Convergent close-coupling calculations for heavy-particle collisions

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with

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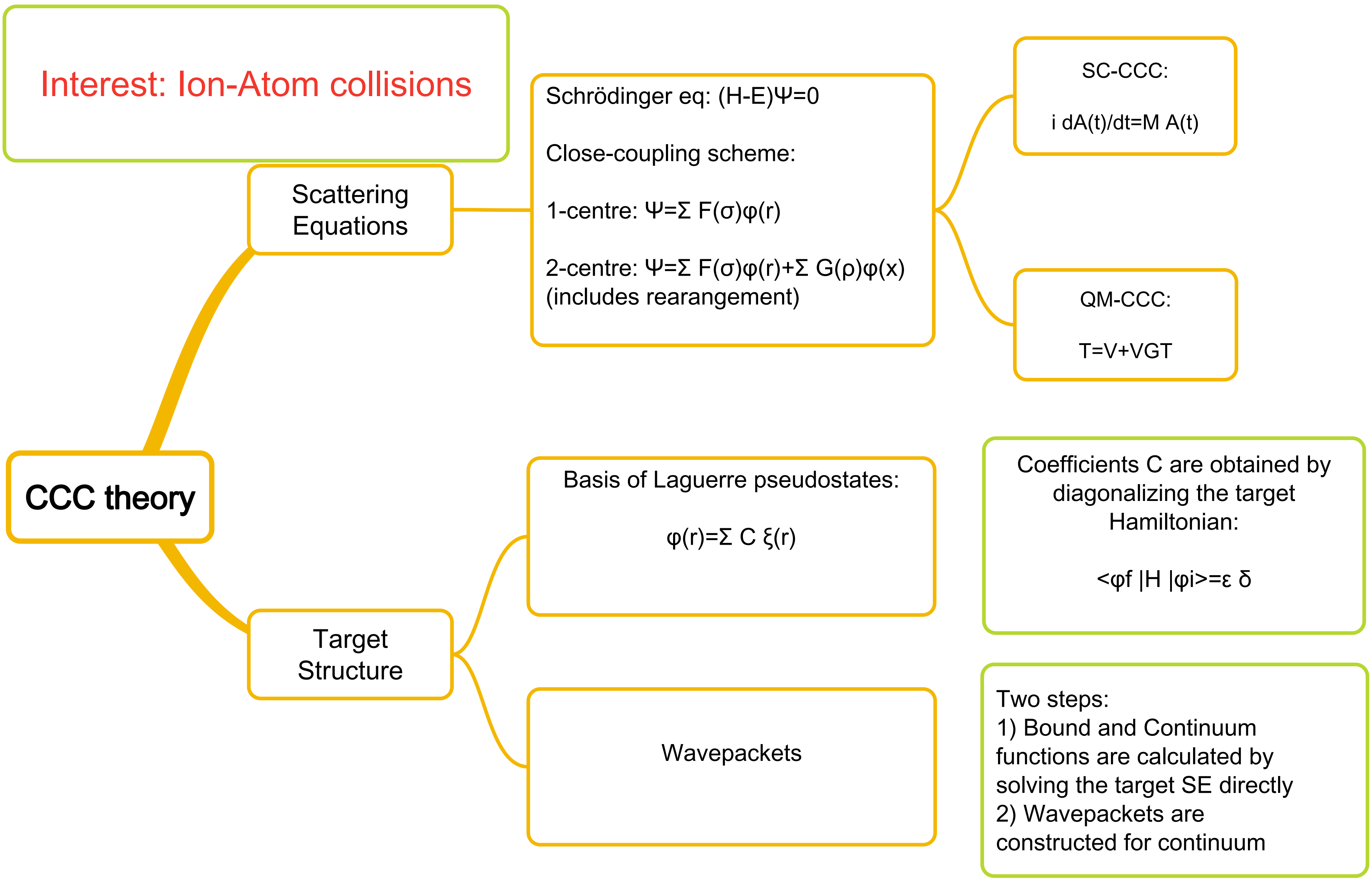
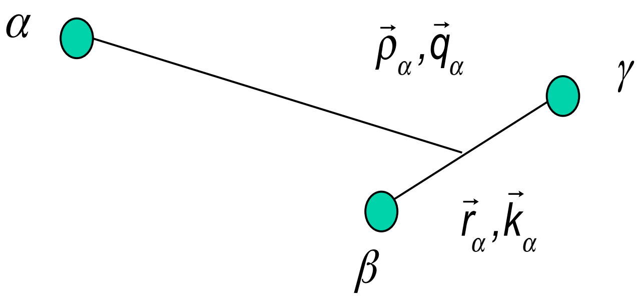
Curtin University

