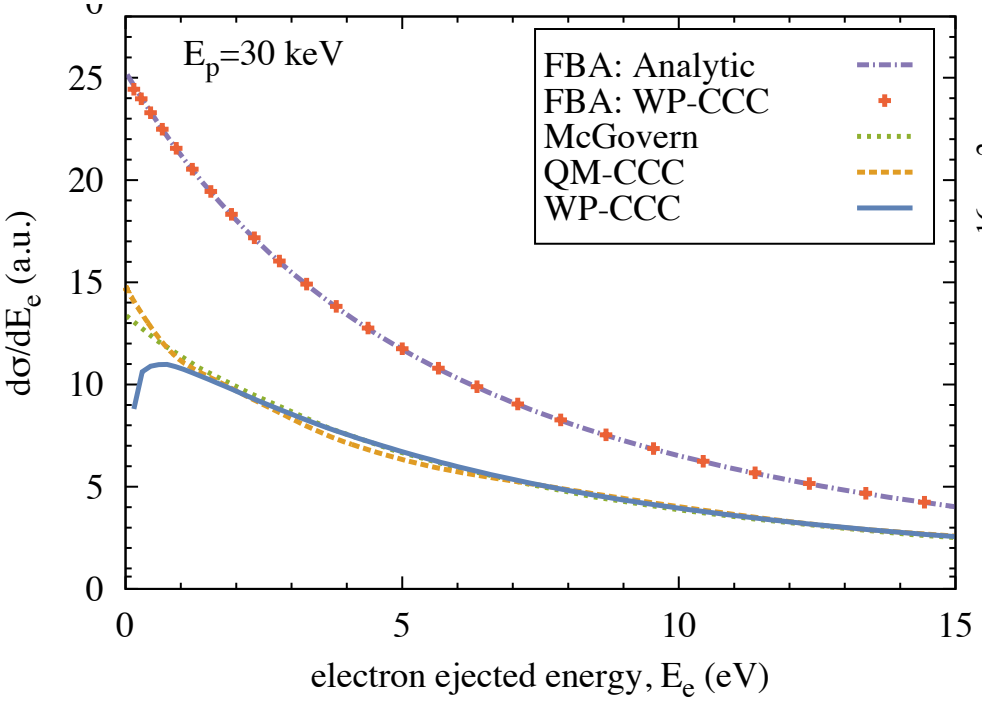
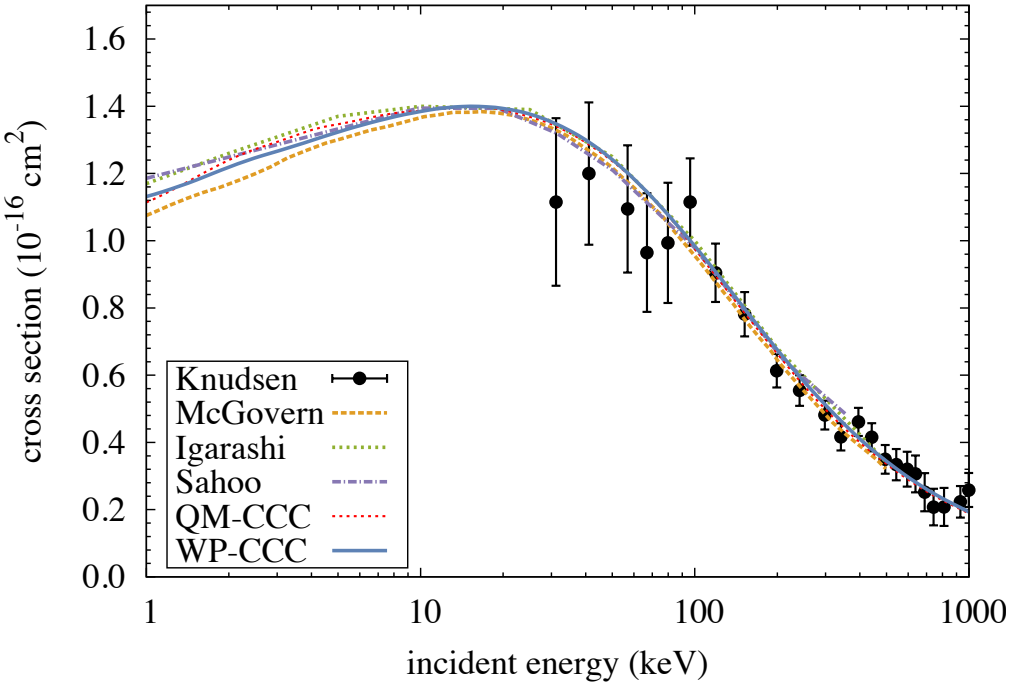
