50 YEARS OF INNOVATION

Curtin University

A global university with campuses in Asia and Western Australia

Perth | Malaysia | Singapore

50 YEARS OF INNOVATION

Curtin University

# Accurate calculations of state-resolved cross sections for … ion-atom collisions

Alisher Kadyrov

19-21 June 2017, IAEA, Vienna

# Coordinated Research Project

- Project Title:

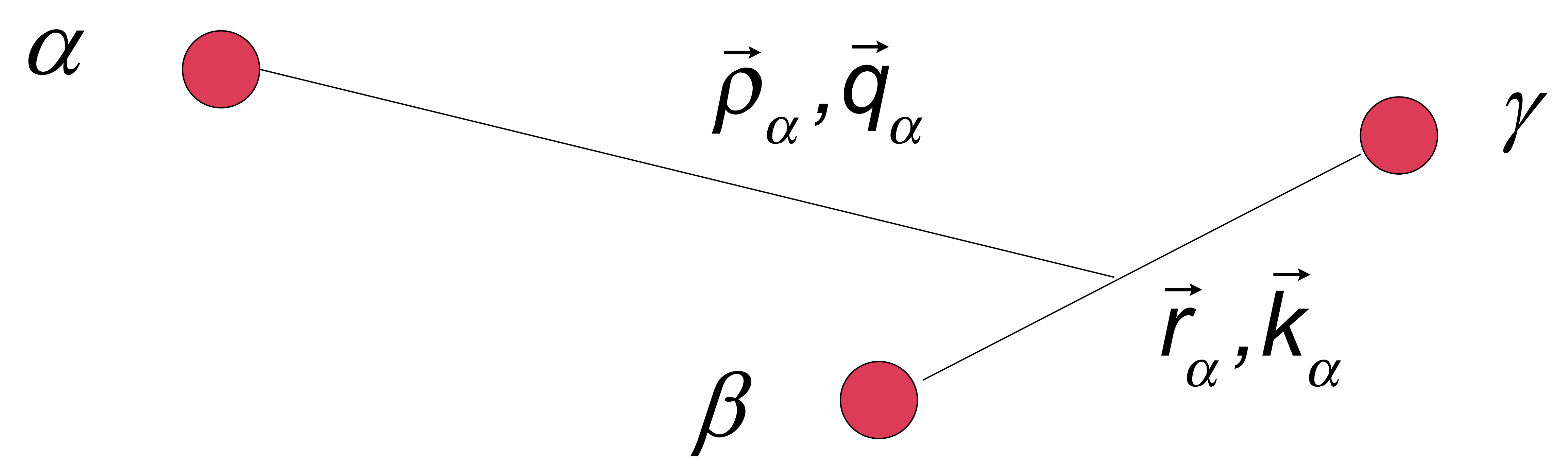
  Accurate calculations of state-resolved cross sections for excitation, ionisation and charge transfer in collisions of hydrogen isotopes with protons, deuterons, tritons and the main impurity ions in fusion plasma

- Primary CSI: Alisher Kadyrov
- Secondary CSI: Igor Bray

# Outline

- Convergent close-coupling (CCC) approach to ion-atom collisions
  - Single-centre CCC
  - Two-centre CCC (including rearrangement)
- CCC approach to proton scattering including electron capture to continuum (ECC)
  - Quantum-mechanical : QM-CCC
  - Semiclassical: SC-CCC
  - Wave-packet: WP-CCC
- Proton-hydrogen collisions: total and differential ionisation cross sections
- Single ionisation of helium by protons
- Multiply-charged ion collisions with hydrogen

# CCC approach to 3-body problem




$$P^{Z+} + H(1s) \rightarrow \Psi_\alpha^+ \rightarrow P^{Z+} + H^*$$

$$\Psi_\alpha^+ \rightarrow P^{Z+} + e^- + p$$

Projectiles: both light and heavy particles

Electrons, positrons, protons, antiprotons, MCI

# Pseudostate expansion

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

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

- Expand the w.f. in a complete 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?

$$\langle\phi_f|H_T|\phi_i\rangle=\varepsilon_f\delta_{fi}$$

- A linear combination of N Laguerre functions

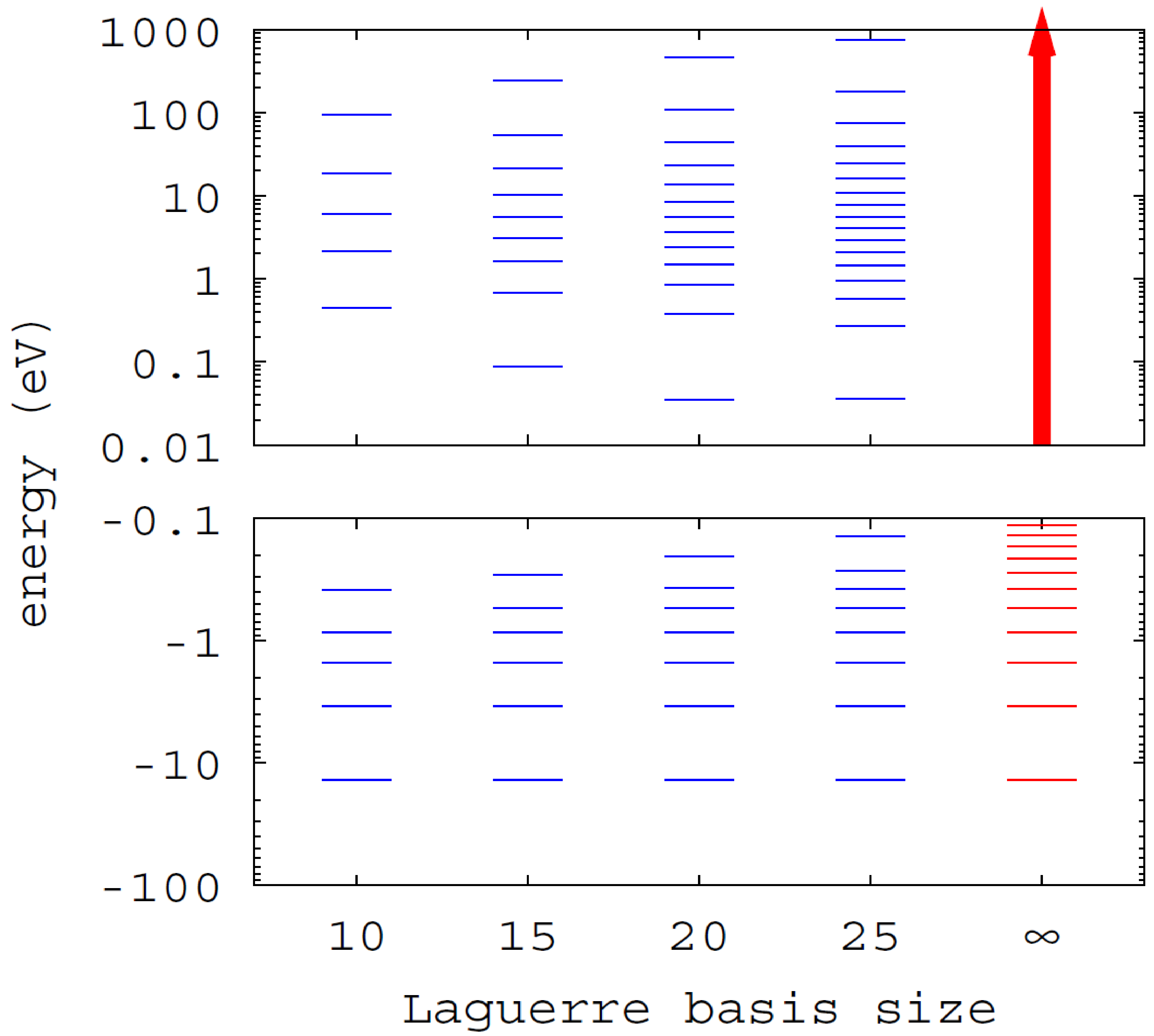
# CCC method: pseudostates

- 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

Hydrogen pseudostates



# CCC equations

- We form a projection operator

$$I = \sum_{n=1}^{\infty} |\varphi_n\rangle\langle\varphi_n| + \int d\varepsilon |\psi_\varepsilon\rangle\langle\psi_\varepsilon| \approx \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n| \equiv I_N$$

- Pseudostate expansion

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

- For any given N we require that

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

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

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

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

# CCC method in a nutshell

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

- We have developed 2 ways of solving this system of equations
- Partial-wave method (light projectiles)
- Impact-parameter method (heavy projectiles)

} 3D→1D

- Total breakup cross section is obtained by summing excitation cross sections of the positive-energy states
- Convergence in cross sections is obtained by increasing N
- Continuum-continuum coupling!
- $e^-$ scattering on H, He, He-like targets, alkalis, inert gases, $H_2$
- Details: Bray et al., Phys Rep 520 (2012) 135

# CCC method for ion-atom collisions

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

- This system of 3D equations are reduced to 1D using impact-parameter method

$$\mathcal{T}_{\gamma'\gamma}(q_{\gamma'}, q_\gamma; b) = \mathcal{V}_{\gamma'\gamma}(q_{\gamma'}, q_\gamma; b) + \frac{1}{(2\pi)^2} \sum_{\gamma''}^{N} \int_0^\infty dq_{\gamma''} \mathcal{V}_{\gamma'\gamma''}(q_{\gamma'}, q_{\gamma''}; b)\, G_{\gamma''}(q_{\gamma''}^2) \mathcal{T}_{\gamma''\gamma}(q_{\gamma''}, q_\gamma; b)$$

- Details of QM-CCC: Abdurakhmanov et al., Phys Rev A 84 (2011) 062708

# CCC method for ion-atom collisions

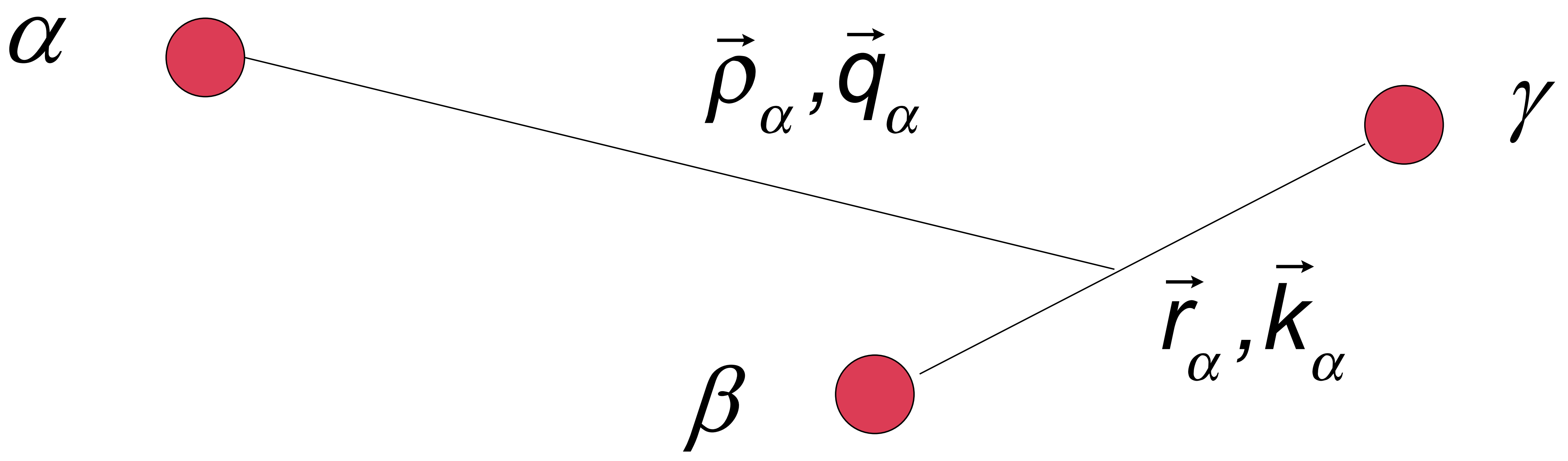
- Cross section for excitation of a pseudostate:

