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Proton scattering from excited states of atomic hydrogen + some other processes

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Outline

① Single-centre semiclassical close-coupling (CC) approach

② Difficulties associated with two-centre semiclassical CC approach

③ Two-centre semiclassical convergent close-coupling (CCC) approach

④ Total and various differential cross sections for ionisation and electron capture in following collisions

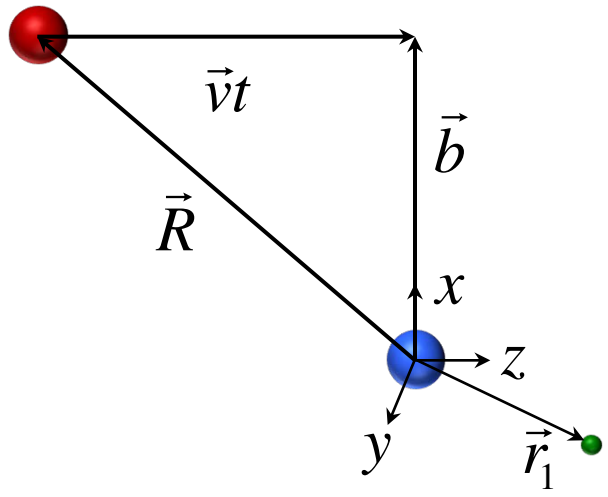
- $p + H(n=2)$
- $C^{6+} + H(1s)$
- $p + He(1s^2)$
- $H(1s) + H(1s)$

1-centre semiclassical CC approach

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

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

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

1-centre semiclassical approach

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

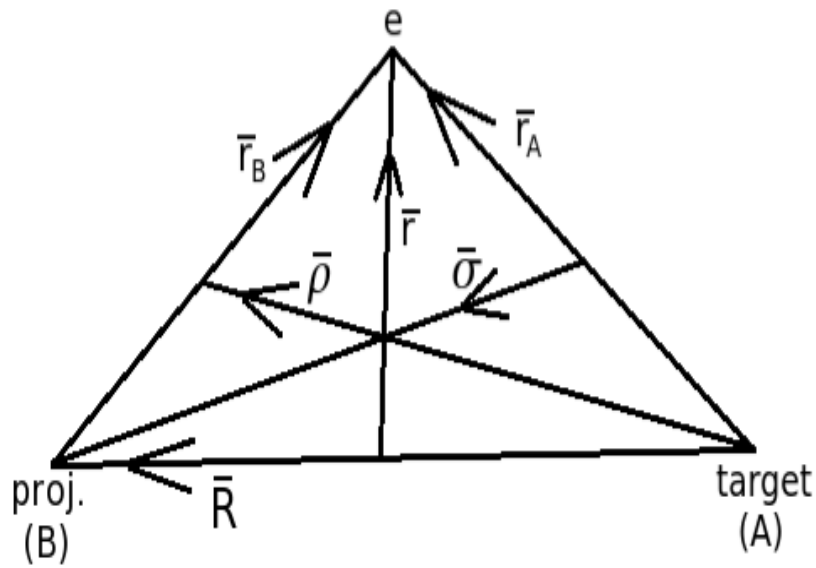
Conventional 2-centre CC approach

In 1-centre case we used

$$\Psi(\vec{r}_A,t)=\sum_\alpha a_\alpha(t)\phi_\alpha^A(\vec{r}_A)e^{-i\varepsilon_\alpha t}$$

It is a solution to TDSE

$$i\frac{\partial\Psi(\vec{r}_A,t)}{\partial t}=(H_A+V_B)\Psi(\vec{r}_A,t)$$

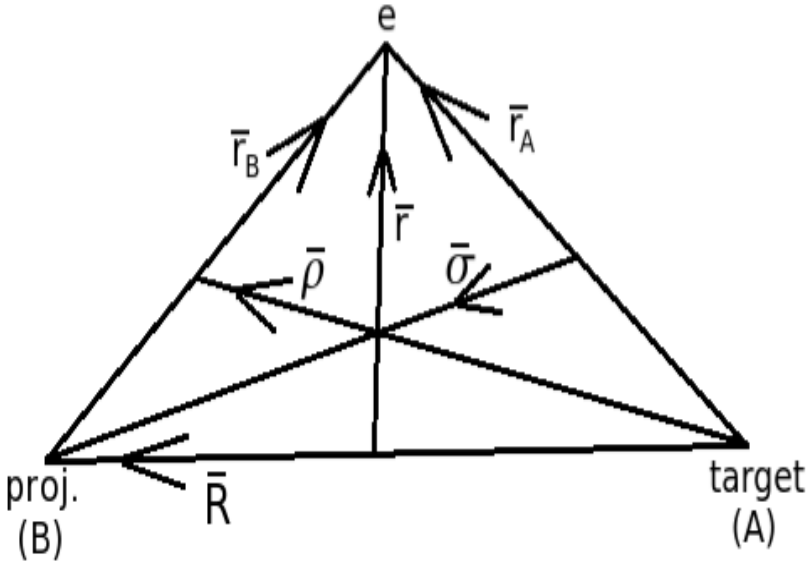


- Now we take into account electron capture
- We need a 2-centre expansion

Conventional 2-centre CC approach

2-centre expansion

$$\Psi(\vec{r},t) = \sum_{\alpha} a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{-i\varepsilon_{\alpha}t} + \sum_{\beta} b_{\beta}(t)\phi_{\beta}^{B}(\vec{r}_{B})e^{-i\varepsilon_{\beta}t}$$



There are 2 problems

We write TDSE in c.m. frame

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

However, this does not solve the problem.

The wave function does not satisfy boundary conditions.

Electronic translational factors

Bates and McCarroll (1958): electronic translational factors (ETF)

2-centre expansion safisfying the boundary conditions

$$\Psi(\vec{r},t)=\sum_{\alpha}a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{-i\varepsilon_{\alpha}t+i\pi_{\alpha}^{A}(\vec{r},t)-iv^{2}t/8}+\sum_{\beta}b_{\beta}(t)\phi_{\beta}^{B}(\vec{r}_{B})e^{-i\varepsilon_{\beta}t+i\pi_{\beta}^{B}(\vec{r},t)-iv^{2}t/8}$$

where $\pi_{\alpha}^{A}(\vec{r},t)$ and $\pi_{\beta}^{B}(\vec{r},t)$ are arbitrary functions.

The only condition is that when $|t|\rightarrow\infty$

$\pi_{\alpha}^{A}(\vec{r},t)\rightarrow-\frac{1}{2}\vec{v}\vec{r}$ and $\pi_{\beta}^{B}(\vec{r},t)\rightarrow\frac{1}{2}\vec{v}\vec{r}$

Science of ETFs

- There is a non-uniqueness problem
- Choice of ETFs and their optimisation (using variational techniques) become elaborate science
- Types of ETFs:
  - common
  - state-dependent
  - plane-wave
  - non-PW etc
- Many papers and reviews have been published
- Bates and McCarroll (1958) solution was incomplete
- We believe there is a better solution

2 problems with the standard approach

- Bates and McCarroll (1958) solution was incomplete

- There is no need for an *ad-hoc* solution using as ETF
- The reason for the problem was 2-fold

1st problem appears in the attempt to represent the 2nd centre w.f. in the same form as the w.f. of the 1st centre

$$\Psi(\vec{r},t)=\sum_{\alpha}a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{-i\varepsilon_{\alpha}t+i\pi_{\alpha}^{A}(\vec{r},t)-iv^{2}t/8}+\sum_{\beta}b_{\beta}(t)\phi_{\beta}^{B}(\vec{r}_{B})e^{-i\varepsilon_{\beta}t+i\pi_{\beta}^{B}(\vec{r},t)-iv^{2}t/8}$$

2nd problem is inTDSE

What is the solution?

- The correct 1-centre expansion should look like

$$\Psi(\vec{r},t)=\sum_{\alpha}a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{-i\varepsilon_{\alpha}t}\Rightarrow\tilde{\Psi}(\vec{r},t)=\sum_{\alpha}a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{i\vec{k}_{\alpha}\vec{\sigma}}$$

- Both satisfy the semi-classical TDSE

$$i\frac{\partial\Psi(\vec{r},\vec{b},t)}{\partial t}=(T_{\vec{r}}+V)\Psi(\vec{r},\vec{b},t)$$

- But $\tilde{\Psi}$ also satisfies the full (exact) TISE $\quad(E-H)\tilde{\Psi}=0$

How does temporal factor emerge?

$$(\boldsymbol{k}_\alpha - \boldsymbol{k}_{\alpha'})\cdot\boldsymbol{\sigma} \approx (\boldsymbol{k}_\alpha - \boldsymbol{k}_{\alpha'})\cdot\boldsymbol{R} = q_{\|}z + \boldsymbol{q}_\perp\cdot\boldsymbol{b}$$

$$q_{\|} = (\epsilon_{\alpha'} - \epsilon_\alpha)/v$$

Since $z = vt$

$$(\boldsymbol{k}_\alpha - \boldsymbol{k}_{\alpha'})\cdot\boldsymbol{\sigma} \approx (\epsilon_{\alpha'} - \epsilon_\alpha)t + \boldsymbol{q}_\perp\cdot\boldsymbol{b}$$

What is the solution?