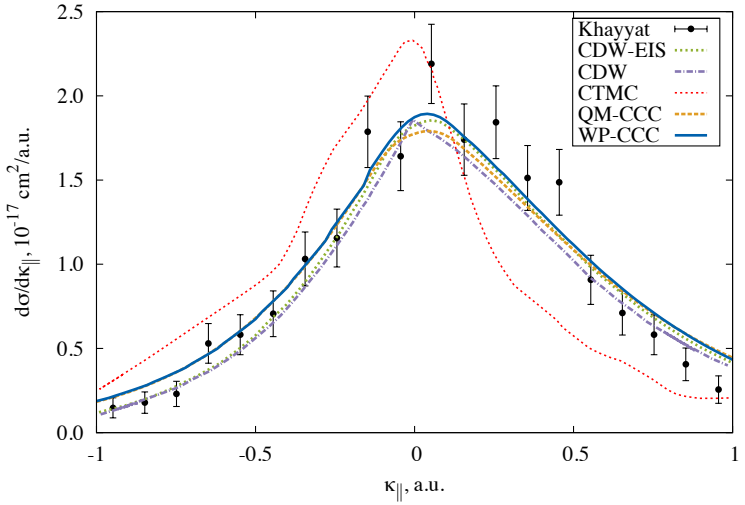