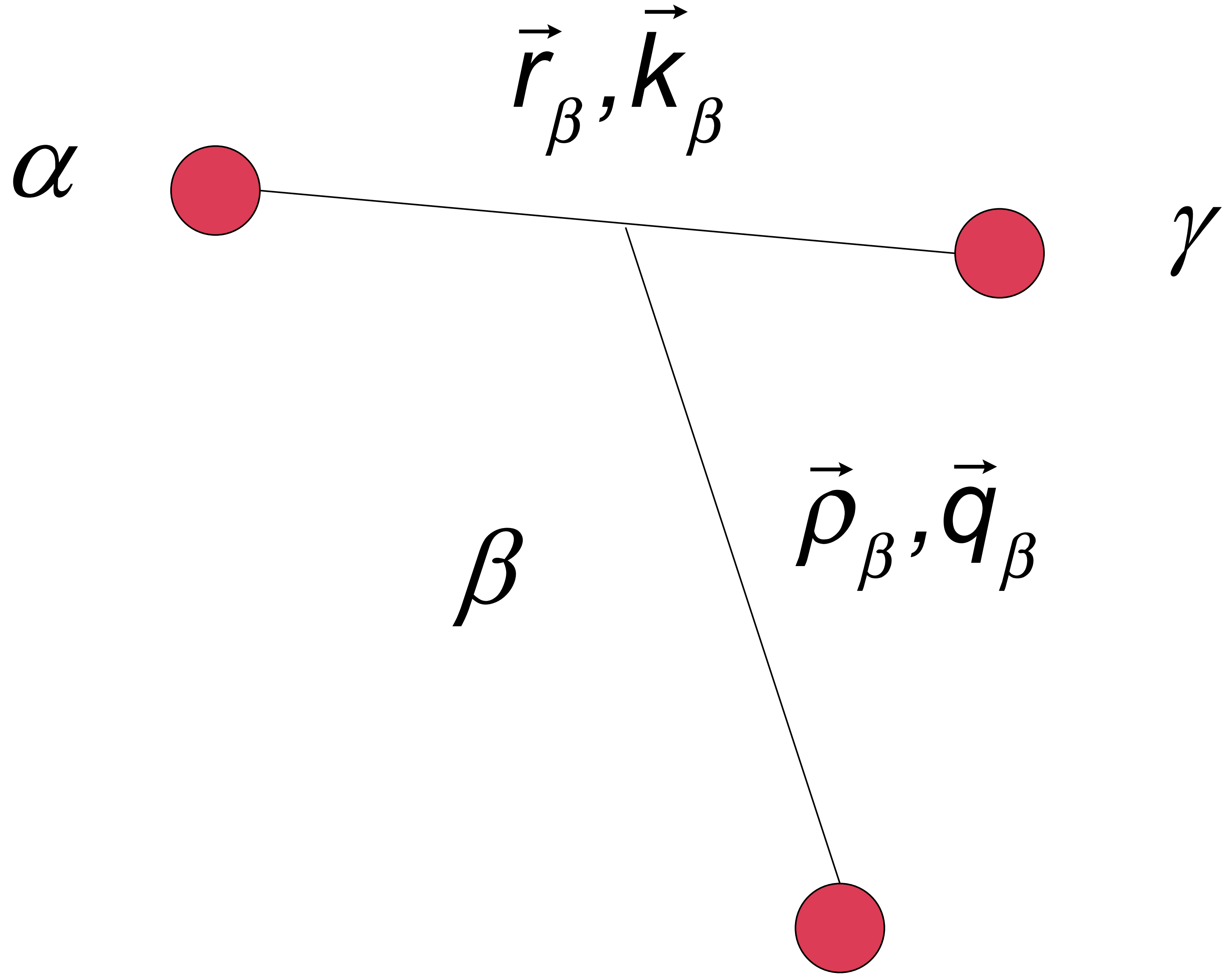
$$\sigma_{nlm} = 2\pi \int_0^{b_{\max}} db\, b\, P_{nlm}(b)$$

- Total breakup cross section is obtained by summing excitation cross sections for the positive-energy states
- Convergence in cross sections is obtained by increasing N

- We used this for antiproton scattering on H, He, inert gases and $H_2$
- Details: Abdurakhmanov et al., Phys Rev Lett 111 (2013) 173201
- $C^{6+}$ - He single ionisation: Abdurahmanov etal, Phys Rev A 86 (2012) 034701

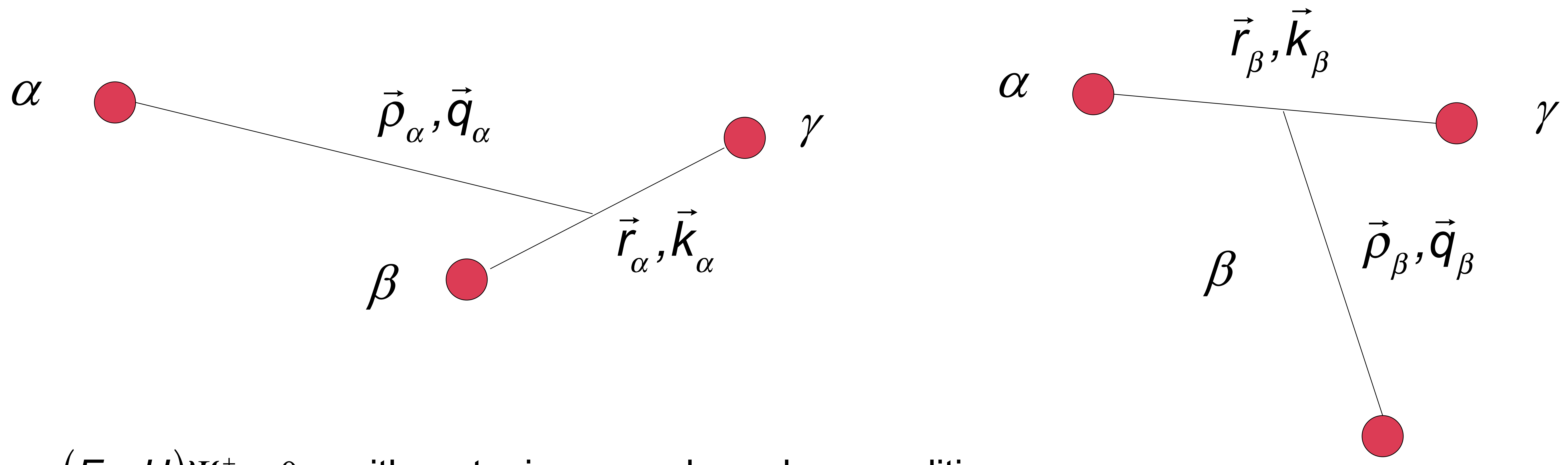
# CCC approach with rearrangement




$$\mathrm{P}^{Z+} + \mathrm{H}(1s) \rightarrow \Psi_\alpha^+ \begin{cases} \nearrow \ \mathrm{P}^{Z+} + \mathrm{H}^* \\ \rightarrow \ \mathrm{P}^{Z+} + e^- + p \\ \searrow \ \left(\mathrm{P}^{Z+} + e^-\right) + p \end{cases}$$

# CCC approach with rearrangement




$(E-H)\Psi_\alpha^+ = 0$ with outgoing-wave boundary condition

- The total w.f. does not fall off at infinity in any of these variables
- The space of functions not falling off at infinity is non-separable
- Can we still use the expansion method?
- Have to combine two orthogonal and complete basis sets: one for each system of coordinates (or centres of the problem)

# 2-centre CCC: associated difficulties

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

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

Target-centered basis is obtained by diagonalising the target atom Hamiltonian with N states

Projectile-centered basis is obtained by diagonalising the (P+e) atom Hamiltonian with M states

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

} problem is ill-conditioned

# 2-centre CCC equations

- Again require our expansion to satisfy the SE

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

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

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

- 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

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

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

- All direct and rearrangement matrix elements coupled
- Electron capture into continuum is included
- Total breakup cross section is obtained by summing excitation cross sections of the positive-energy states of both target atom and projectile atom
- Convergence in cross sections is obtained by increasing N and M
- $e^+$ scattering on H, He, Mg, alkalis, $H_2$
- Topical Review: Kadyrov & Bray, J Phys B 49 (2016) 222002

# Heavy projectiles: QM-CCC approach

- QM-CCC [Abdurakhmanov et al., Phys Rev A 84 (2011) 062708]:

$$\mathcal{T}_{\gamma'\gamma}(q_{\gamma'}, q_\gamma; b) = \mathcal{V}_{\gamma'\gamma}(q_{\gamma'}, q_\gamma; b) + \frac{1}{(2\pi)^2} \sum_{\gamma''}^{N} \int_0^\infty dq_{\gamma''} \mathcal{V}_{\gamma'\gamma''}(q_{\gamma'}, q_{\gamma''}; b) G_{\gamma''}(q_{\gamma''}^2) \mathcal{T}_{\gamma''\gamma}(q_{\gamma''}, q_\gamma; b)$$

where

$$\mathcal{V}_{\gamma'\gamma}(q_{\gamma'}, q_\gamma; b) = 2\pi \int_{-\infty}^{\infty} dz \exp(i(q_\gamma - q_{\gamma'})z) v_{\gamma'\gamma}(b\ ,\ z)$$

- We used this for antiproton scattering on H, He, inert gases and $H_2$
- Calculations were slow. Much slower than semi-classical
- Can we do the off-shell integration analytically?

# Off-shell integration → algebraic eqns.

- After some algebra we obtain a set of algebraic equations

$$t_{\gamma'\gamma}(b\ ,\ z) = v_{\gamma'\gamma}(b\ ,\ z) + \frac{1}{(2\pi)^2}\sum_{\gamma''}^{N} \exp(iq_{\gamma'}z)t_{\gamma''\gamma}(b\ ,\ z)F(z)$$

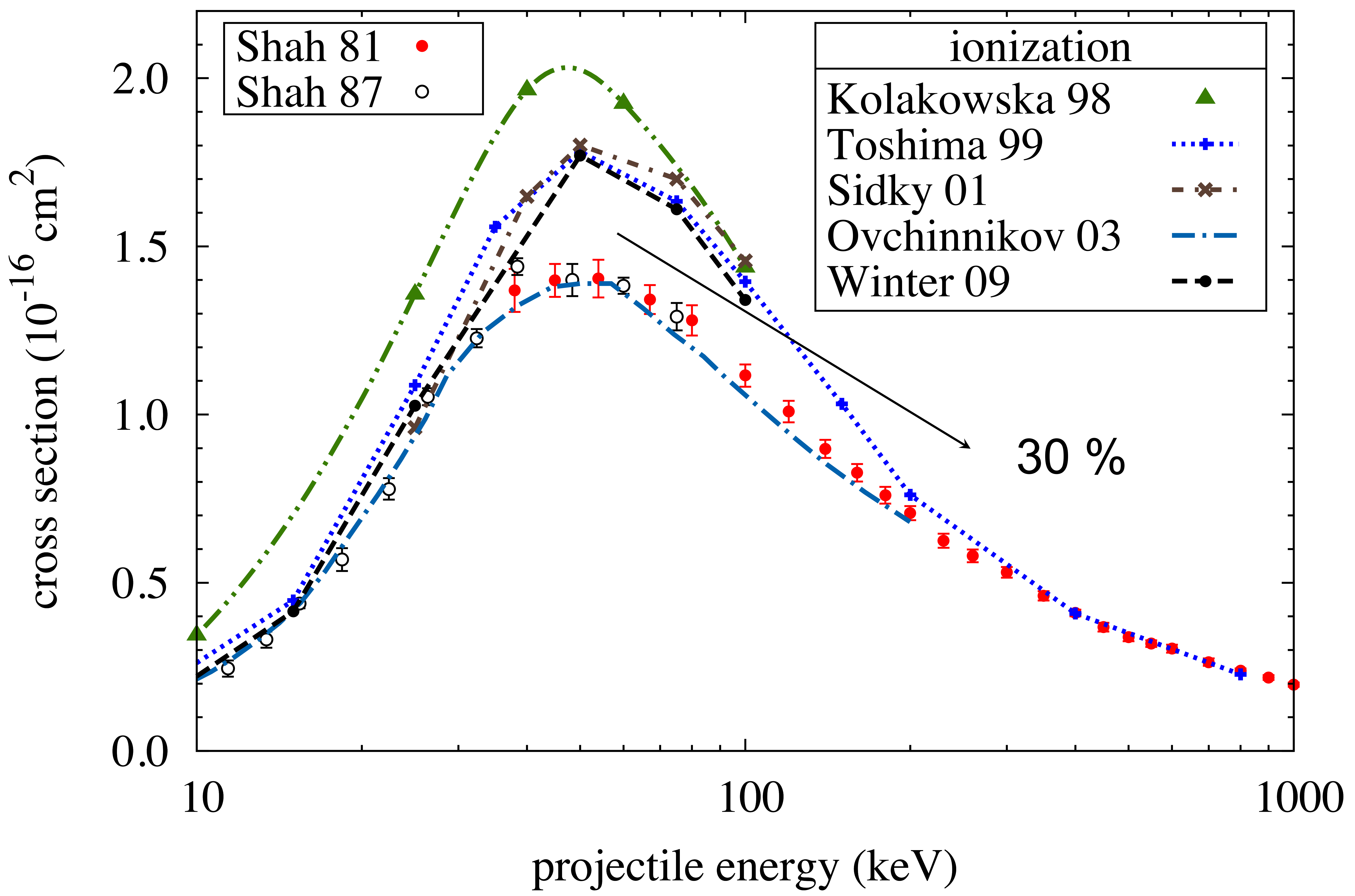
- Then we can recover the transition amplitudes from

$$\mathcal{T}_{\gamma'\gamma}(q_{\gamma'}, q_{\gamma}; b) = 2\pi\int_{-\infty}^{\infty} dz \exp(i(q_{\gamma} - q_{\gamma'})z)t_{\gamma'\gamma}(b\ ,\ z)$$