- The correct 2-centre expansion is

$$\tilde{\Psi}(\vec{r},t) = \sum_{\alpha} a_{\alpha}(t)\phi_{\alpha}^{A}(\vec{r}_{A})e^{i\vec{k}_{\alpha}\vec{\sigma}} + \sum_{\beta} b_{\beta}(t)\phi_{\beta}^{B}(\vec{r}_{B})e^{i\vec{k}_{\beta}\vec{\rho}}$$

- This w.f. does not satisfy TDSE

$$i\frac{\partial\tilde{\Psi}(\vec{r},t)}{\partial t} \neq (T_{\vec{r}} + V)\tilde{\Psi}(\vec{r},t)$$

- But satisfies the full TISE $(E - H)\tilde{\Psi} = 0$

How does ETF appear?

$$\boldsymbol{k}_\beta \cdot \boldsymbol{\sigma}_\mathrm{P} - \boldsymbol{k}_{\alpha'} \cdot \boldsymbol{\sigma}_\mathrm{T} = p_{\beta\|} z + \boldsymbol{p}_{\beta\perp} \cdot \boldsymbol{b} + \boldsymbol{v} \cdot \boldsymbol{r}_\mathrm{T}$$

$$p_{\beta\|} = -v/2 + (\epsilon_{\alpha'} - \epsilon_\beta)/v$$

$$\boldsymbol{k}_\beta \cdot \boldsymbol{\sigma}_\mathrm{P} - \boldsymbol{k}_{\alpha'} \cdot \boldsymbol{\sigma}_\mathrm{T} = (\epsilon_{\alpha'} - \epsilon_\beta) t - v^2 t/2 + \boldsymbol{p}_{\beta\perp} \cdot \boldsymbol{b} + \boldsymbol{v} \cdot \boldsymbol{r}_\mathrm{T}$$

ETF

- These 2 terms were introduced *ad-hoc* to fix the problem
- In our approach they appear naturally
- Details: Abdurakhmanov etal, PRA 97, 032707 (2018)

2-centre semi-classical equations

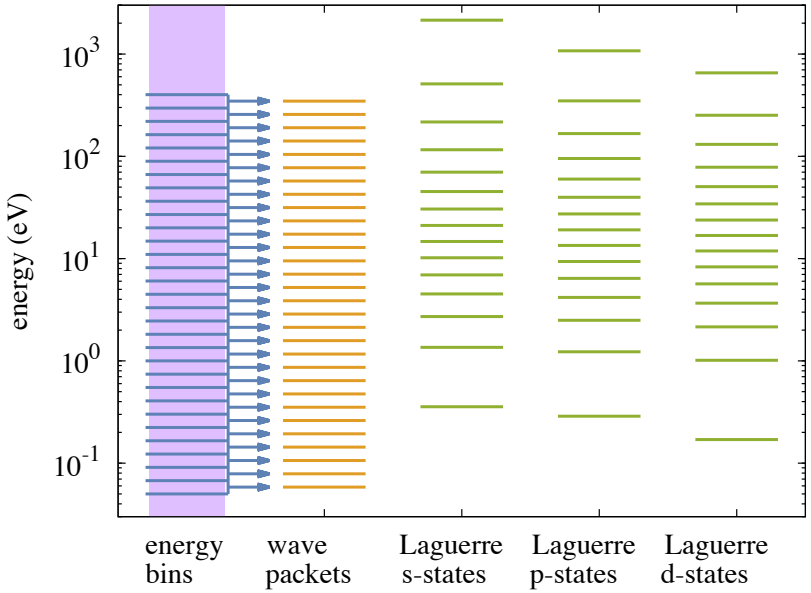
- Inserting $\tilde{\Psi}$ into TISE $(E-H)\tilde{\Psi}=0$ and using semi-classical approximation we get the same result as we would get using PW ETFs

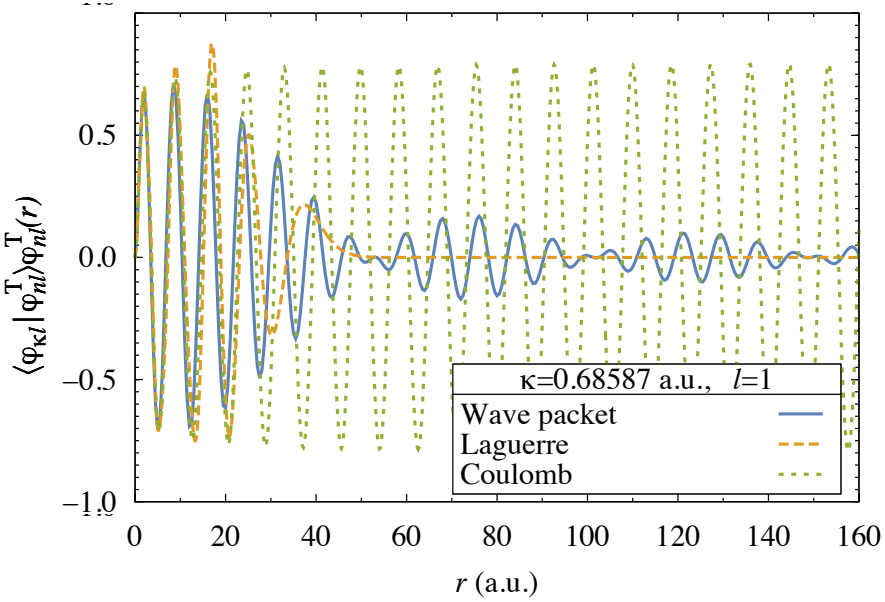
$$i\begin{pmatrix} \boldsymbol{I} & \boldsymbol{G}^A \\ \boldsymbol{G}^B & \boldsymbol{I} \end{pmatrix}\begin{pmatrix} \dot{\boldsymbol{a}} \\ \dot{\boldsymbol{b}} \end{pmatrix}=\begin{pmatrix} \boldsymbol{D}^A & \boldsymbol{Q}^A \\ \boldsymbol{Q}^B & \boldsymbol{D}^B \end{pmatrix}\begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix}$$

NB: Compare with 1-centre case: $\boldsymbol{i\dot{a}}=\boldsymbol{D}^A\boldsymbol{a}$

- Thus there is no SC TDSE when rearrangment inlcuded

Wave-packet continuum discretisation





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

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

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

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

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.*, Ann Phys 324 (2009) 1516:

Kadyrov et al, PRL 101 (2008) 230405

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

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

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

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

Breakup amplitude including ECC

- Surface-integral formulation of scattering theory:

$$T^{post} = \left\langle \Phi_0^- \left| \overleftarrow{H} - E \right| \Psi_i^+ \right\rangle \approx \langle \Phi_0^- (I_N^T + I_M^P) \,|\, \overleftarrow{H} - E \,|\, (I_N^T + I_M^P) \Psi_i^+ \rangle$$
$$\equiv \langle \Phi_0^- I_N^T \,|\, \overleftarrow{H} - E \,|\, \Psi_i^{NM+} \rangle + \langle \Phi_0^- I_M^P \,|\, \overleftarrow{H} - E \,|\, \Psi_i^{NM+} \rangle$$

Thus the breakup amplitude splits into two:

direct ionisation (DI) and electron capture to continuum (ECC)

$$T^T = \left\langle \vec{q}_f, \psi_{\vec{k}}^T \left| I_N \left(\overleftarrow{H} - E \right) \right| \Psi_i^{NM+} \right\rangle = \left\langle \psi_{\vec{k}}^T \left| \phi_f^T \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad k^2 / 2 = \varepsilon_f$$

$$T^P = \left\langle \vec{q}_f, \psi_{\vec{p}}^P \left| I_P \left(\overleftarrow{H} - E \right) \right| \Psi_i^{NM+} \right\rangle = \left\langle \psi_{\vec{p}}^P \left| \phi_f^P \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad p^2 / 2 = \varepsilon_f$$

where $\psi_{\vec{k}}^T$ and $\psi_{\vec{p}}^P$ are the continuum states of target and projectile.

p + H(n=2)