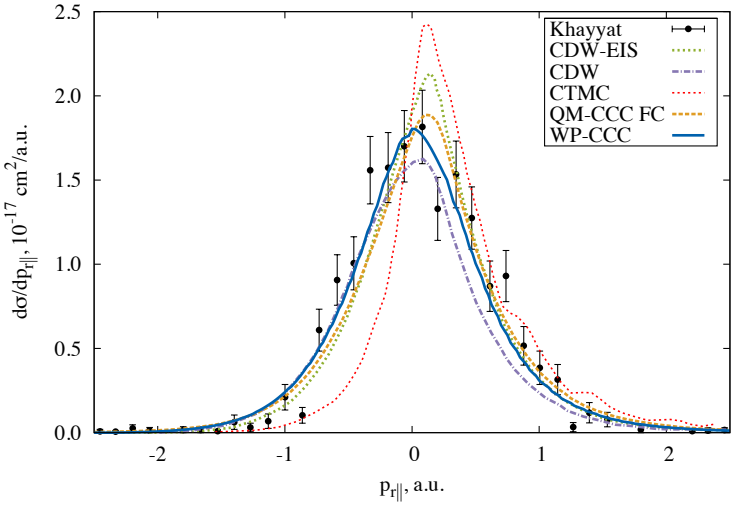


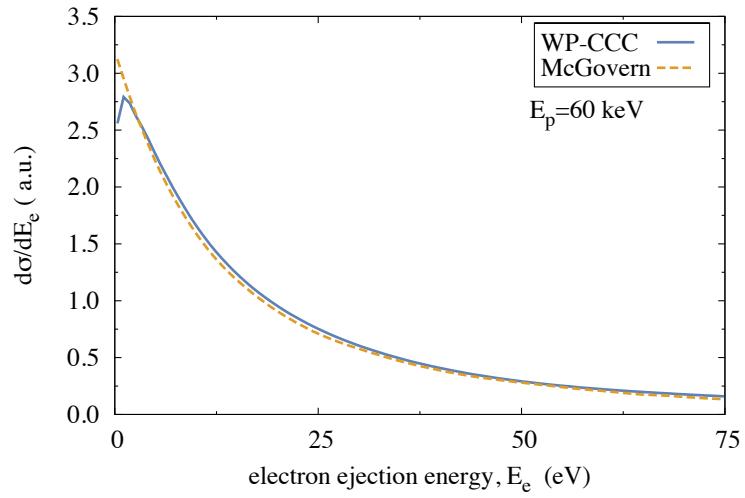
Relativistic method: Bondarev et al 2017 PRA 95, 052709

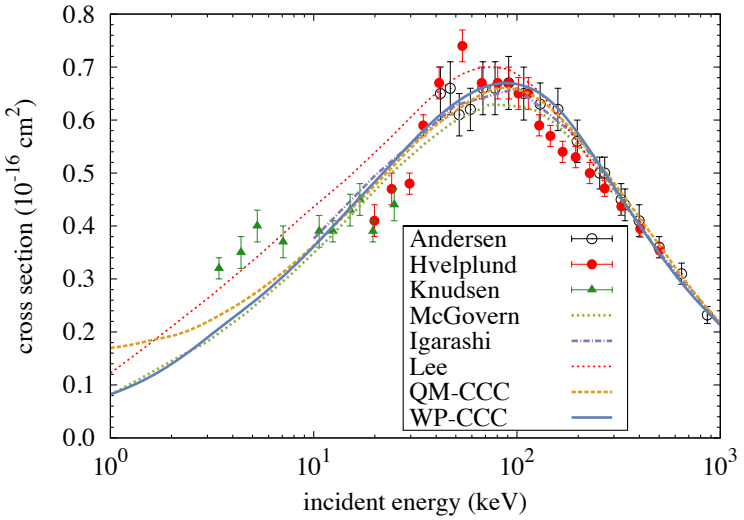
WP-CCC: Abdurakhmanov et al. 2016, PRA 94, 022703
QM-CCC: Abdurakhmanov et al. 2011 JPB 44, 075204