- This makes QM-CCC algebraic
- New code is tested against the old integral-equation code: full agreement
- Calculations become fast – as fast as semi-classical ones

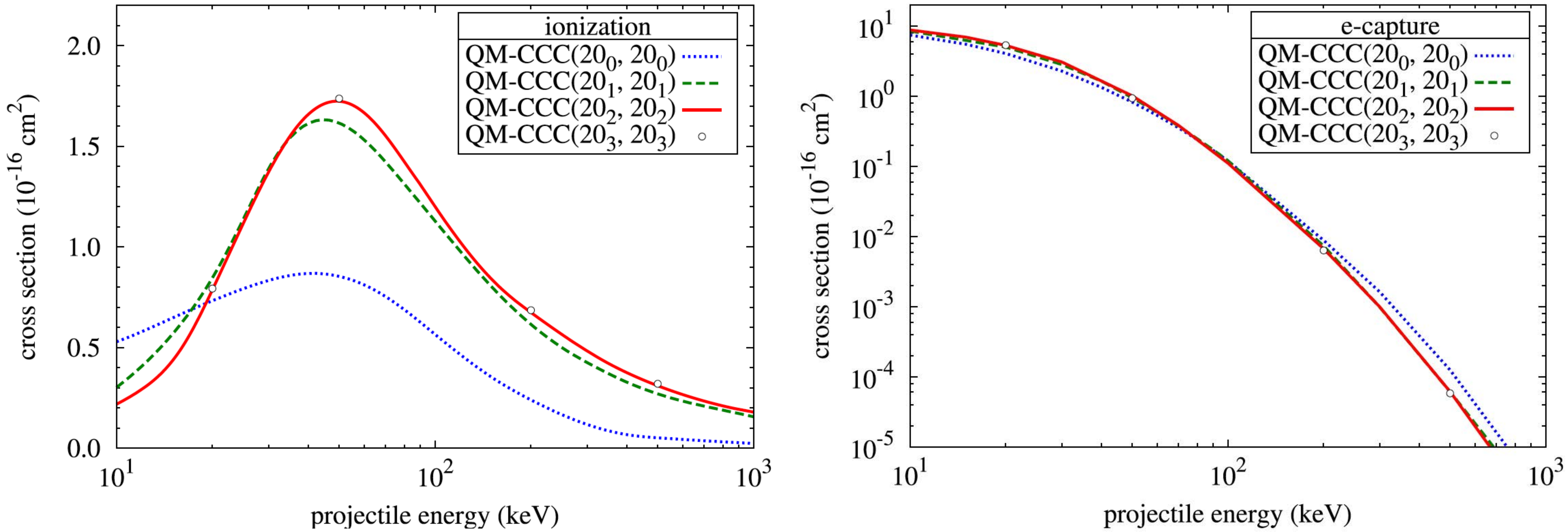
- Details: Abdurakhmanov et al., J Phys B 49 (2016) 115203