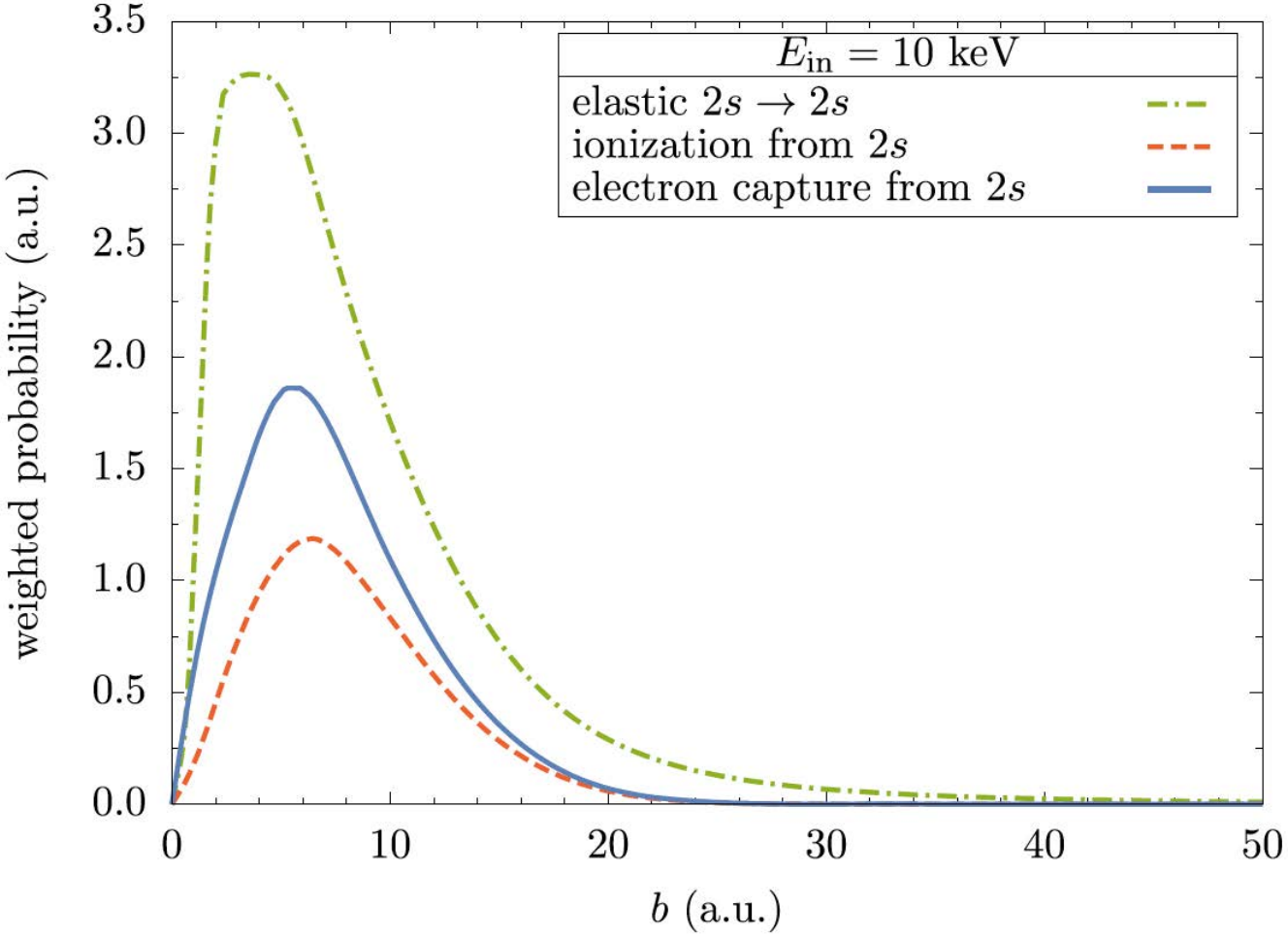


Figure 1. The weighted elastic bP_{2s}^{el}, total ionization bP_{2s}^{ion} and total electron-capture bP_{2s}^{tec} probabilities as a function of impact parameter for 10 keV protons scattering off atomic hydrogen in the $2s$ state.

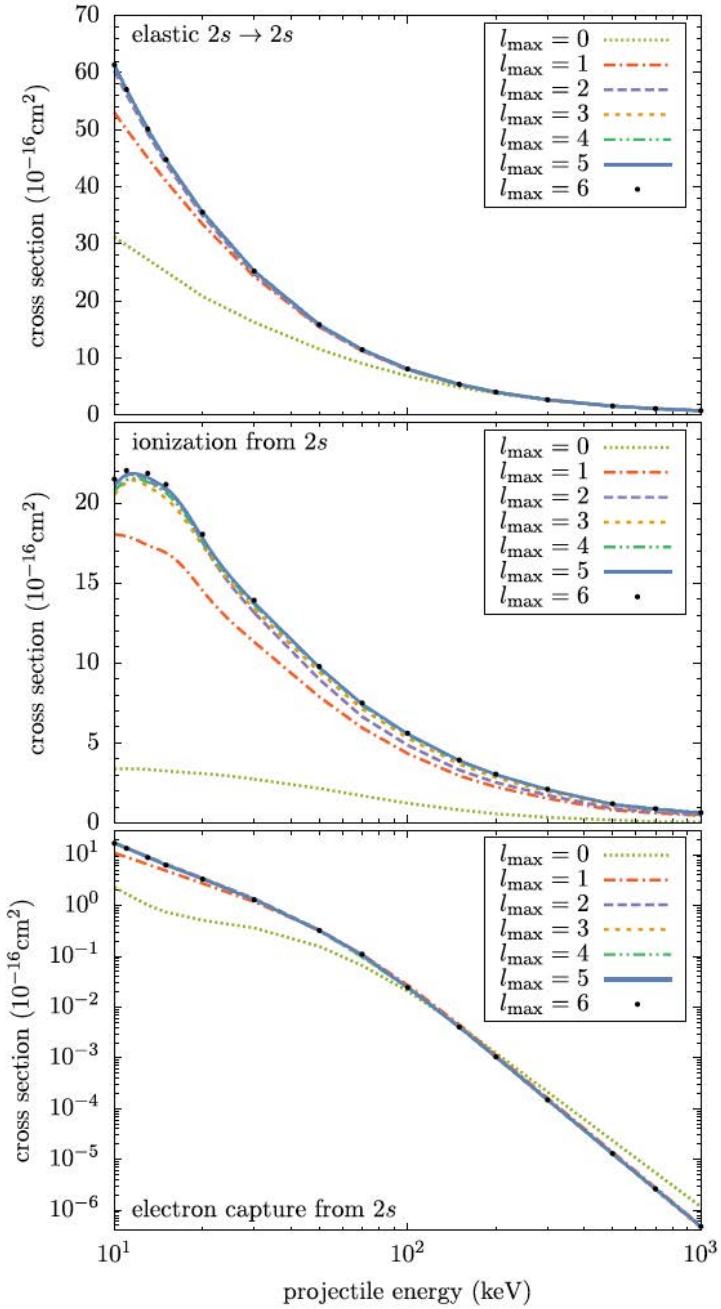


Figure 2. Convergence of the elastic, total ionization and total electron-capture cross sections for proton scattering off atomic hydrogen in the metastable $2s$ state.

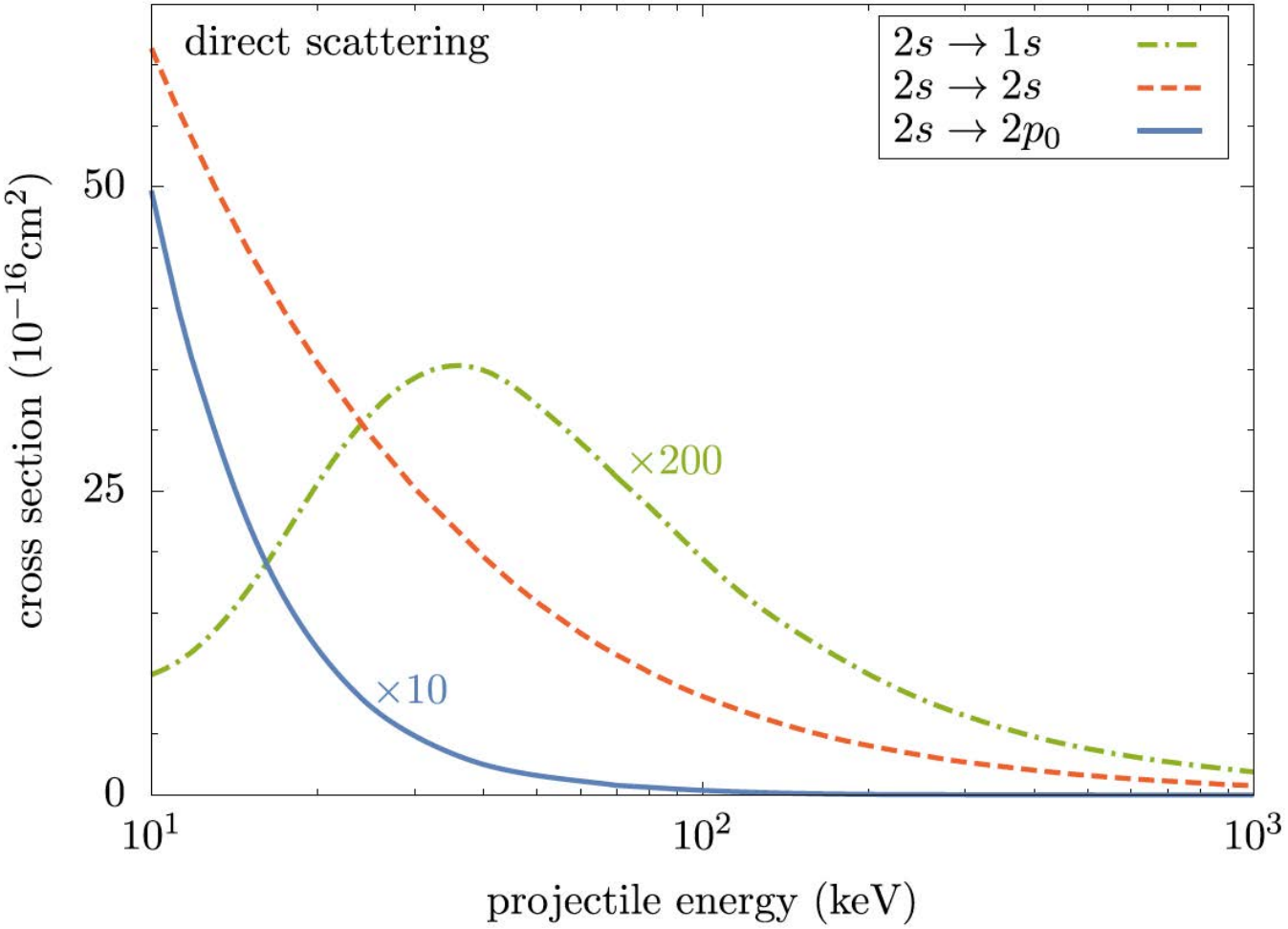


Figure 3. The cross sections for super-elastic, elastic and quasi-elastic scattering in p–H($2s$) collisions.