Motivation

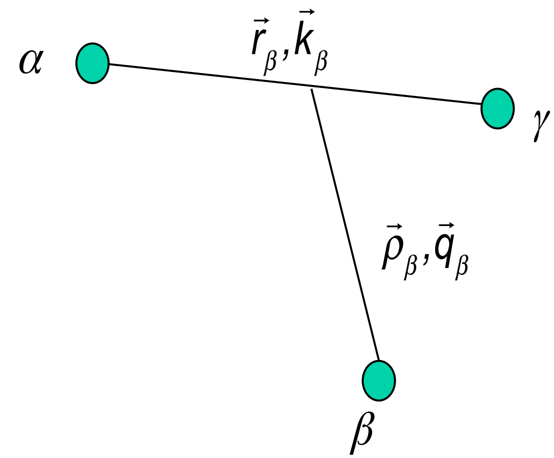
- Fundamental Science
- Hadron therapy of cancer
- Collisions of particular interest to ITER
- Charge exchange reactions of particular interest to X-ray observatories


Interest: Ion-Atom collisions
CCC theory
Scattering Equations
Schrödinger eq: (H-E)Ψ=0
Close-coupling scheme:
1-centre: Ψ=Σ F(σ)φ(r)
2-centre: Ψ=Σ F(σ)φ(r)+Σ G(ρ)φ(x)
(includes rearangement)
SC-CCC:
i dA(t)/dt=M A(t)
QM-CCC:
T=V+VGT
Target Structure
Basis of Laguerre pseudostates:
φ(r)=Σ C ξ(r)
Coefficients C are obtained by diagonalizing the target Hamiltonian:
<φf |H |φi>=ε δ
Wavepackets
Two steps:
1) Bound and Continuum functions are calculated by solving the target SE directly
2) Wavepackets are constructed for continuum

Close coupling scheme

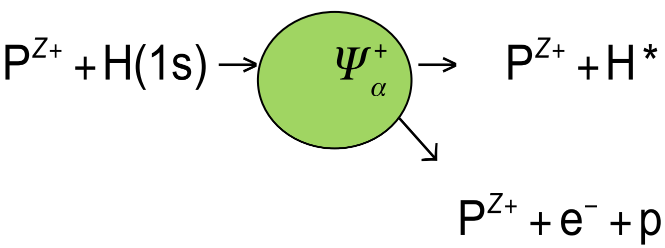


1-centre CCC

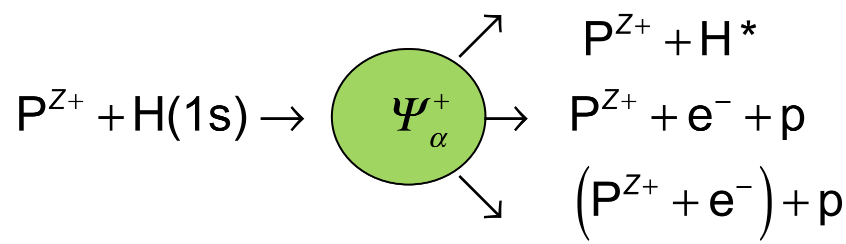


2-centre CCC

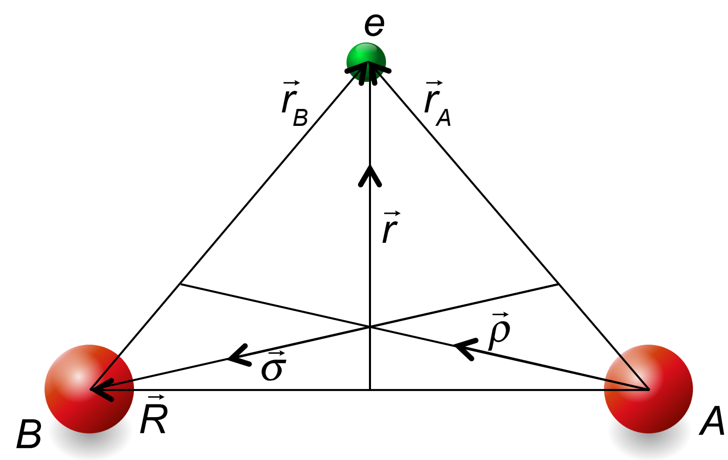
$$\Psi = \sum_{\alpha}^{N_\alpha} F_\alpha(\boldsymbol{\rho}_\alpha)\psi_\alpha(\boldsymbol{r}_\alpha)$$



$$\Psi = \sum_{\alpha}^{N_\alpha} F_\alpha(\boldsymbol{\rho}_\alpha)\psi_\alpha(\boldsymbol{r}_\alpha) + \sum_{\beta}^{N_\beta} F_\beta(\boldsymbol{\rho}_\beta)\psi_\beta(\boldsymbol{r}_\beta)$$