# p-H ionisation: which theory is correct?



# Electron capture and ionisation in p-H

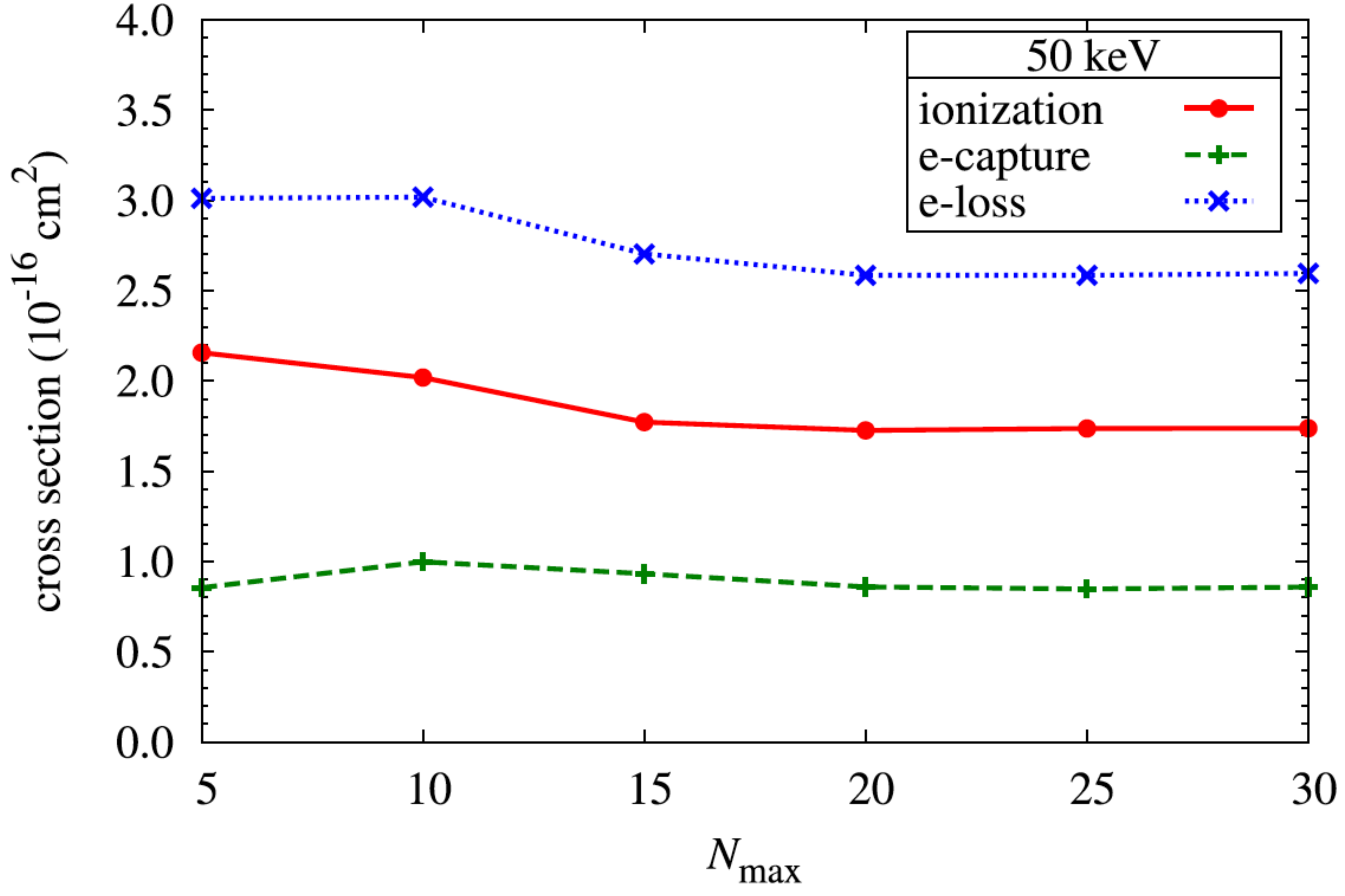
Convergence in terms of $\ell_{max}$

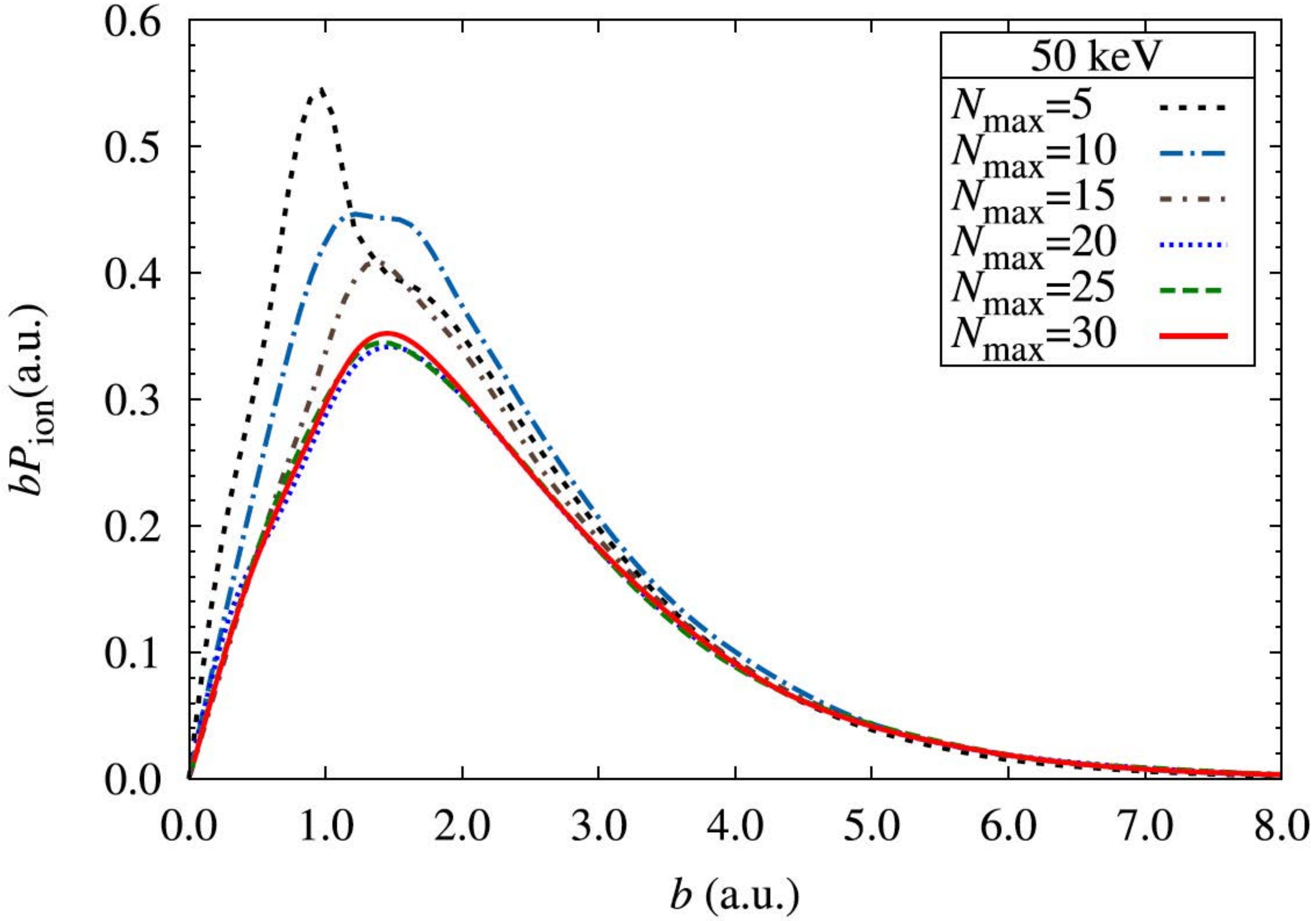



2-centre QM-CCC: Abdurakhmanov et al., J Phys B 49 (2016) 115203

# Electron capture and ionisation in p-H

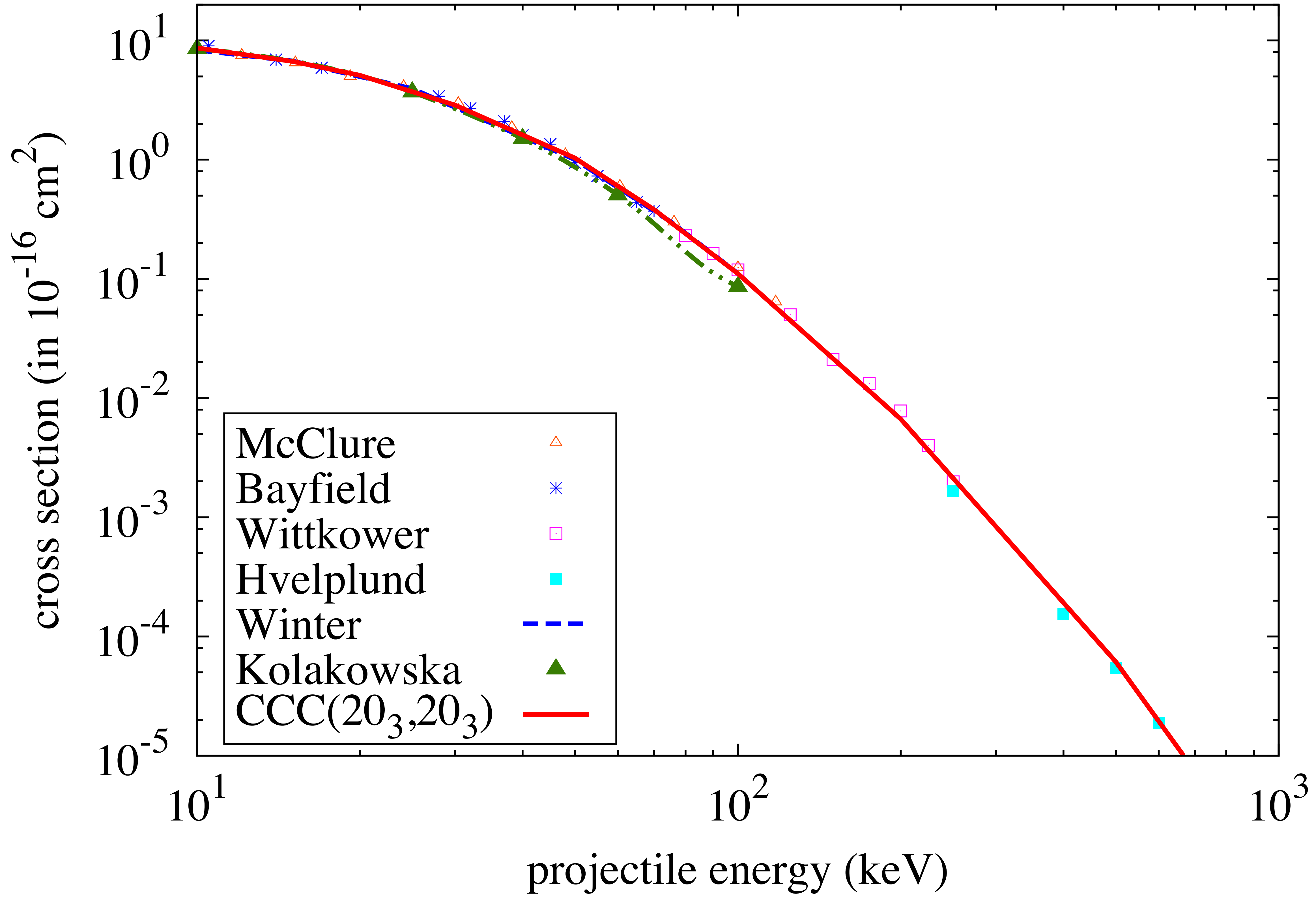
Convergence in terms of $N_{max}$

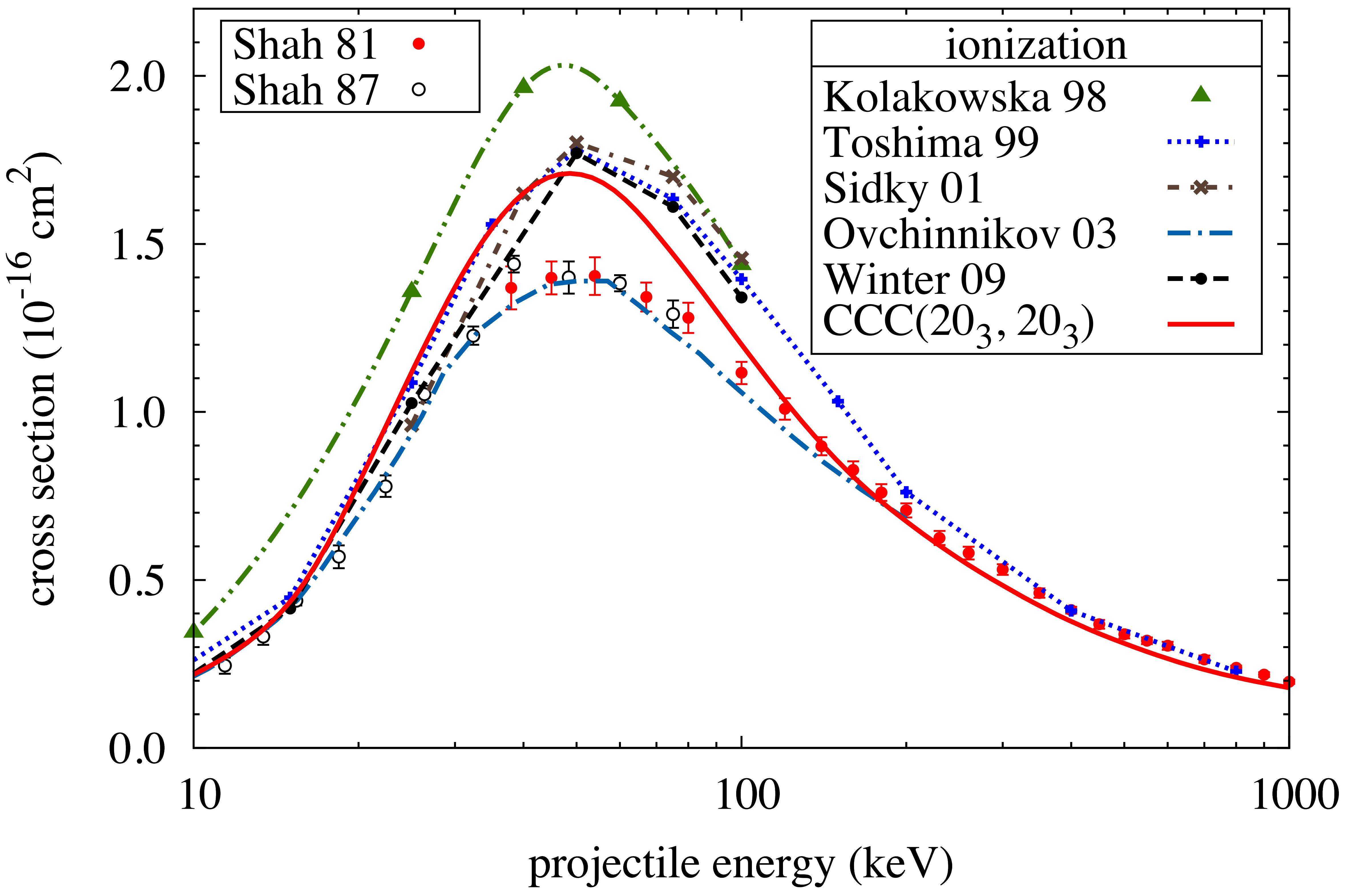



2-centre QM-CCC: Abdurakhmanov et al., J Phys B 49 (2016) 115203

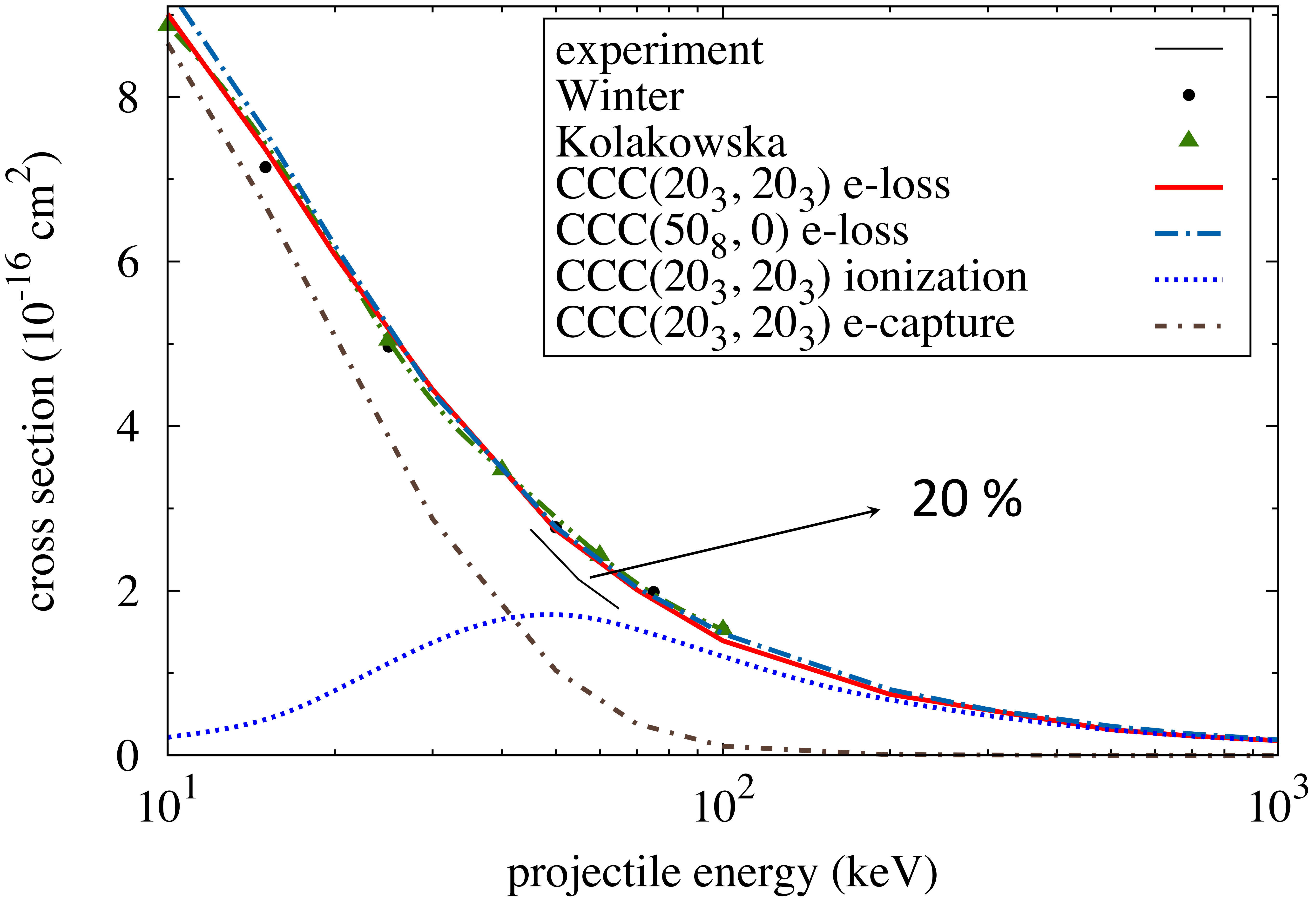
# Electron capture and ionisation in p-H




2-centre QM-CCC: Abdurakhmanov et al., J Phys B 49 (2016) 115203

# Electron loss in p-H




Level of convergence:

CCC($50_8$,0)