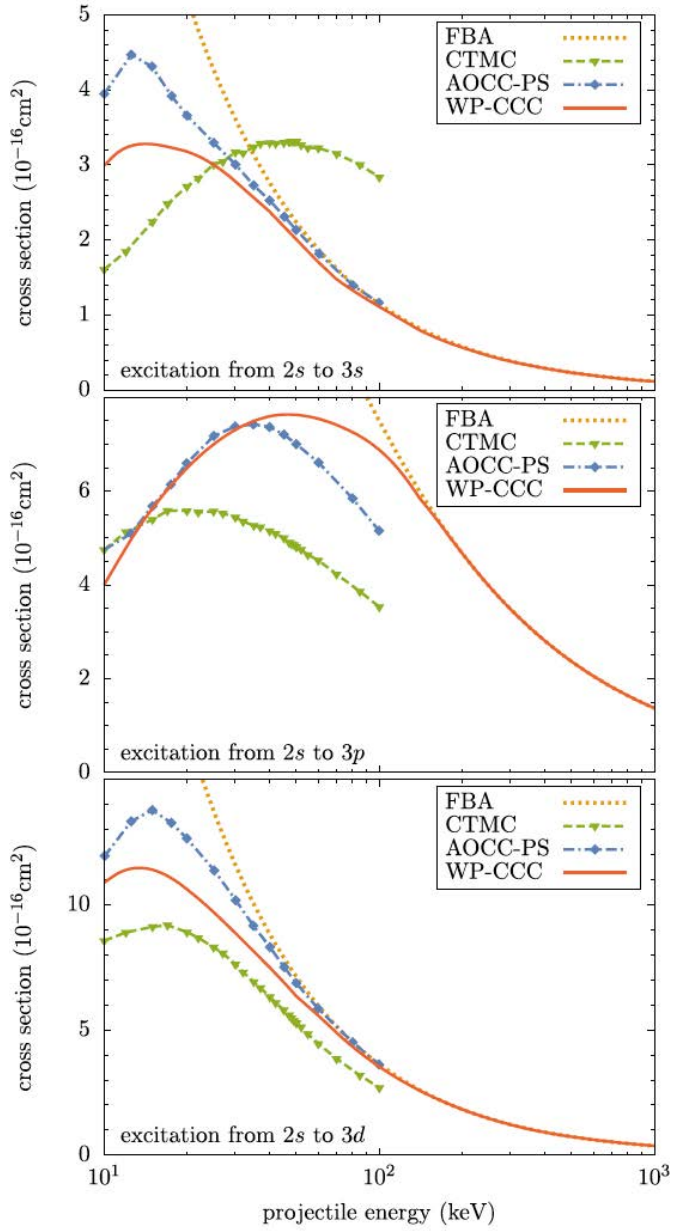


Figure 4. The cross sections for excitation of the $n = 3$-shell states in p–H(2s) collisions. The cross sections for excitations to the p and d states are summed over the magnetic quantum number. The CTMC and AOCC-PS results of Pindzola *et al* [9], and the FBA cross sections are also shown for comparison.

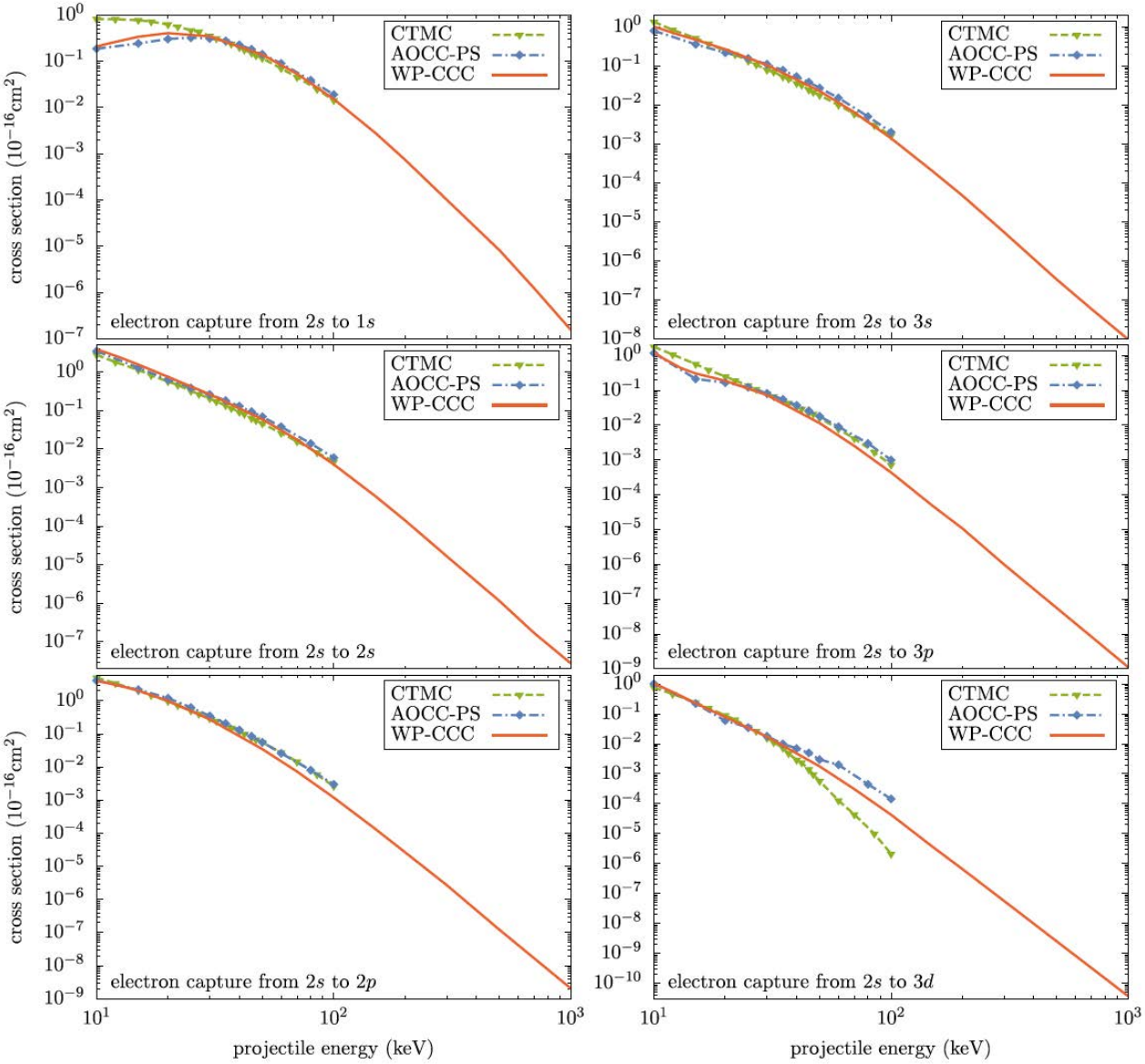


Figure 5. Select electron-capture cross sections for p–H(2*s*) collisions. The CTMC and AOCC-PS calculations of Pindzola *et al* [9] (see text) are also shown for comparison. The cross sections for electron-capture to the *p* and *d* states are summed over the magnetic quantum number.

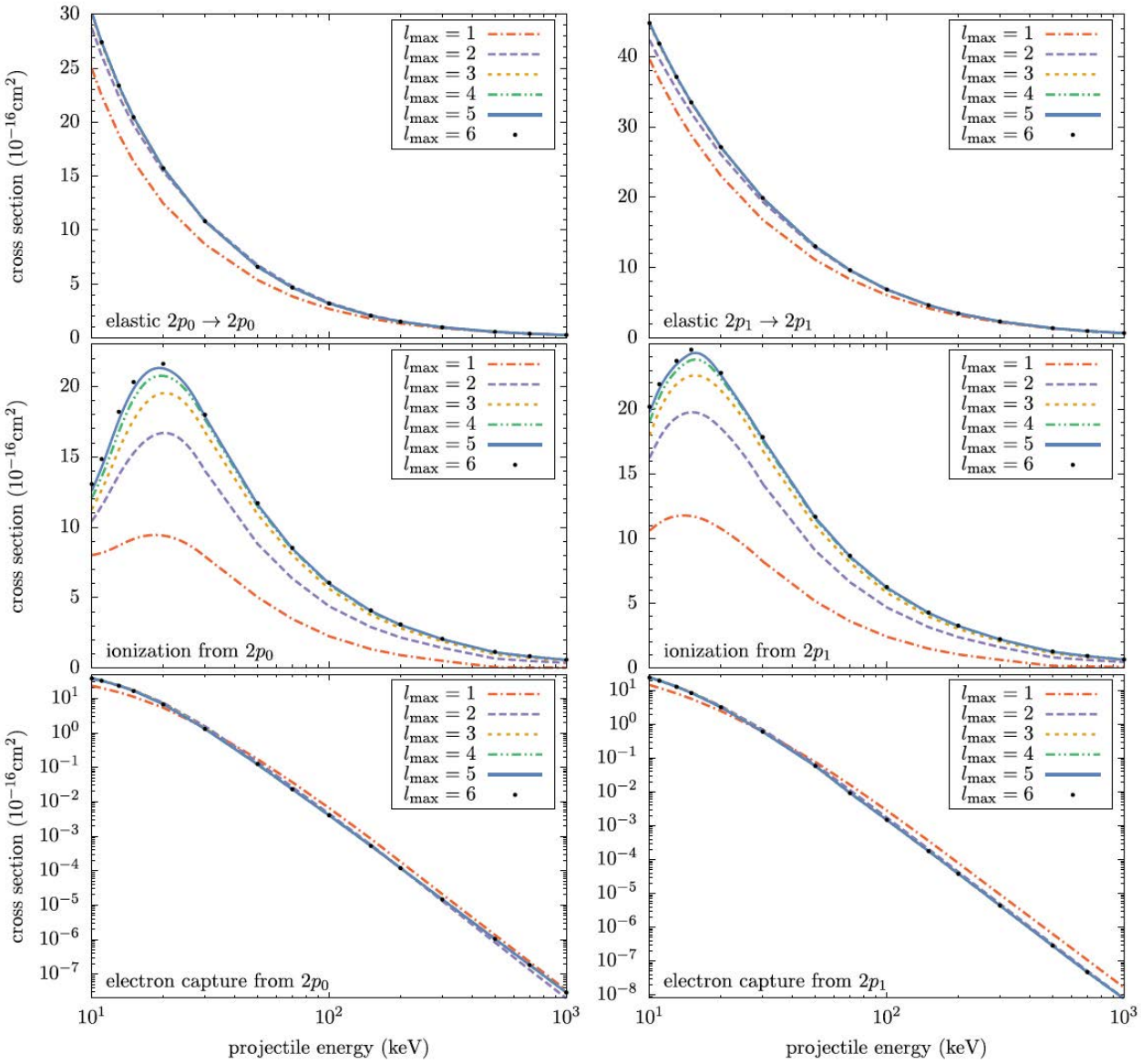


Figure 6. Convergence of the elastic, total ionization and total electron-capture cross sections for proton scattering off atomic hydrogen in the $2p_0$ and $2p_1$ states.