He single ionisation by antiprotons



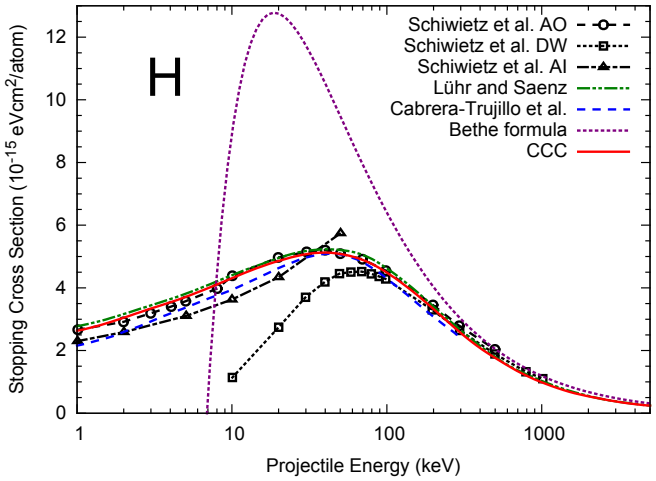


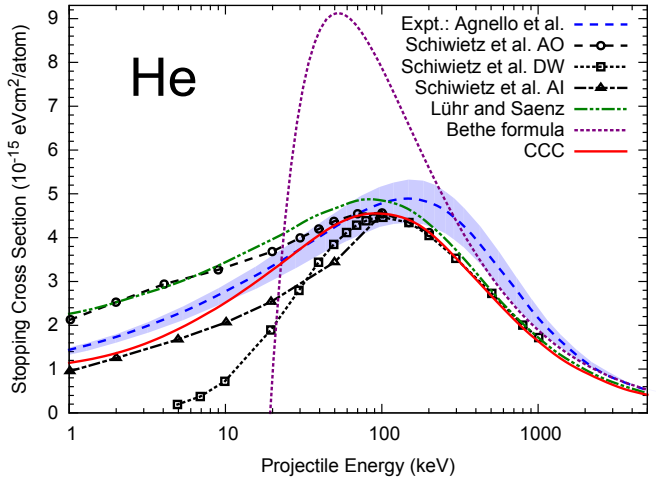


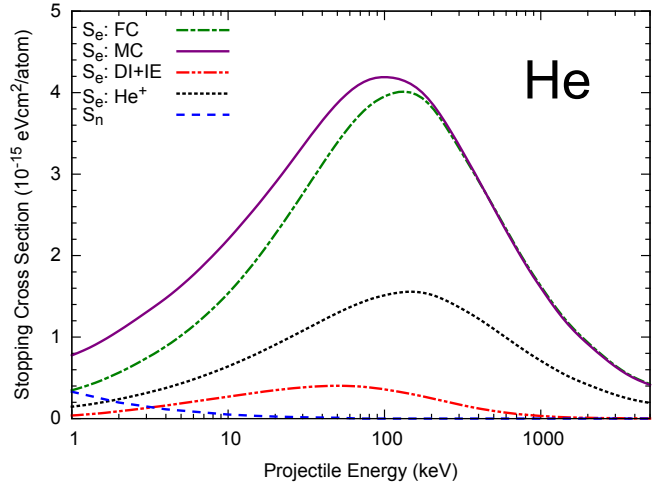


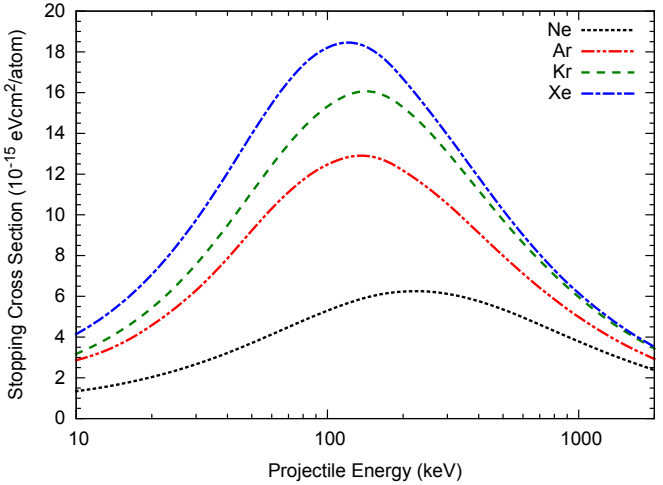
WP-CCC: Abdurakhmanov et al. 2017, PRA 96, 022702