CCC($50_7$,0) 0.4 %

CCC($49_8$,0) 0.04 %

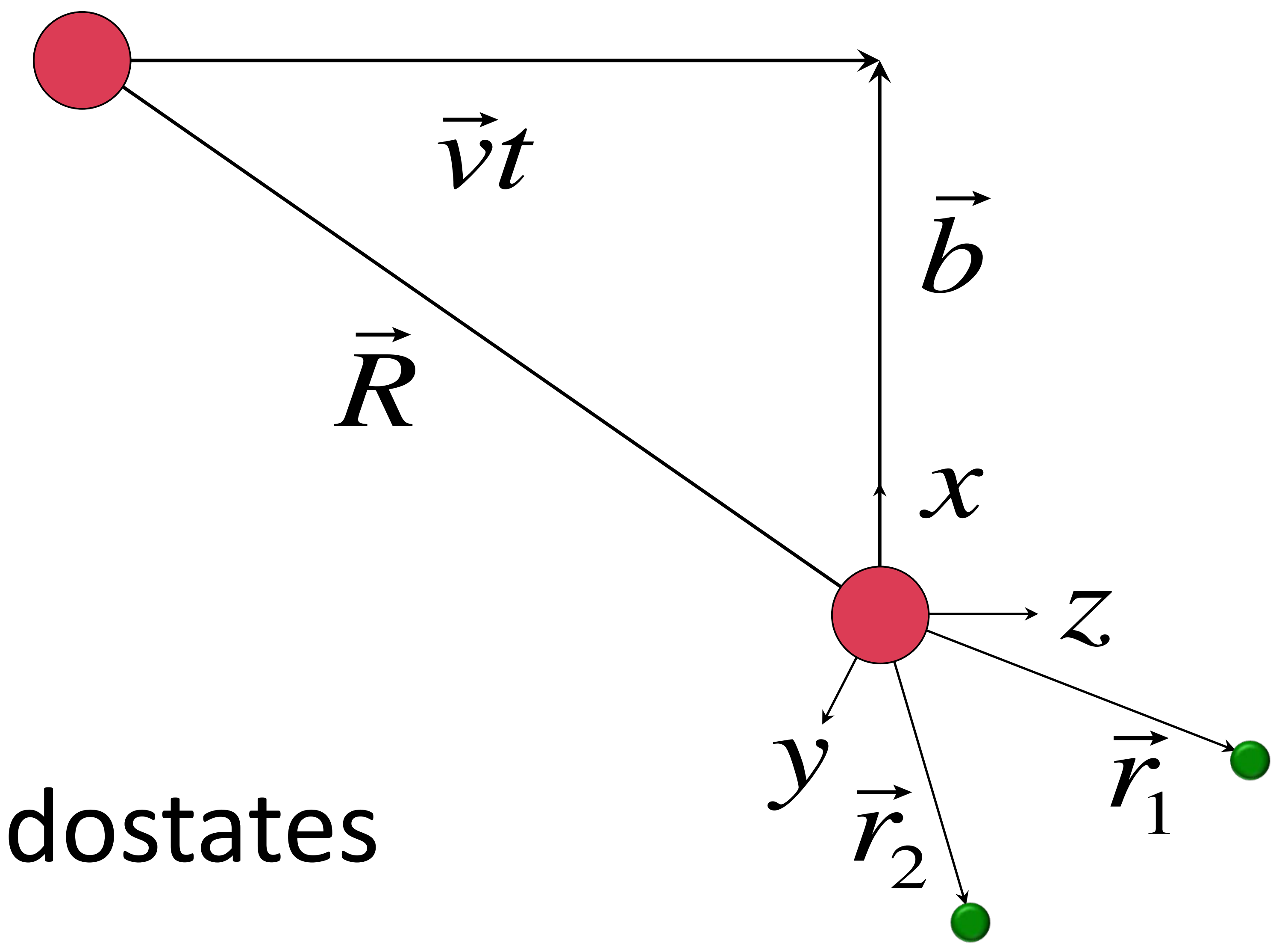
Net error < 0.5 %

So, 20% difference is impossible

# Semi-classical CCC approach

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

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



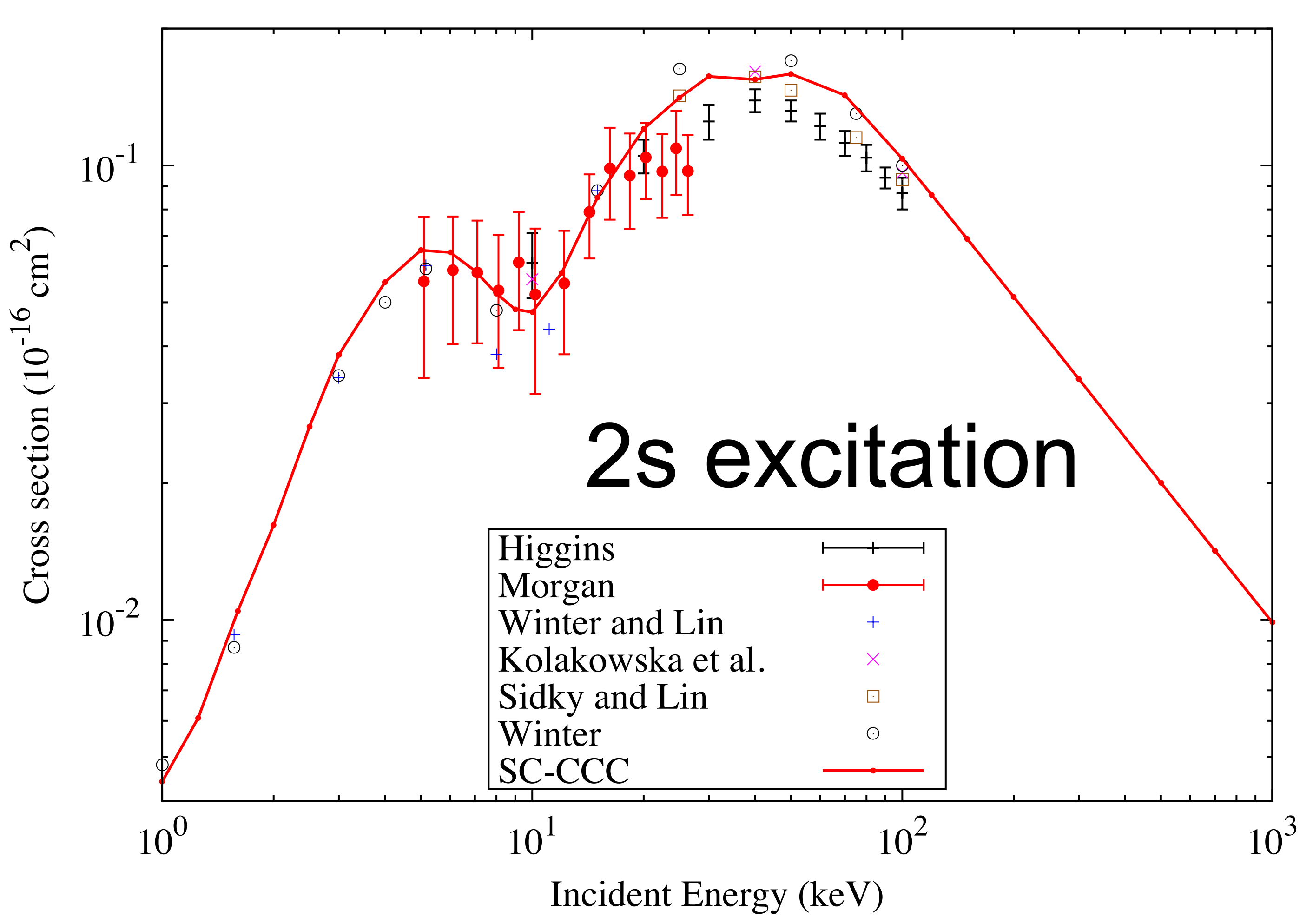

The w.f. is a solution to SC TDSE

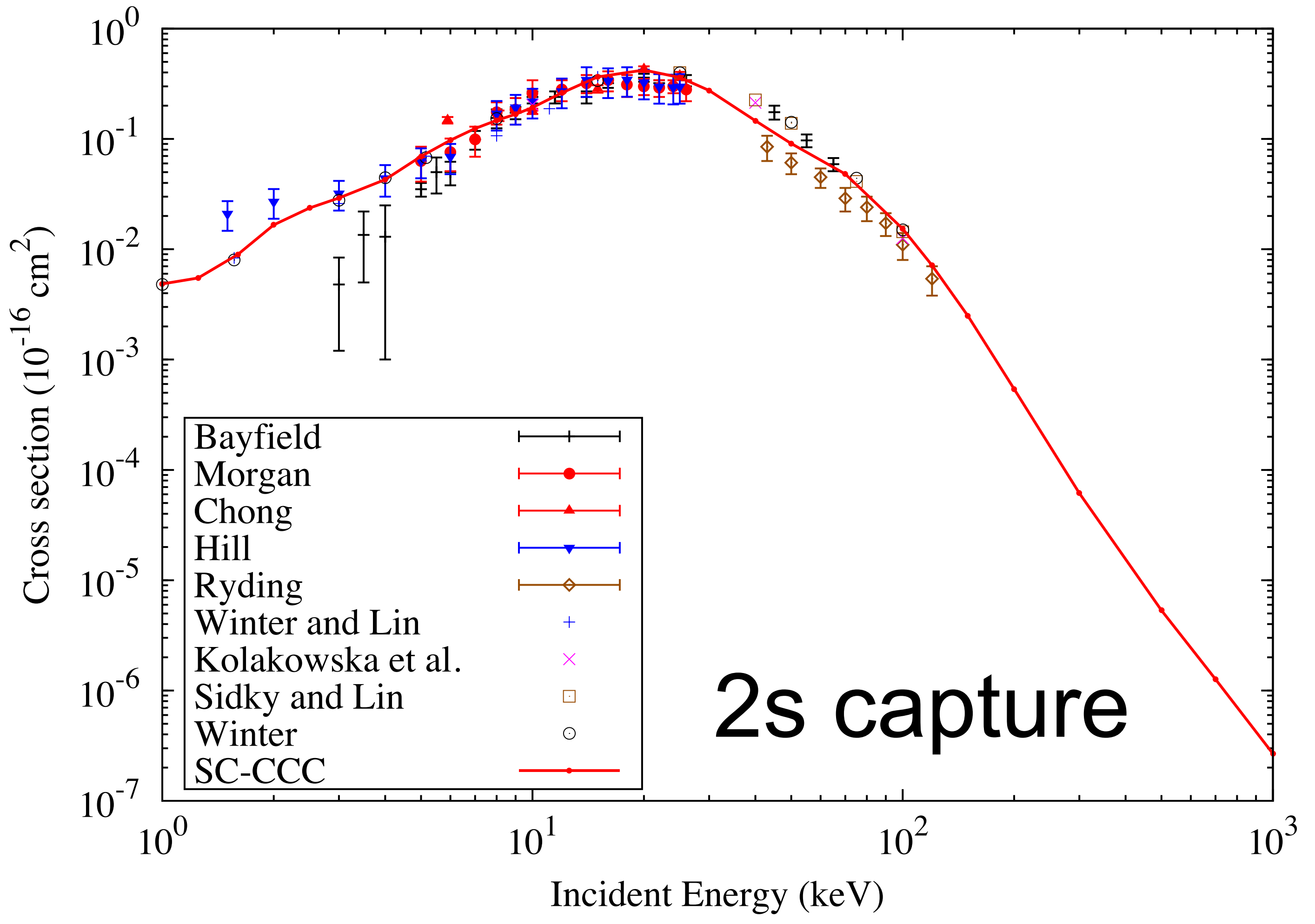
$$i\frac{\partial\Psi(\vec{r},t)}{\partial t} = (H_T + V_P)\Psi(\vec{r},t)$$