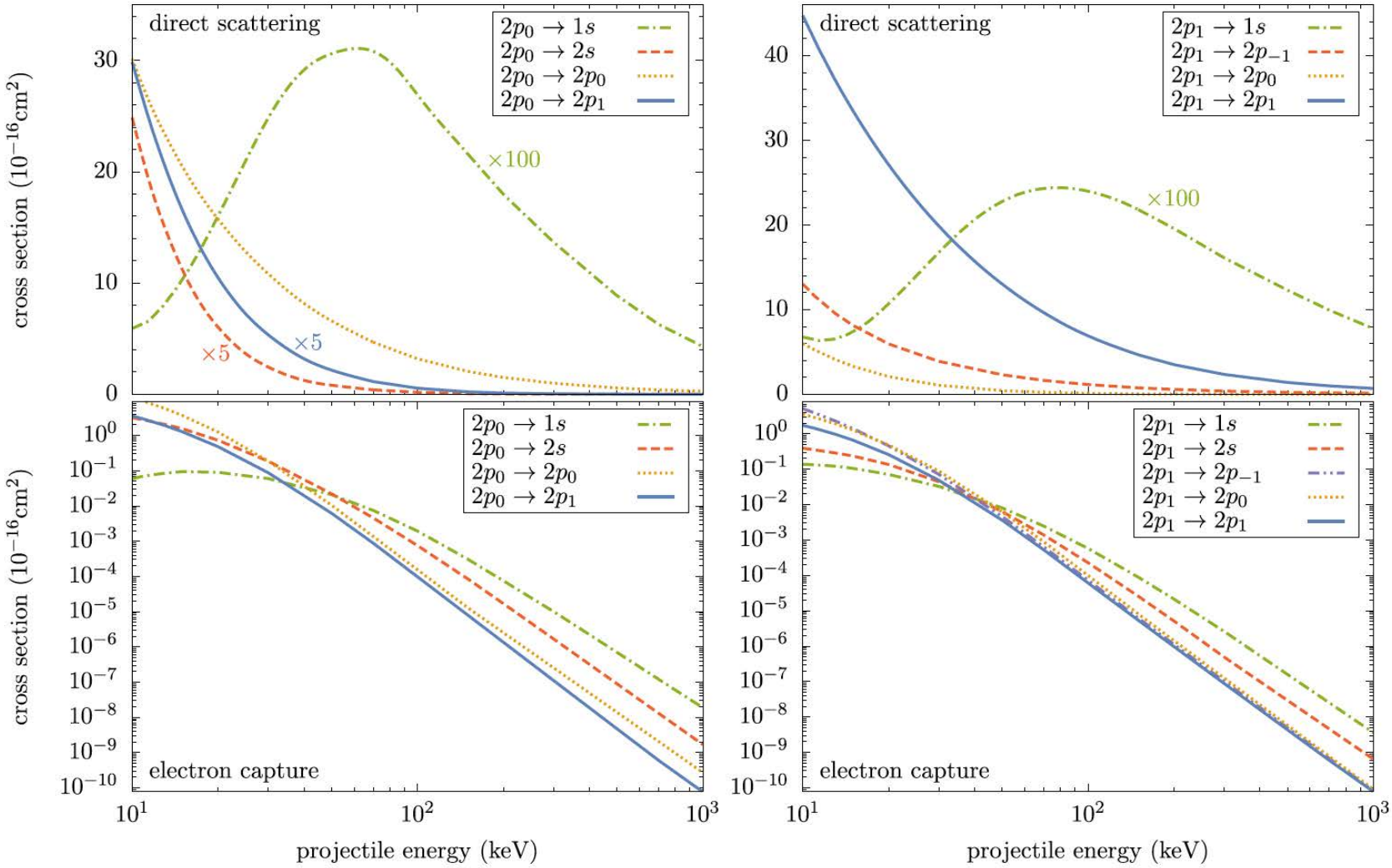


Figure 7. The super-elastic, elastic and quasi-elastic scattering, and electron-capture cross sections for proton scattering on atomic hydrogen in the $2p_0$ and $2p_1$ states.

Density matrix*

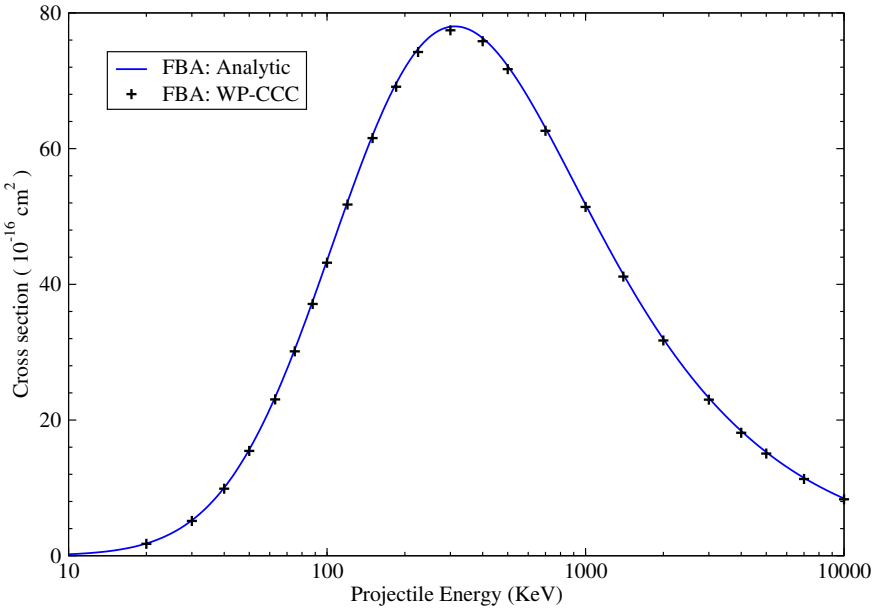
$$\rho^{i}_{\alpha'\alpha} = 2\pi \int_0^{\infty} \mathrm{d}b b F^{*}_{\alpha' i}(+\infty, b) F_{\alpha i}(+\infty, b)$$

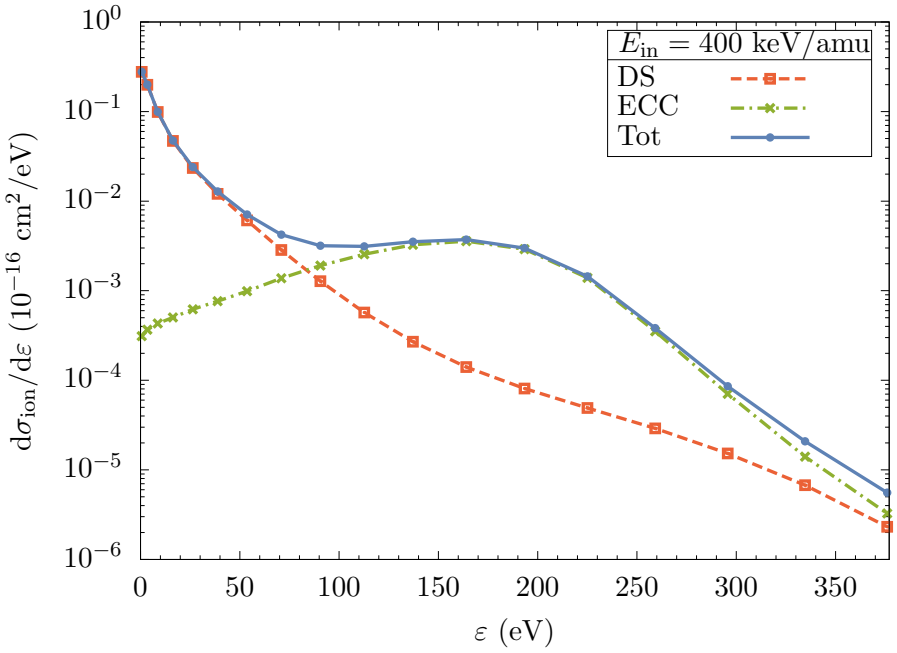
Table 3. Density matrix elements $\rho^{2p_1}_{\alpha'\alpha}$ (in 10^{-16} cm^2) for excitation of H($2p_1$) into the final n = 1–4 shell states of the target by proton impact at 50 keV.