Stopping power for antiproton in atoms









Bailey etal. 2015, Phys Rev A 92, 022707 and PRA 92, 052711

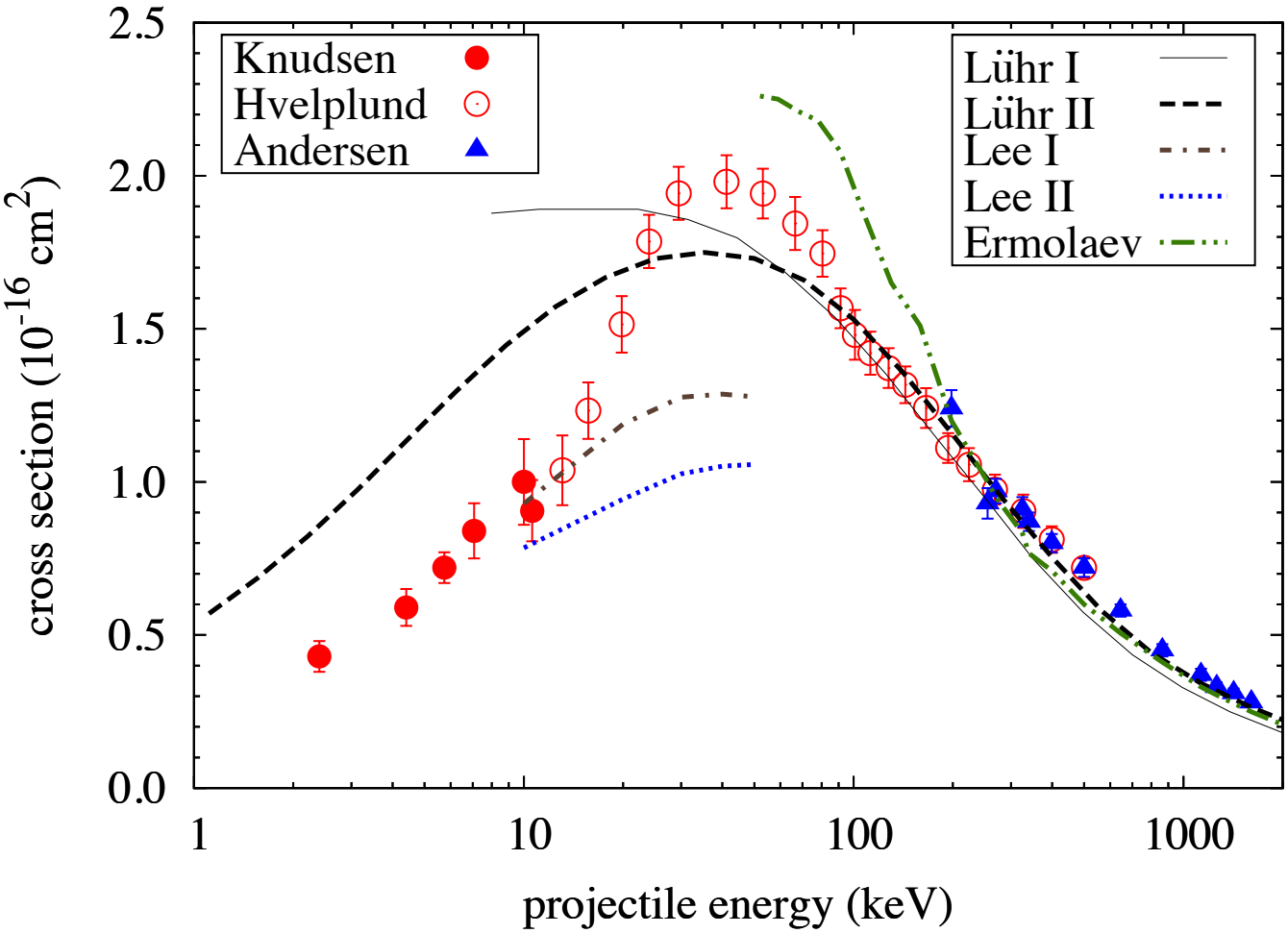
Conclusions

- Quantum-mechanical CCC approach is applied to antihydrogen formation in Ps collisions with antiproton
- Quantum suppression of the antihydrogen-formation cross section
- Results of the CTMC simulations might be too optimistic

- Developed CCC approach to antiproton scattering on atomic and molecular targets (H, He, inert gases, H_2, H_2O)
  - Quantum-mechanical: QM-CCC
  - Semiclassical: SC-CCC
  - Wave-packet: WP-CCC