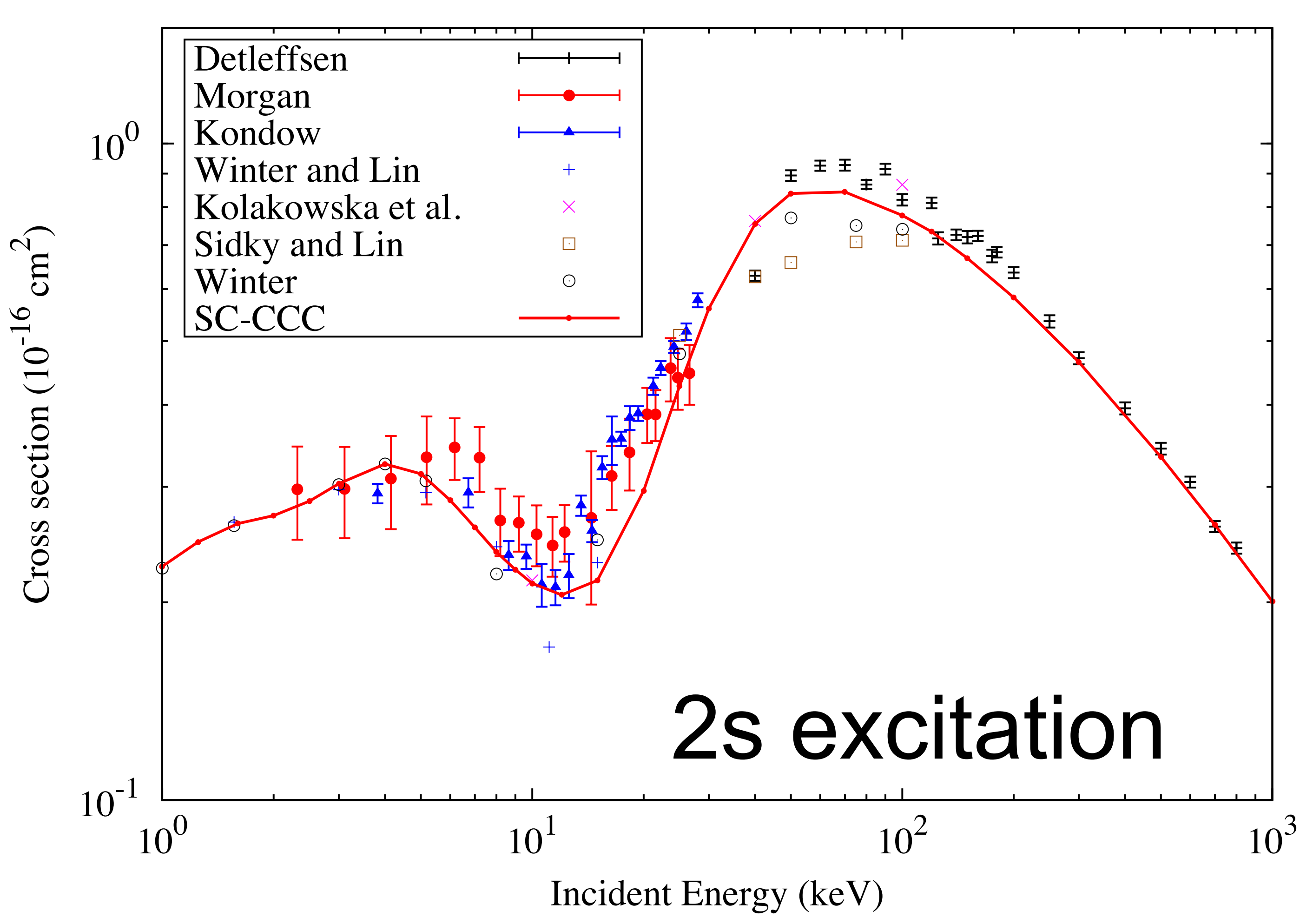
Expand in terms of target and projectile-centered pseudostates

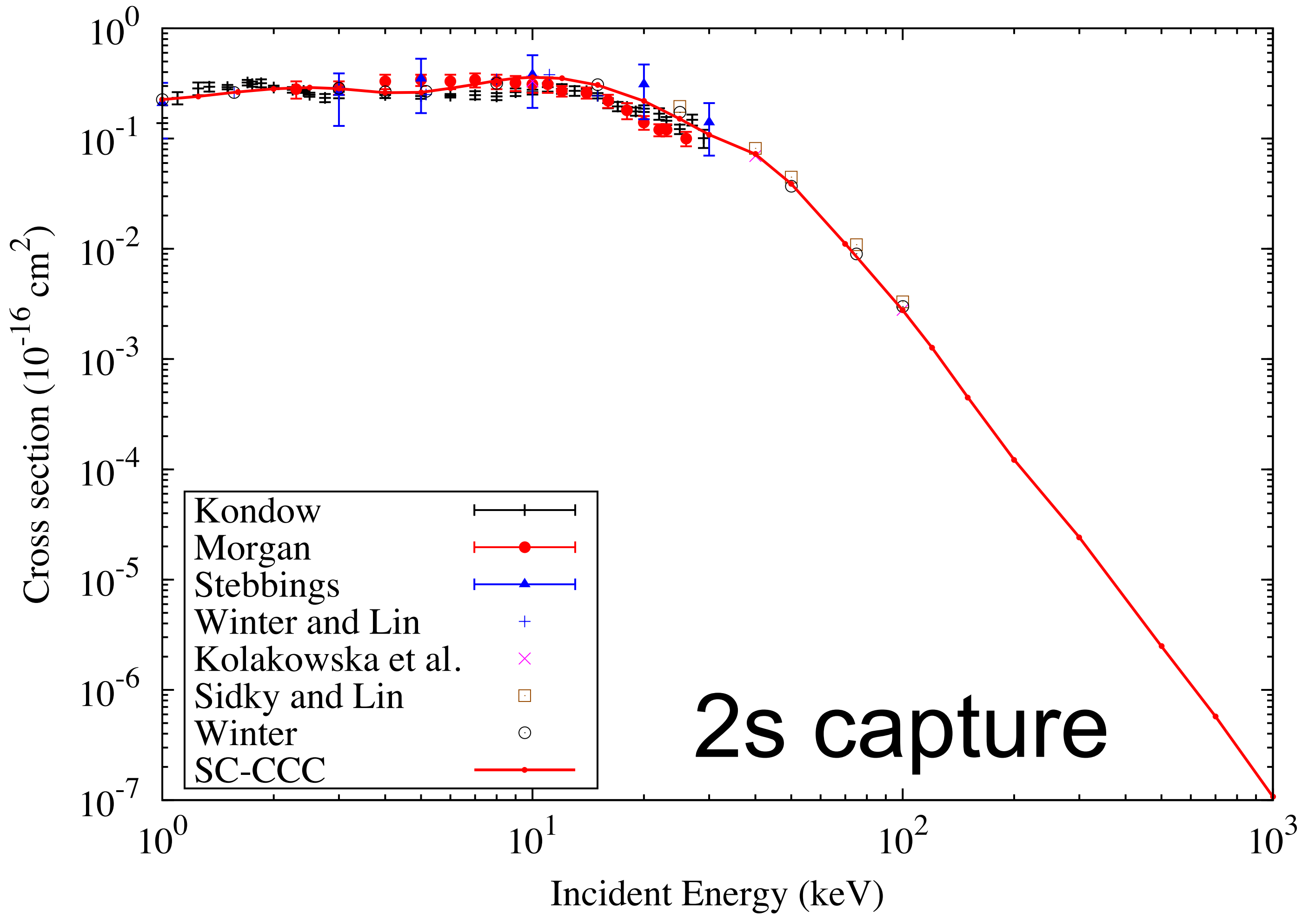
$$\Psi(t,\boldsymbol{r},\boldsymbol{R}) = \sum_{\alpha=1}^{N_\alpha} a_\alpha(t,\boldsymbol{b})\psi_\alpha^T(\boldsymbol{r}_T)\exp\left[-i\epsilon_\alpha^T t\right] + \sum_{\beta=1}^{N_\beta} b_\beta(t,\boldsymbol{b})\psi_\beta^P(\boldsymbol{r}_P)\exp\left[-i\epsilon_\beta^P t\right]\exp[-i(\boldsymbol{v}\cdot\boldsymbol{r}_T + v^2t/2)]$$

# 2-centre semi-classical CCC: p-H



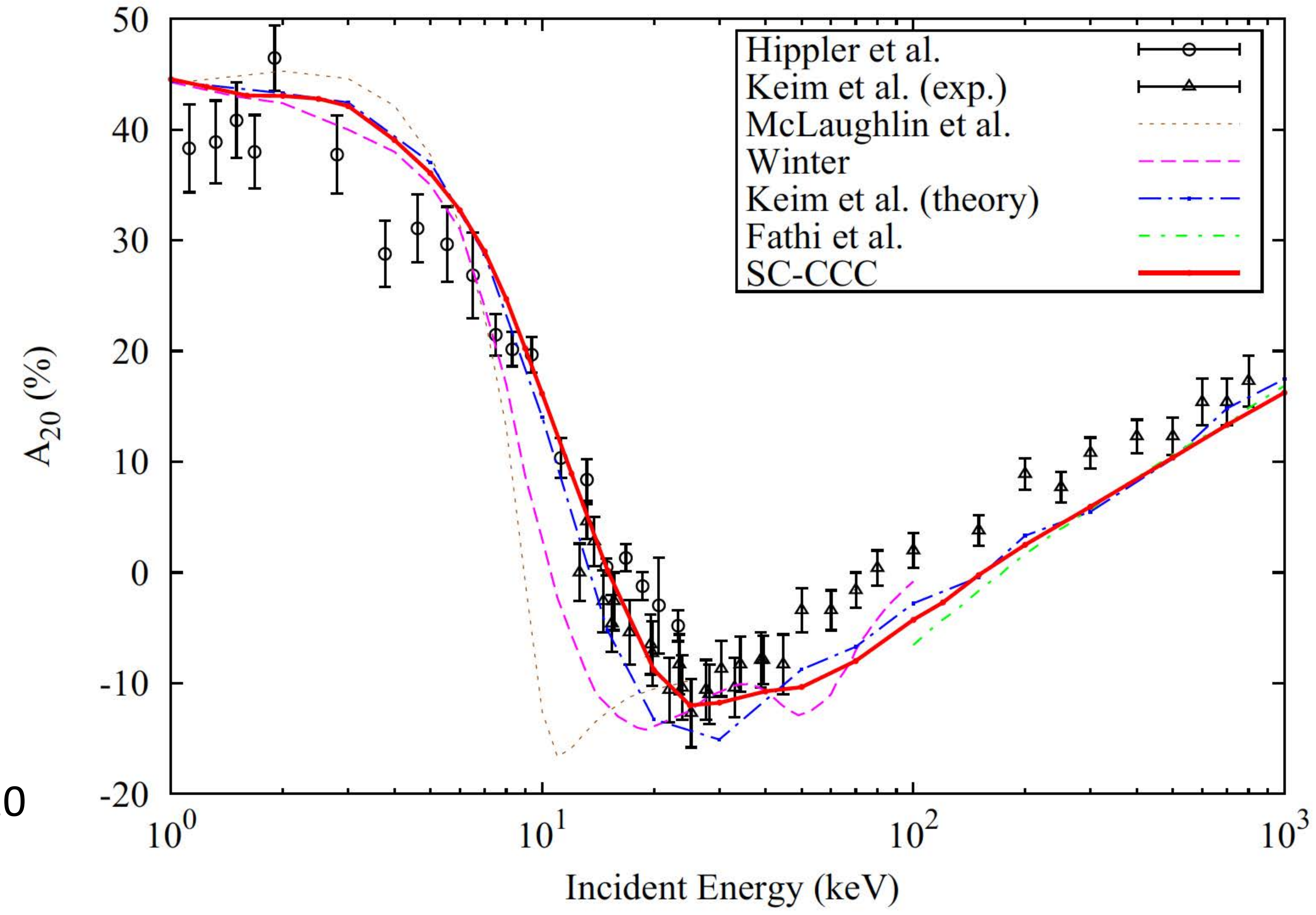

Details of SC-CCC: Avazbaev etal, Phys Rev A 93 (2016) 022710

# 2-centre semi-classical CCC: p-H

$$A_{20} = \frac{\sigma_{2p_1} - \sigma_{2p_0}}{2\sigma_{2p_1} + \sigma_{2p_0}}$$

$$\sigma_{2p_0} = \sigma_{2p_0}^{\mathrm{di}} + \sigma_{2p_0}^{\mathrm{ex}}$$

$$\sigma_{2p_1} = \sigma_{2p_1}^{\mathrm{di}} + \sigma_{2p_1}^{\mathrm{ex}}$$




Details of SC-CCC:
Avazbaev etal,
Phys Rev A 93 (2016) 022710

# Ionisation amplitude

- Surface-integral formulation of scattering theory:

  Kadyrov etal, Phys Rev Lett 101 (2008) 230405

  Kadyrov *et al.*, Ann Phys 324 (2009) 1516

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

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

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

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

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

# Breakup amplitude including ECC

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

Thus the breakup amplitude splits into two:

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

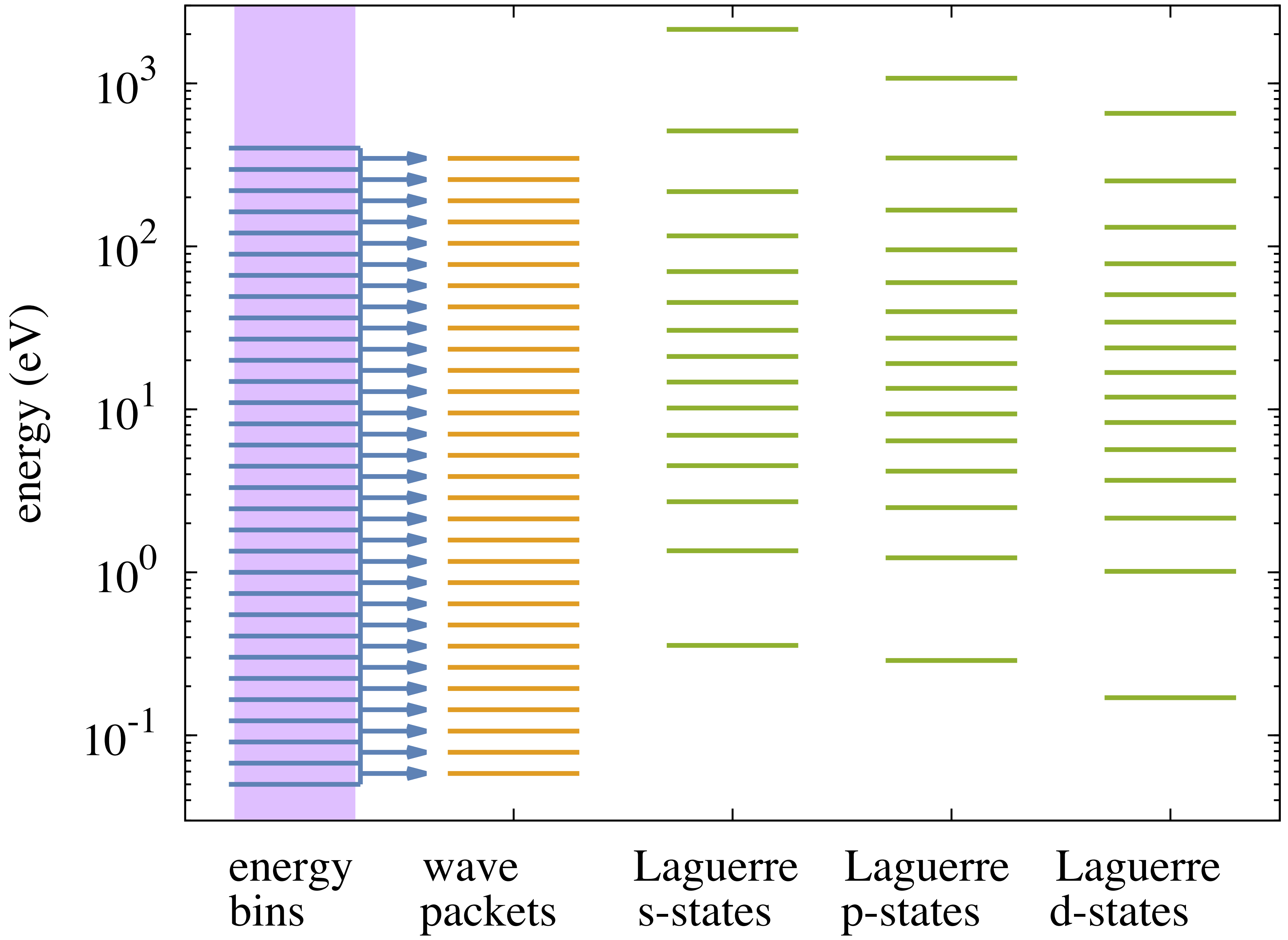
$$T^T = \left\langle \vec{q}_f, \psi_{\vec{k}}^T \left| I_N \left( \overleftarrow{H} - E \right) \right| \Psi_i^{NM+} \right\rangle = \left\langle \psi_{\vec{k}}^T \middle| \phi_f^T \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad k^2/2 = \varepsilon_f$$

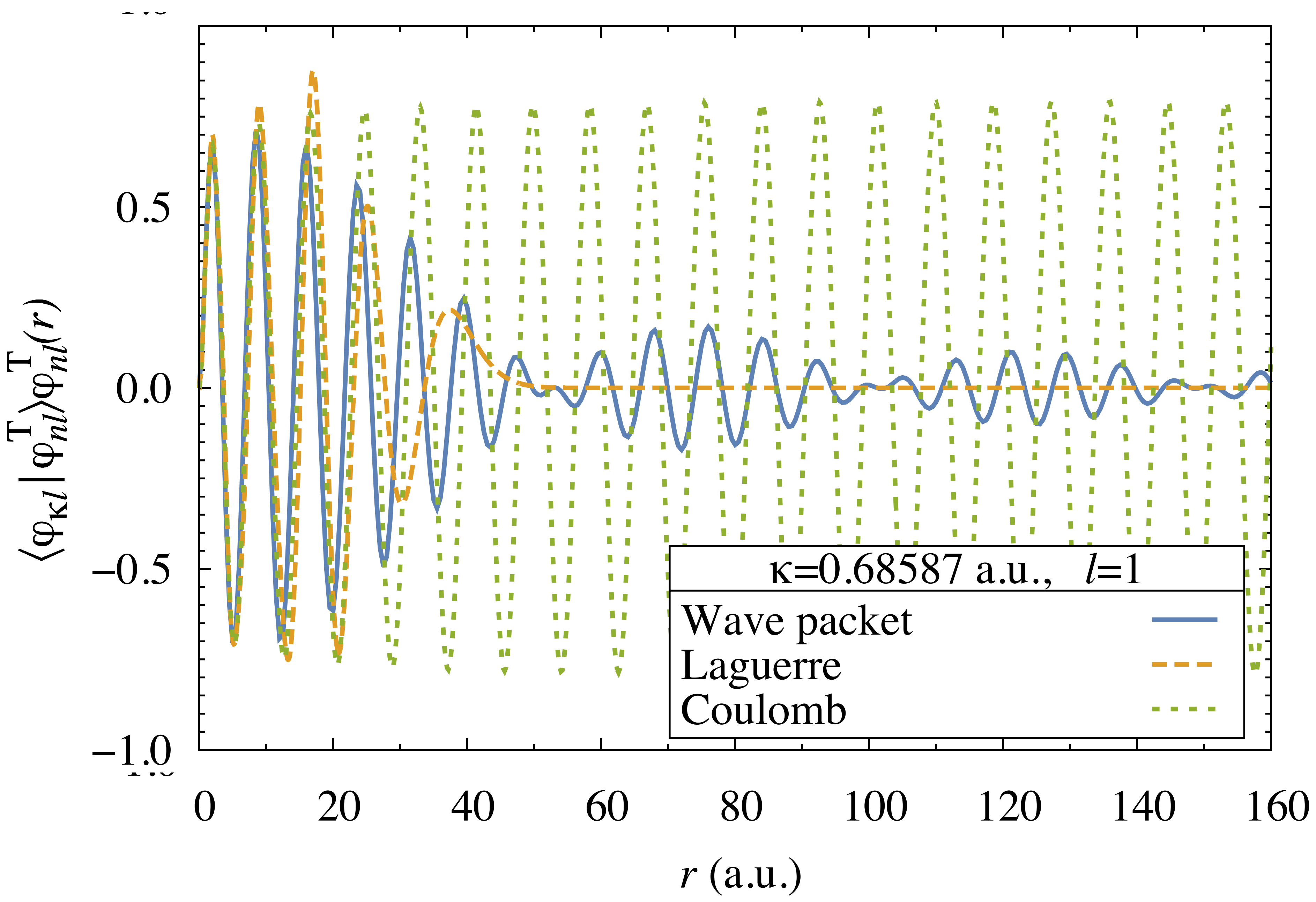
$$T^P = \left\langle \vec{q}_f, \psi_{\vec{p}}^P \left| I_P \left( \overleftarrow{H} - E \right) \right| \Psi_i^{NM+} \right\rangle = \left\langle \psi_{\vec{p}}^P \middle| \phi_f^P \right\rangle \tilde{T}_{fi}^T \quad \text{for} \quad p^2/2 = \varepsilon_f$$

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

- It appears that 2 amplitudes must be combined coherently: a fundamental question

# 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

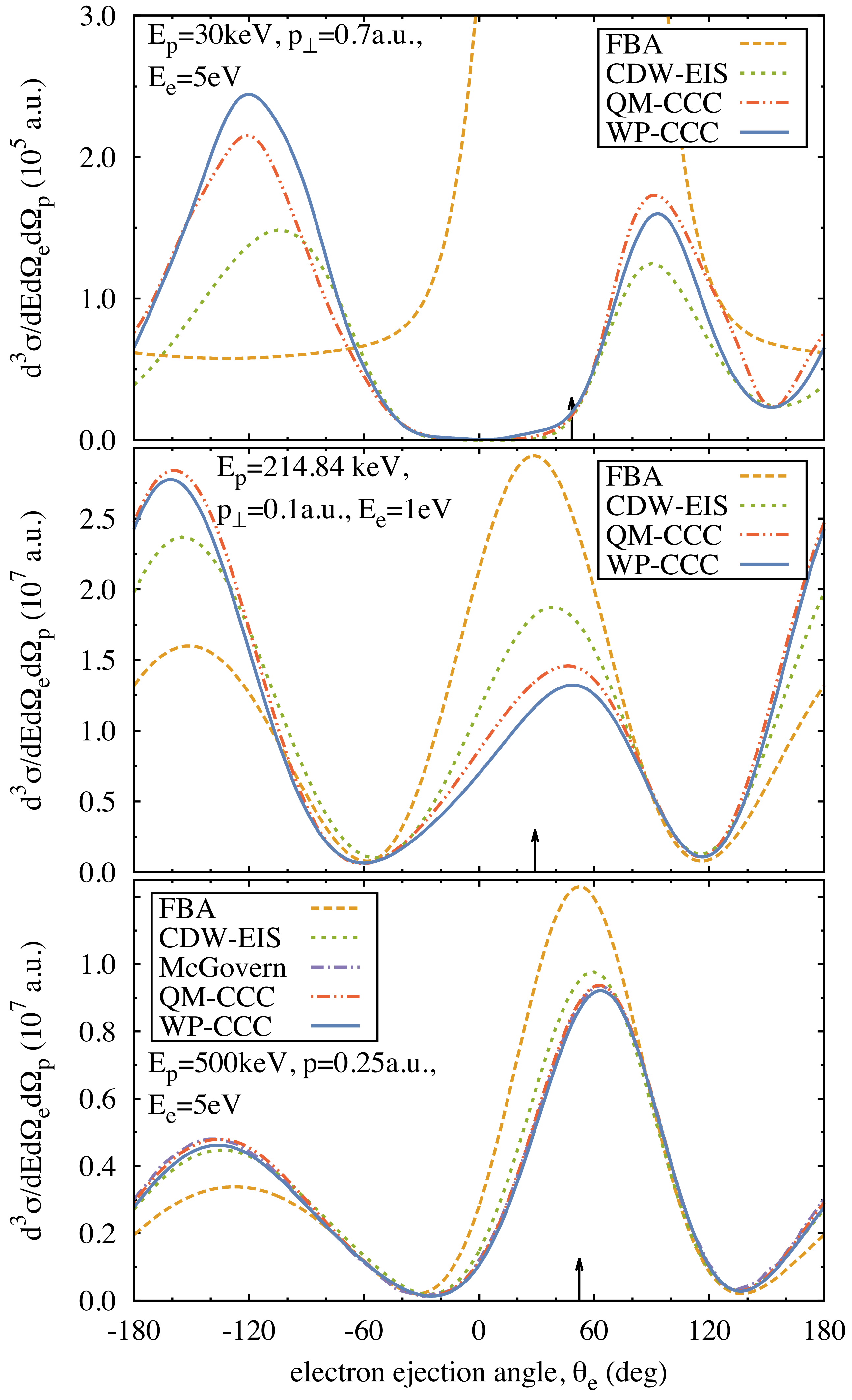
$$\left\langle \phi_{jl}^{WP} \middle| H_T \middle| \phi_{il}^{WP} \right\rangle = \delta_{ji} \varepsilon_i$$