α'	α	Re	Im	α'	α	Re	Im	α'	α	Re	Im	α'	α	Re	Im
100	100	2.28[−1]	0	210	321	−8.87[−1]	7.04[−1]	310	420	−1.69[−1]	−3.33[−2]	400	431	1.29[−2]	8.12[−4]
100	200	−1.23	2.32[−1]	210	322	−1.17	−1.28	310	421	2.58[−2]	−2.82[−1]	400	432	−2.96[−2]	2.05[−2]
100	210	−1.84[−1]	1.60[−1]	210	410	−4.66[−2]	−4.82[−2]	310	422	4.19[−1]	1.95[−2]	400	433	−3.68[−2]	−2.76[−2]
100	211	6.69[−1]	−1.29	210	411	3.79[−1]	−7.70[−2]	310	430	8.06[−2]	−2.76[−2]	410	410	2.08[−2]	0
100	300	−1.75[−1]	−6.42[−2]	210	420	1.36[−1]	2.12[−1]	310	431	2.90[−2]	1.55[−1]	410	411	−1.12[−2]	5.09[−2]
100	310	6.68[−2]	2.27[−2]	210	421	−3.80[−1]	3.27[−1]	310	432	−1.55[−1]	9.14[−2]	410	420	−5.62[−2]	−2.81[−2]
100	311	−3.80[−1]	5.19[−1]	210	422	−5.28[−1]	−5.43[−1]	310	433	−1.27[−1]	−1.26[−1]	410	421	3.11[−2]	−8.77[−2]
100	320	−1.57[−1]	5.04[−3]	210	430	−9.08[−2]	−3.96[−2]	311	311	2.28	0	410	422	1.29[−1]	4.29[−2]
100	321	−1.40[−1]	−4.39[−1]	210	431	1.74[−1]	−2.06[−1]	311	321	−1.77	1.15	410	430	3.31[−2]	−1.30[−3]
100	322	6.86[−1]	−2.16[−1]	210	432	2.79[−1]	6.56[−2]	311	322	−1.89	−2.61	410	431	−1.20[−3]	5.12[−2]
100	400	−6.72[−2]	−3.14[−2]	210	433	1.03[−2]	2.76[−1]	311	411	1.00	4.02[−2]	410	432	−5.92[−2]	1.56[−2]
100	410	1.35[−2]	1.03[−2]	211	211	13.0	0	311	421	−8.49[−1]	5.82[−1]	410	433	−3.16[−2]	−5.67[−2]
100	411	−1.93[−1]	2.27[−1]	211	311	−3.90	−6.00[−1]	311	422	−9.26[−1]	−1.17	411	411	4.58[−1]	0
100	420	−7.26[−2]	3.79[−3]	211	321	2.64	−5.18[−1]	311	431	4.40[−1]	−3.59[−1]	411	421	−3.29[−1]	2.35[−1]
100	421	−4.16[−2]	−2.40[−1]	211	322	7.40[−1]	4.54	311	432	4.97[−1]	1.95[−1]	411	422	−3.62[−1]	−4.54[−1]
100	422	3.59[−1]	−8.02[−2]	211	411	−1.90	−3.09[−1]	311	433	−5.87[−2]	4.94[−1]	411	431	1.78[−1]	−1.43[−1]
100	430	8.67[−4]	−1.58[−2]	211	421	1.36	−3.70[−1]	320	320	1.45	0	411	432	1.85[−1]	7.88[−2]
200	200	∞	0	211	433	4.48[−1]	−5.79[−1]	320	421	1.20[−1]	9.04[−1]	420	422	−5.60[−1]	2.98[−2]
200	210	1.88	−2.30	300	300	3.29[−1]	0	320	422	−1.33	2.13[−1]	420	430	−9.32[−2]	6.68[−2]