- Antiproton scattering on residual gas in ELENA ring

TICS nondissociative ionisation of H_2



SC-CCC: Abdurakhmanov et al. 2013, PRL 111, 173201

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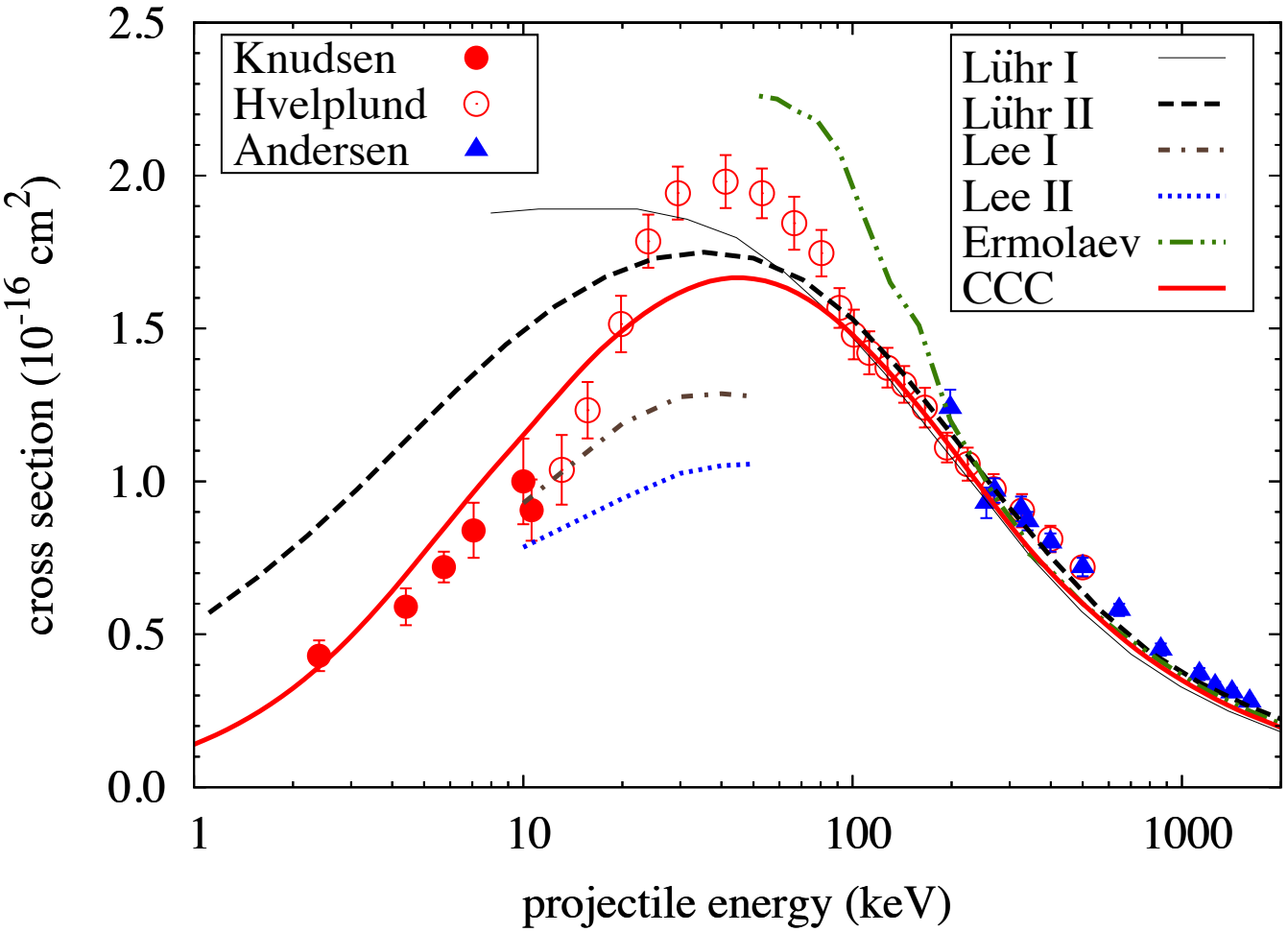
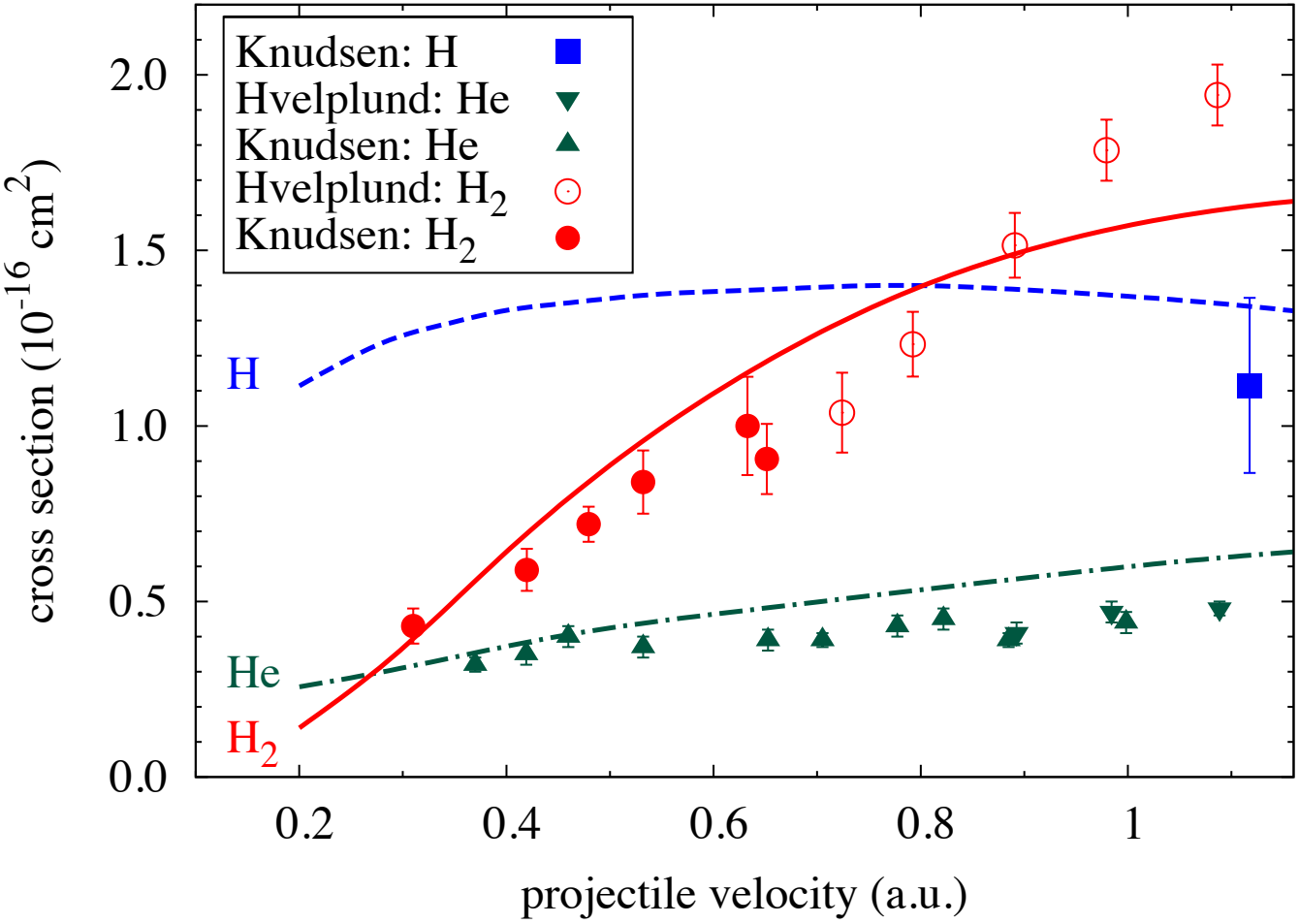
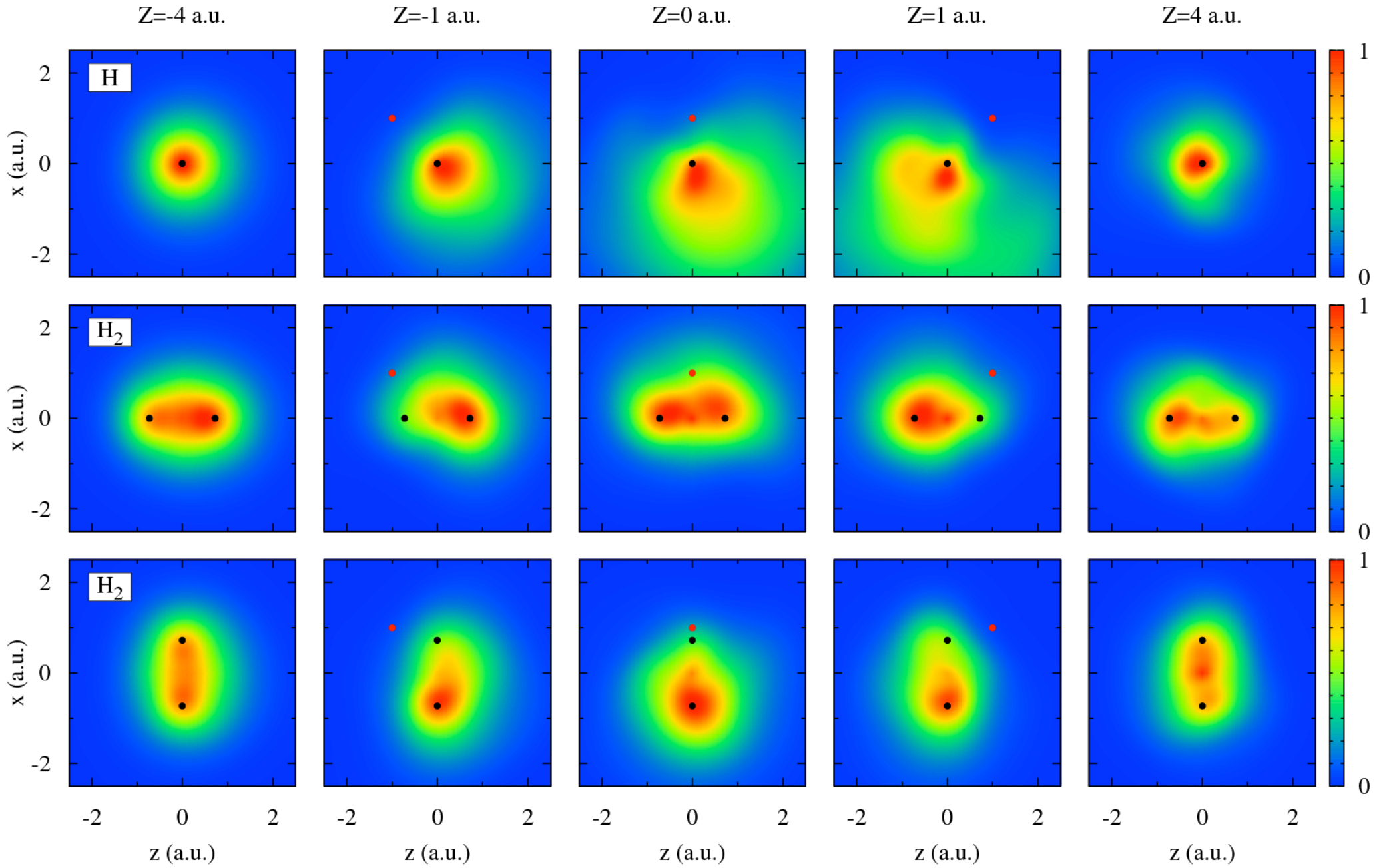


SC-CCC: Abdurakhmanov et al. 2013, PRL 111, 173201

TICS: H, He and H_2

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Z=-1 a.u.
Z=0 a.u.
Z=1 a.u.
Z=4 a.u.
H
H2
H2
x (a.u.)
z (a.u.)
2
0
-2
1
0