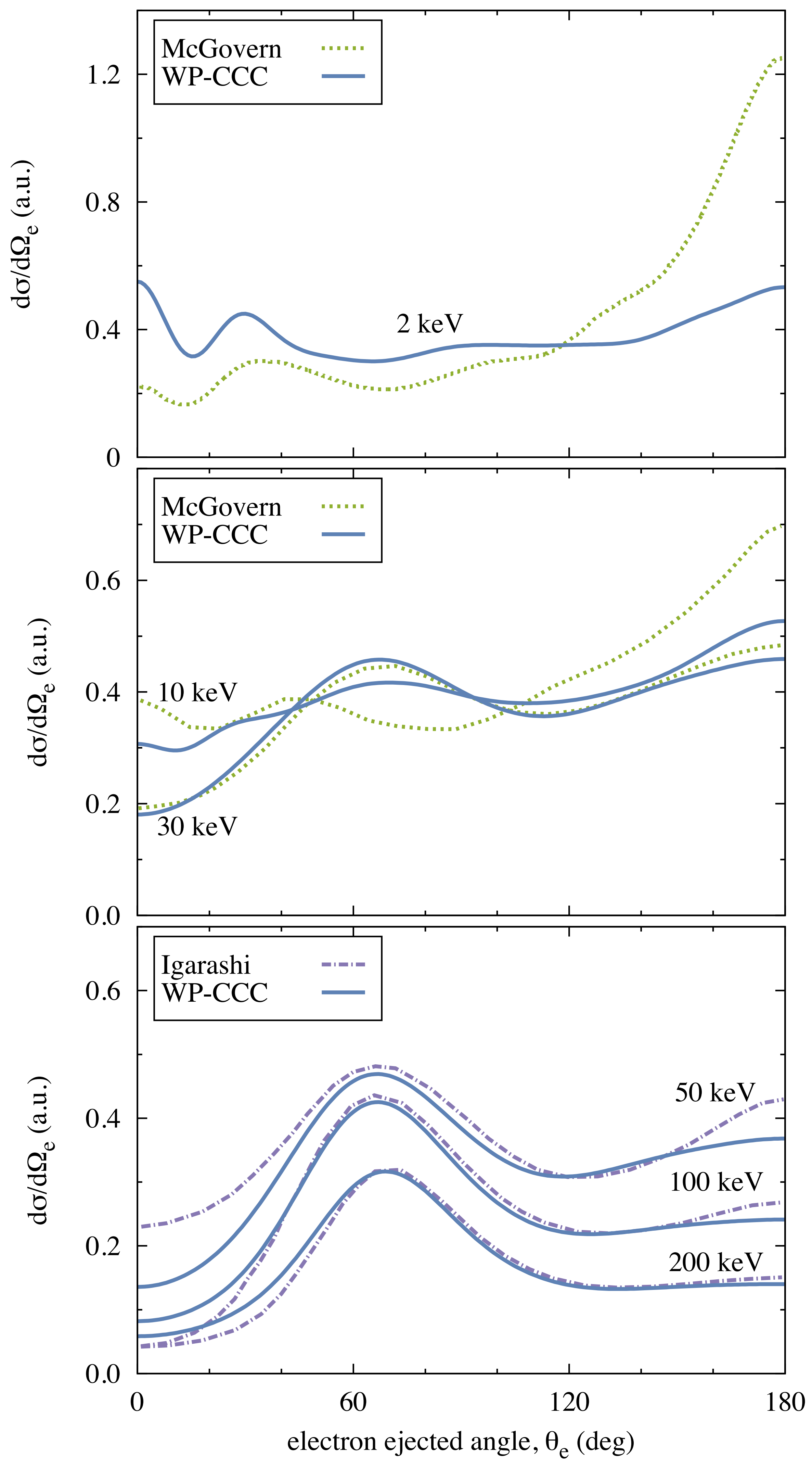
- Advantages of WP: there are 3

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

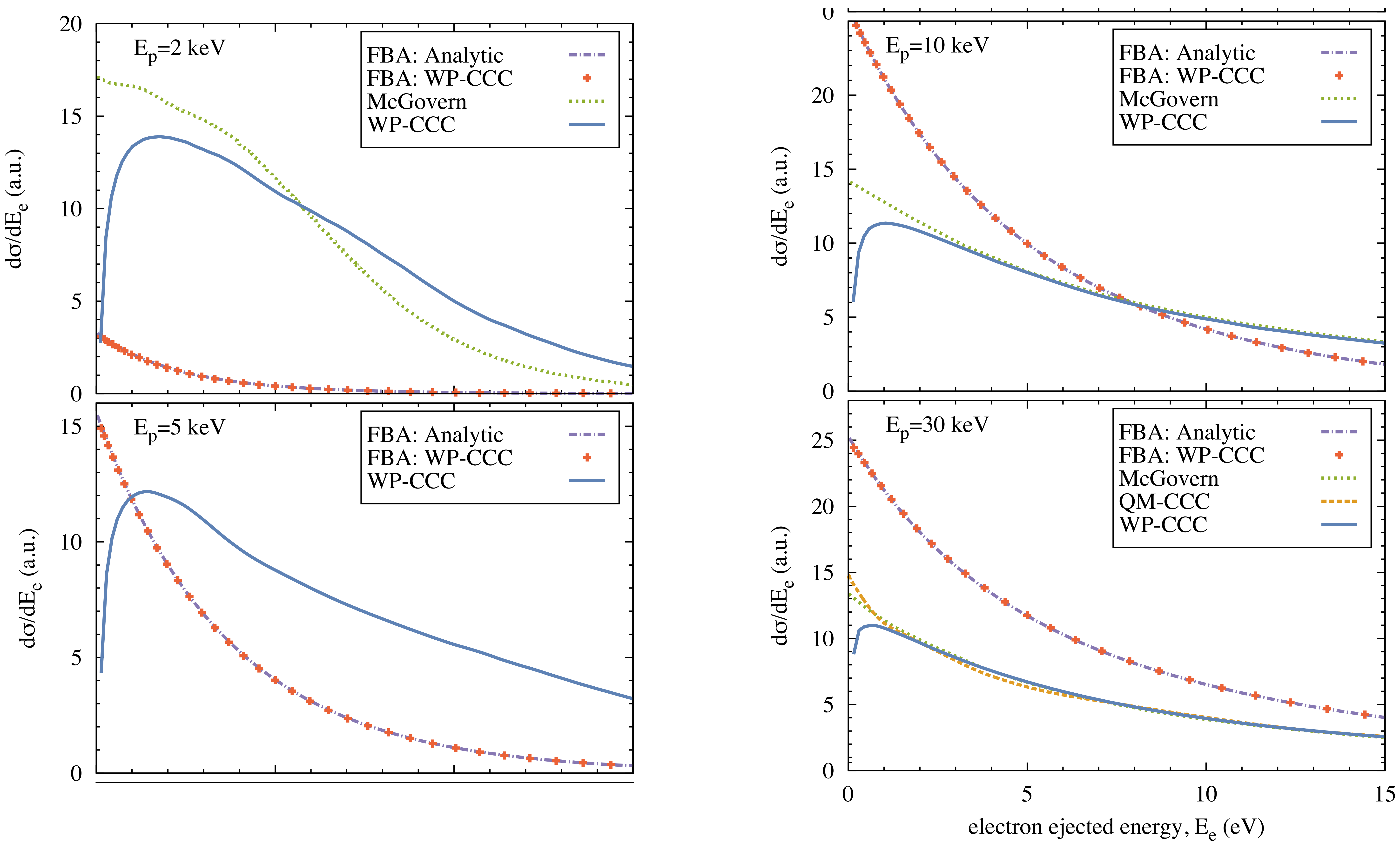
$$b_{nl}(k) = \int_0^\infty dr \varphi_{kl}(r)\ \varphi_n^{WP}(r) = \frac{1}{\sqrt{w_n}}$$

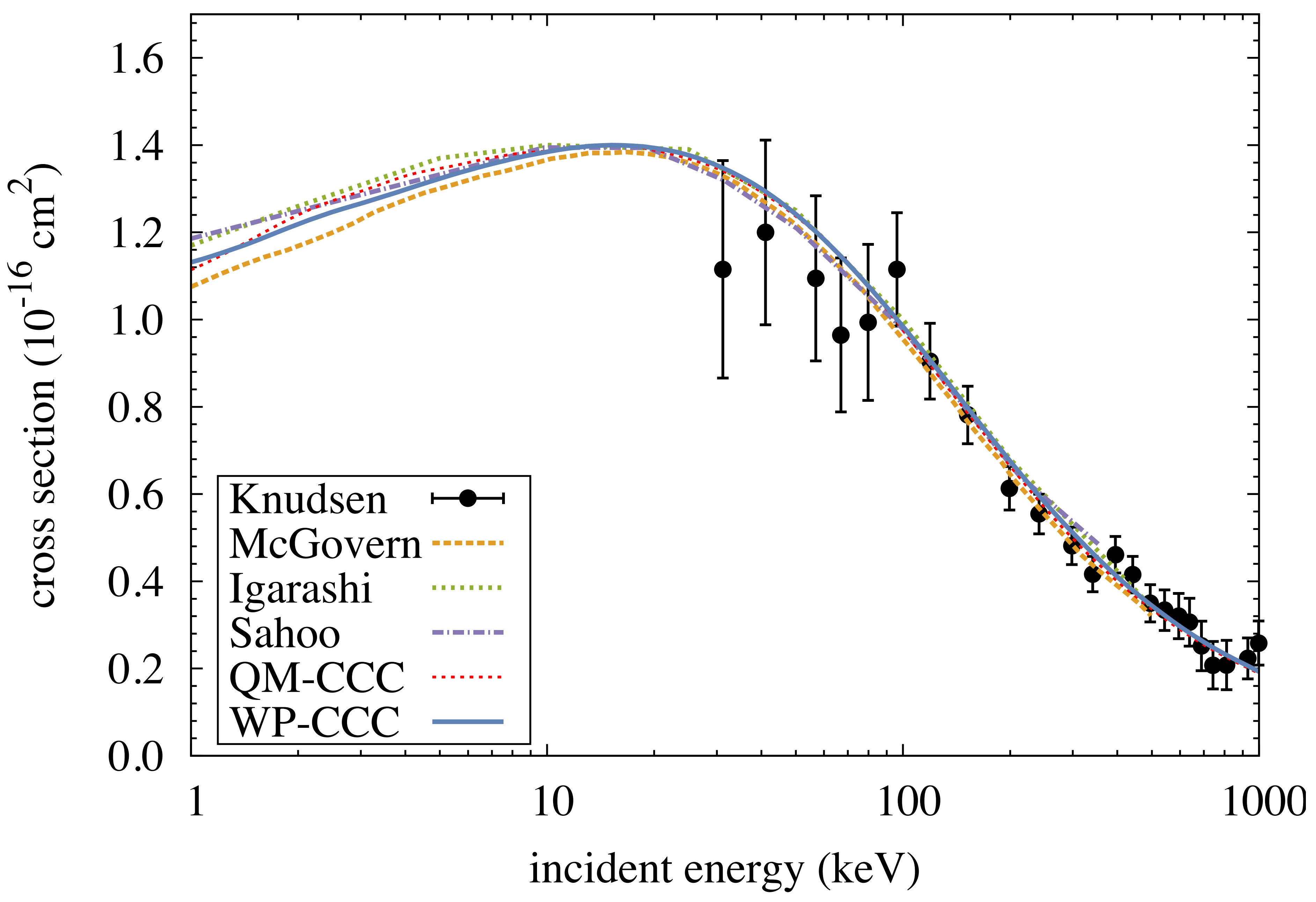
# Wave-packet CCC: $\bar{p}$ + H(1s) ionisation



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




Details of WP-CCC: Abdurakhmanov et al., Phys Rev 94 (2016) 022703

# Conclusions

- Developed 2-centre CCC approach ion scattering including ECC
    - QM-CCC
    - SC-CCC
    - WP-CCC

- Fully differential breakup calculations of p + H
- Single ionisation of helium in p + He
- Multiply-charged ion collisions with hydrogen: $He^{2+}$ and $C^{6+}$

- We can provide fully *nlm*-resolved cross sections for excitation and electron capture
- We can provide data for any initial state H(nml) [within reasonable limits]

# Team

- Prof Igor Bray
- Dr Ilkhom Abdurakhmanov
- Dr Sanat Avazbaev
- Jackson Bailey
- Charlie Rawlins
- Shukhrat Alladustov
- Kym Massen-Hane
- Ozlem Erkilic
- Joshua Faulkner

- Supported by Australian Research Council

YEARS 50 OF INNOVATION

# Thank you

Make tomorrow better.