Abdurakhmanov et al, Plasma Phys. Control. Fusion 60 (2018) 095009

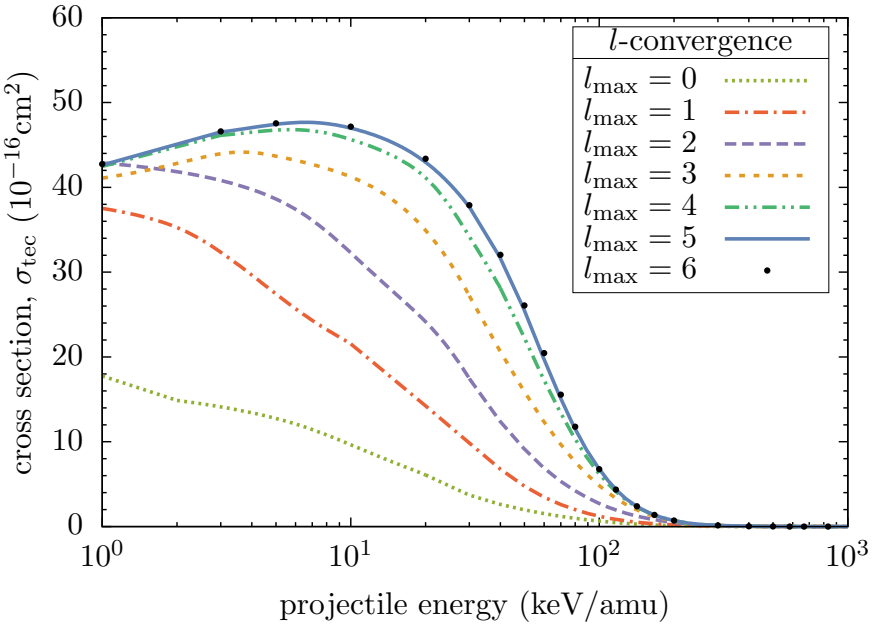
C^{6+} + H(1s) ionisation: test



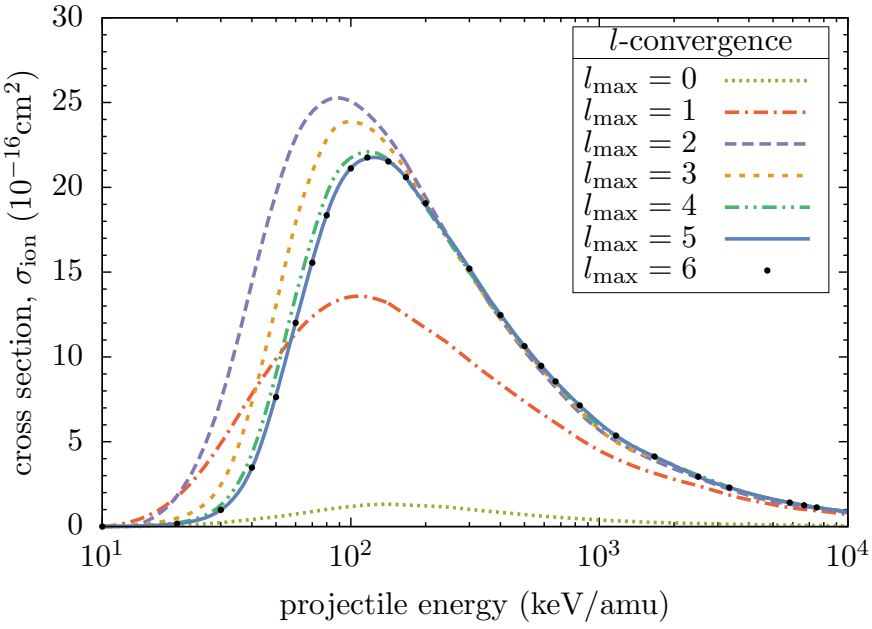


e-capture and ionisation: convergence

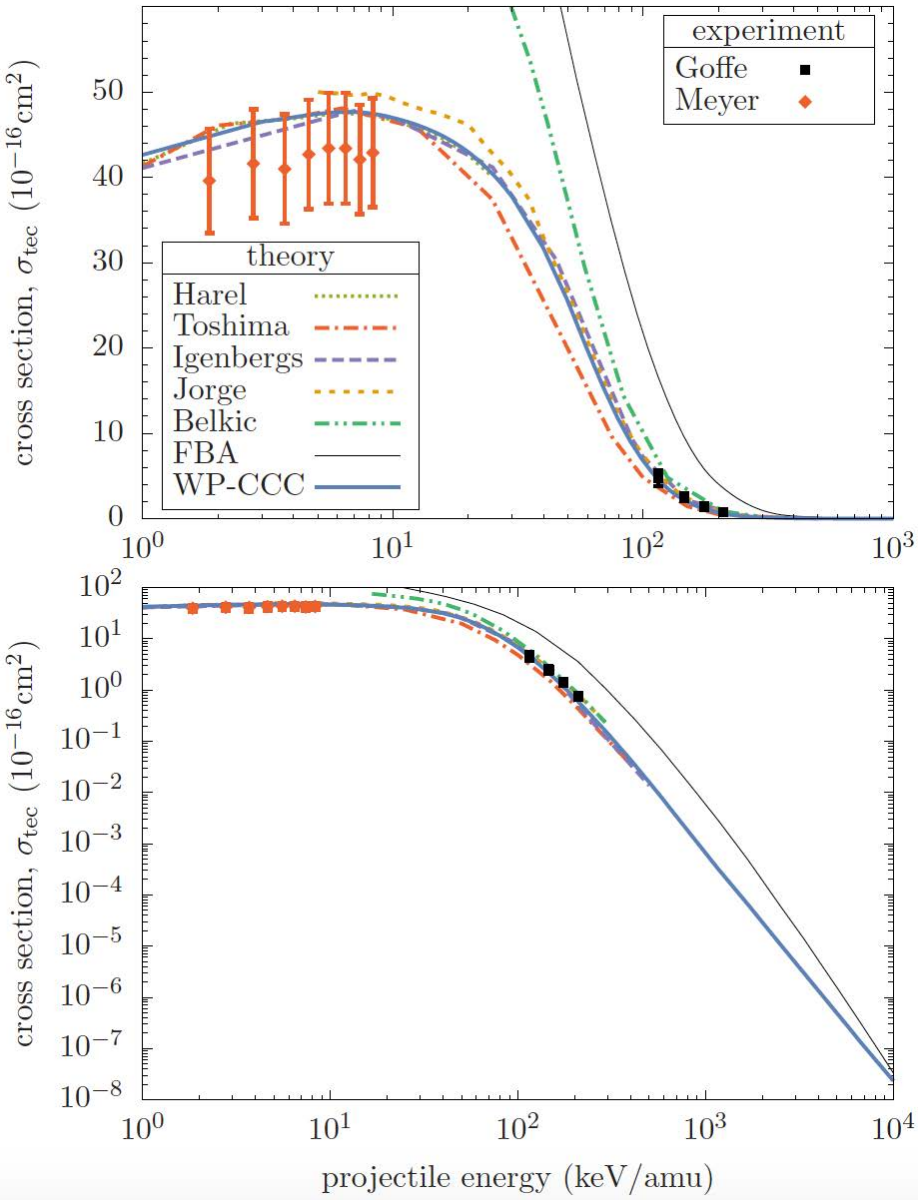
electron capture

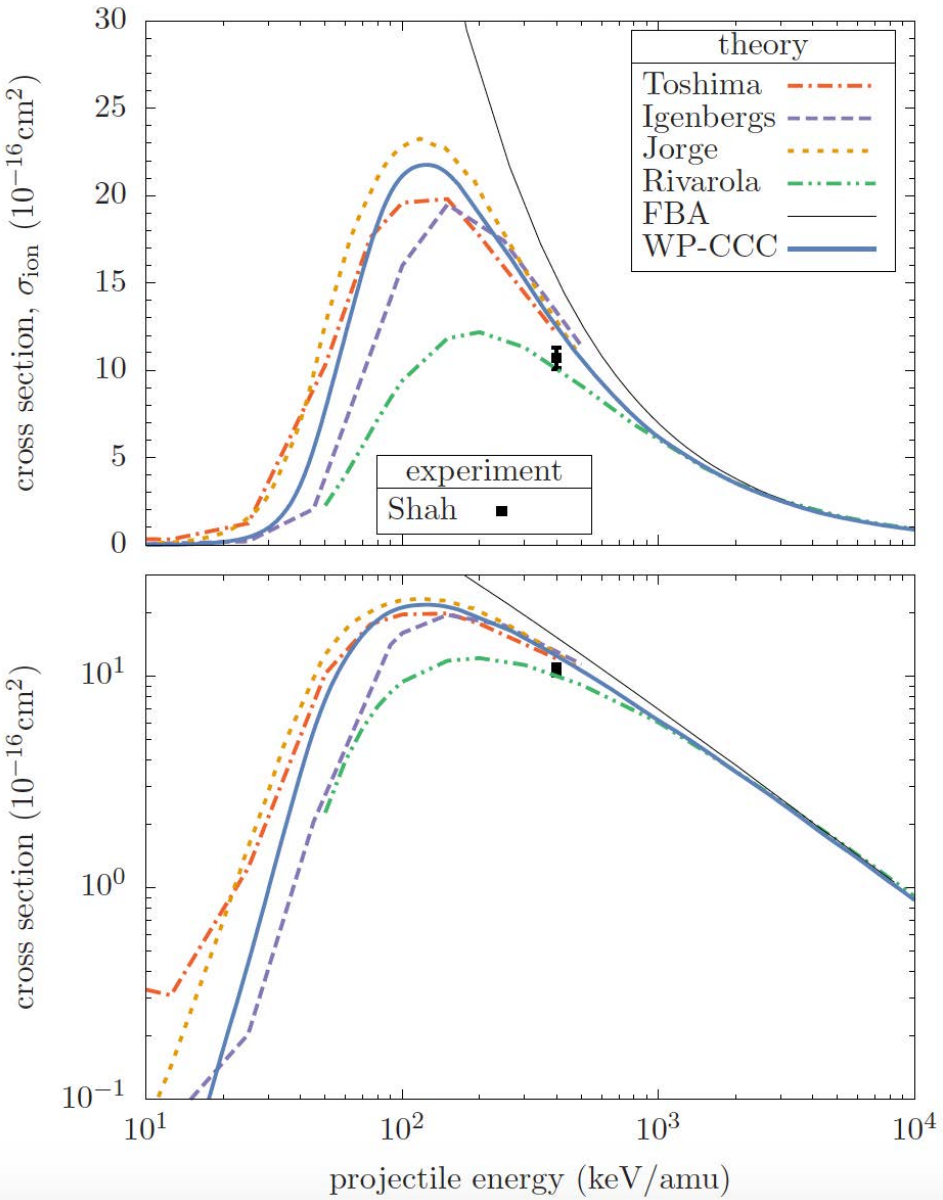


ionisation

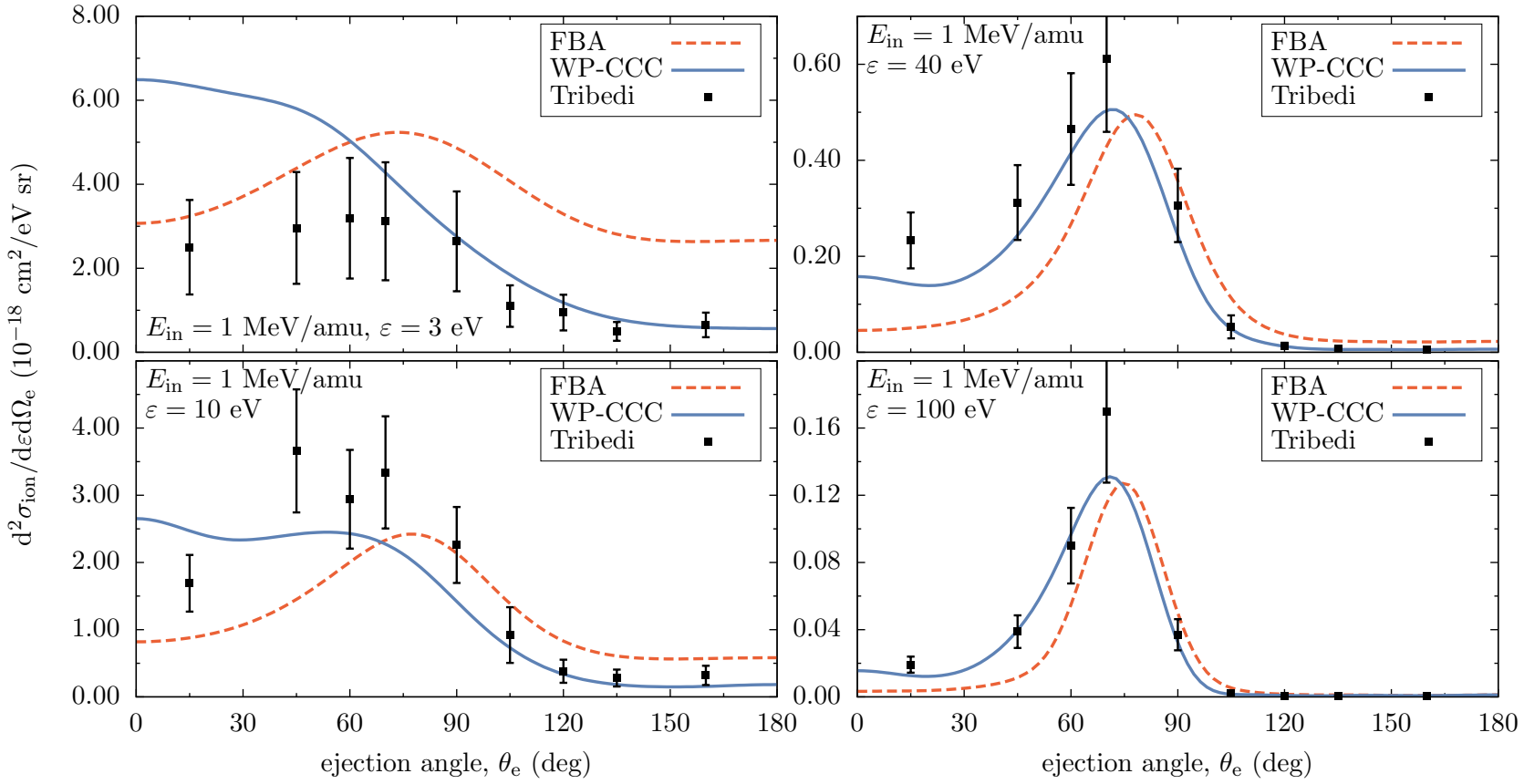


Electron capture and ionisation



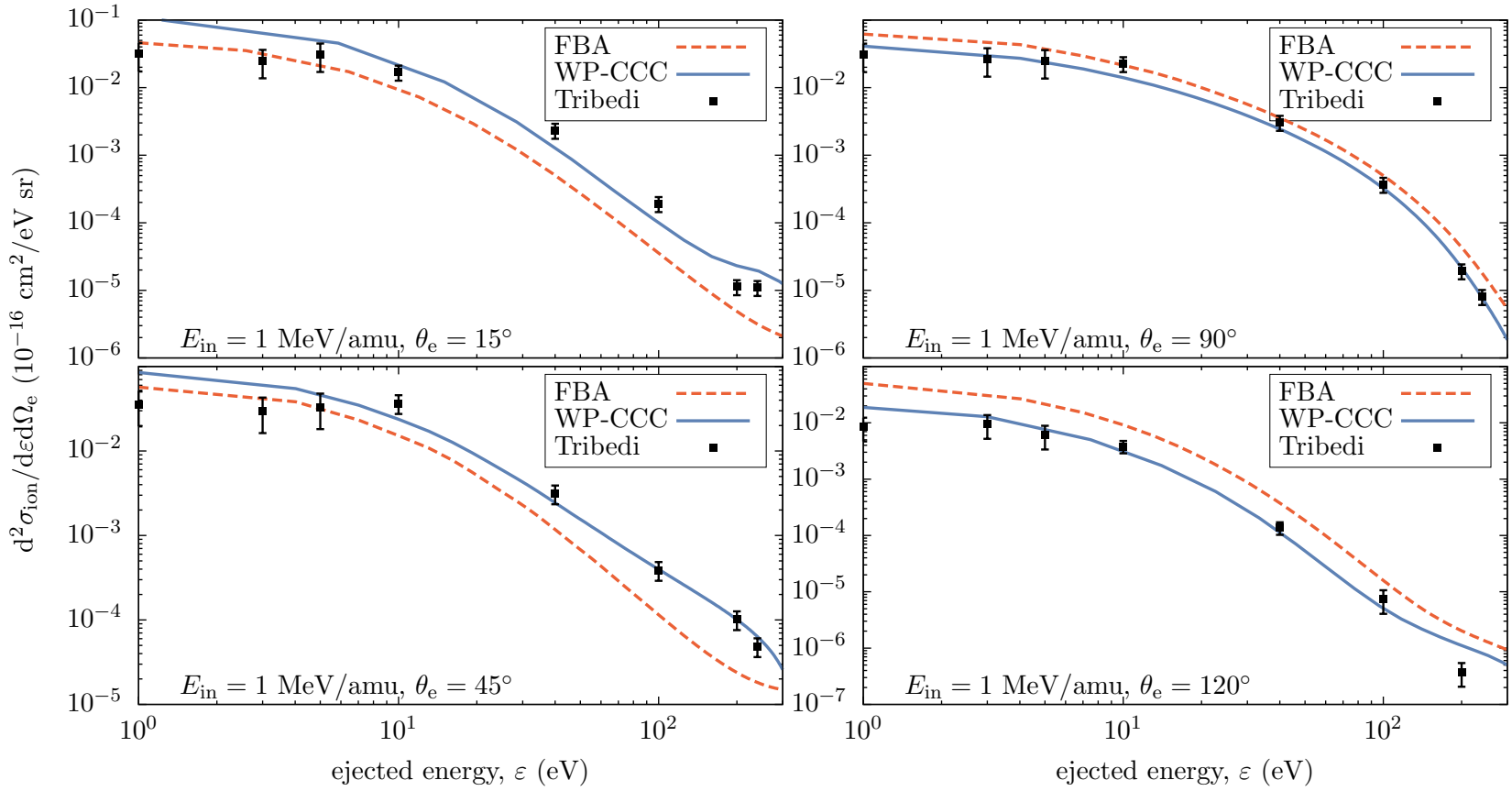


C^{6+}-H DDCS at 1 MeV/amu



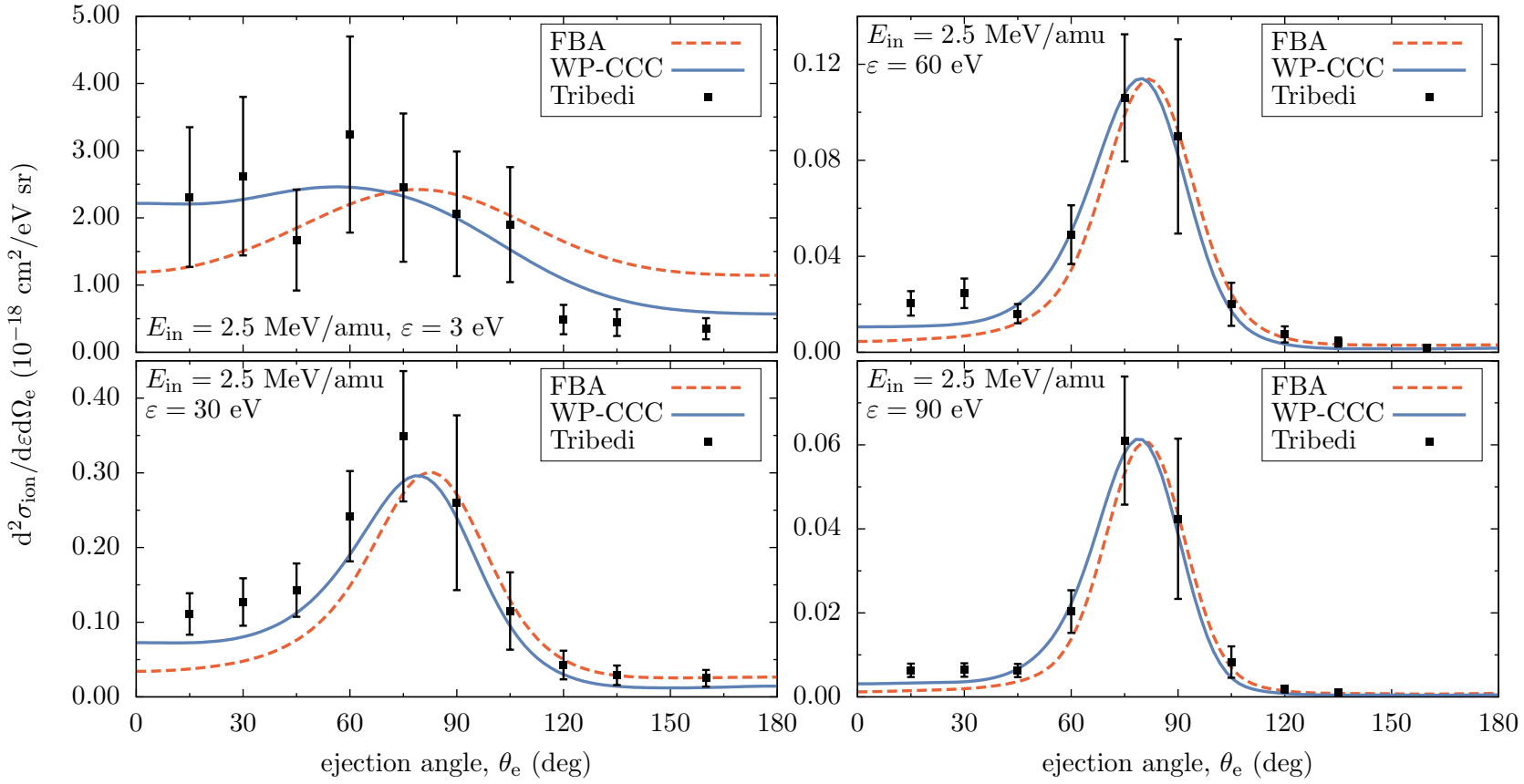
Exp: Tribedi et al., Phys Rev A 63, 062723 (2001)

C^{6+}-H DDCS at 1 MeV/amu



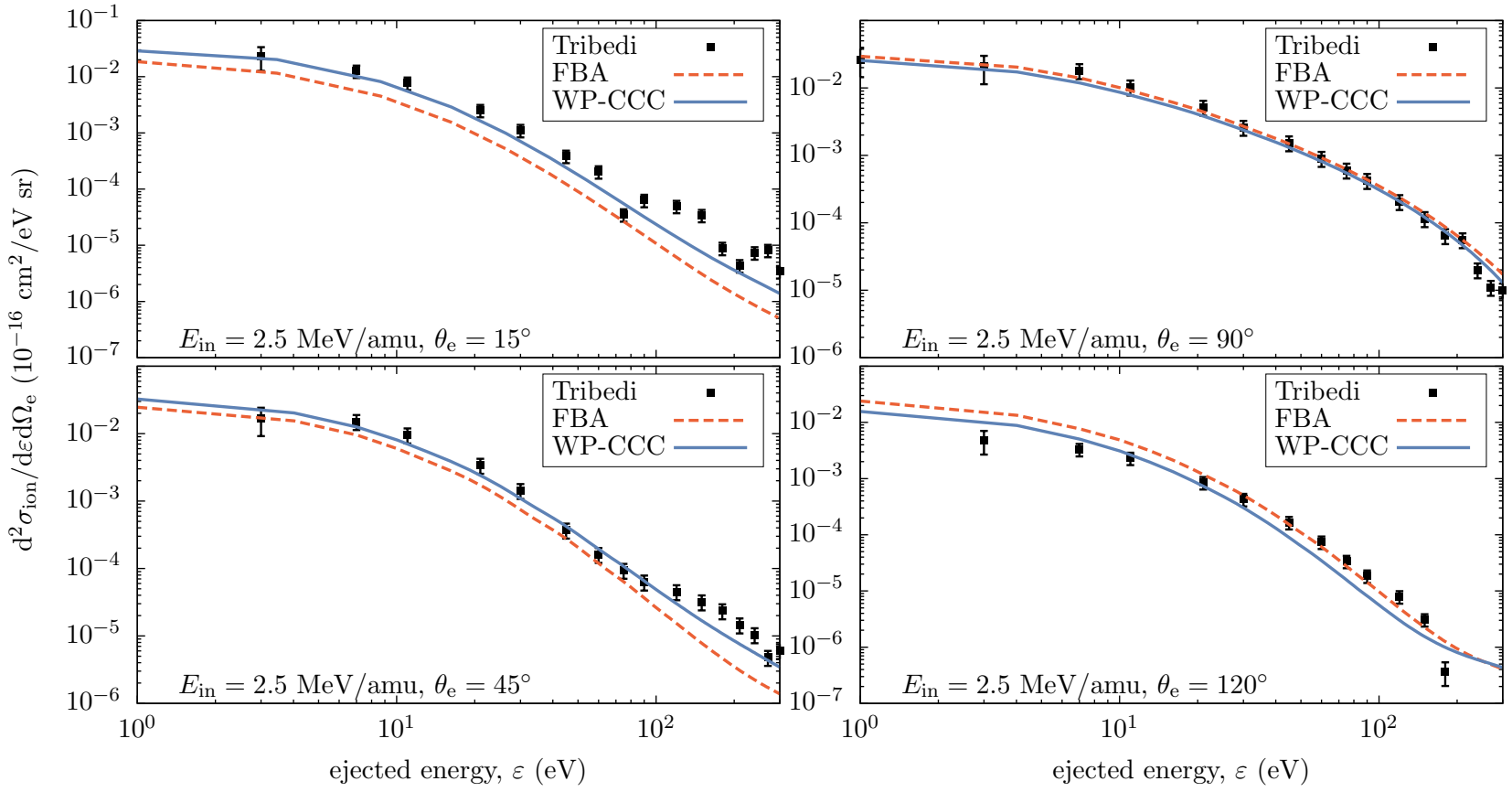
Exp: Tribedi et al., Phys Rev A 63, 062723 (2001)

C^{6+}-H DDCS at 2.5 MeV/amu



Exp: Tribedi et al., J Phys B 31, L369 (1998)

C^{6+}-H DDCS at 2.5 MeV/amu



Exp: Tribedi et al., J Phys B 31, L369 (1998)

Conclusions

- Developed 2-centre CCC approach to HCI-atom collisions including ECC
- Resolved the notorious ETF problem. Details: PRA 97, 032707 (2018)
- Accurate calculations of the total and various differential cross sections for ionisation and electron capture in p + H and C^{6+} + H collisions
- p + He and H + H collisions
- C^{6+} + H: DDCS and SDCS: good agreement at 2.5 MeV/amu
- DDCS: some disagreement when low-energy electrons are ejected near the forward direction at 1 MeV/amu
- SDCS: some disagreement with the experiment seen in the forward direction at 1 MeV/amu
- p + He: integrated cross sections in good agreement with experiment
- H + H: good agreement with experiment for electron-loss cross section

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Thank you for attention!