Two-center QM CCC approach



- Schrödinger Eq: $(H-E)\Psi = 0$

- Two-centre expansion:

$$\Psi = \sum_{\alpha} F_{\alpha}^{A}(\vec{\sigma})\phi_{\alpha}^{A}(\vec{r}_A) + \sum_{\beta} F_{\beta}^{B}(\vec{\rho})\phi_{\beta}^{B}(\vec{r}_B)$$

- Require our expansion to satisfy the SE:

$$(E-H)\left(\sum_{\alpha} F_{\alpha}^{A}(\vec{\sigma})\phi_{\alpha}^{A}(\vec{r}_A) + \sum_{\beta} F_{\beta}^{B}(\vec{\rho})\phi_{\beta}^{B}(\vec{r}_B)\right) \approx 0$$

- Project this on each pseudostate Bubnov-Galerkin principle)

$$\begin{cases} \left\langle \phi_{\alpha'}^{A} \middle| (E-H)\sum_{\alpha} F_{\alpha}^{A} \middle| \phi_{\alpha}^{A} \right\rangle + \left\langle \phi_{\alpha'}^{A} \middle| (E-H)\sum_{\beta} F_{\beta}^{B} \middle| \phi_{\beta}^{B} \right\rangle \approx 0 \\ \left\langle \phi_{\beta'}^{B} \middle| (E-H)\sum_{\alpha} F_{\alpha}^{A} \middle| \phi_{\alpha}^{A} \right\rangle + \left\langle \phi_{\beta'}^{B} \middle| (E-H)\sum_{\beta} F_{\beta}^{B} \middle| \phi_{\beta}^{B} \right\rangle \approx 0 \end{cases}$$

Two-center QM CCC approach

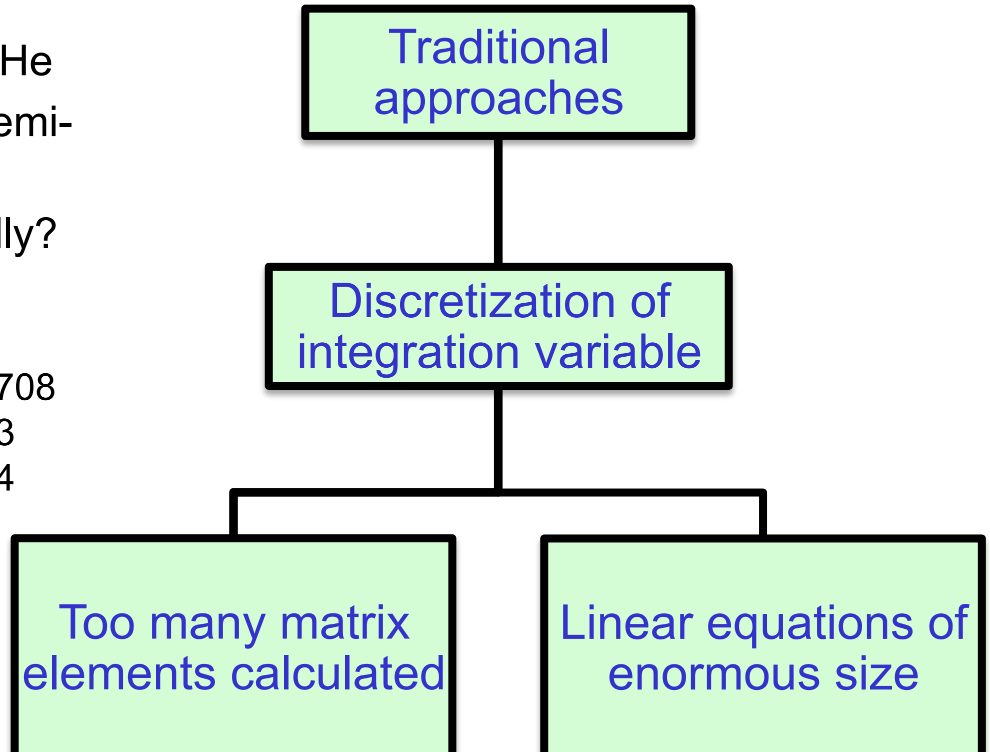
- Lippmann-Schwinger integral equations for the T-matrix in the impact-parameter sp.

$$T_{fi}(k_f,k_i,b)=V_{fi}(k_f,k_i,b)+\frac{k_i}{\pi}\sum_{n=1}^{N_A+N_B}\int_{-\infty}^{\infty}dk\,\frac{V_{fn}(k_f,k,b)T_{ni}(k,k_i,b)}{k_n^2-k^2+i0}$$

k_f, k_i , k are parallel components of momentum

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

Details:
IB Abdurakhmanov et al. 2011 Phys. Rev. A 84 062708
IB Abdurakhmanov et al. 2011 J. Phys. B 44 165203
IB Abdurakhmanov et al. 2011 J. Phys. B 44 075204



Alternative approach

- Off-shell momentum dependent parts of V and T are factored out

$$V_{fi}(k_f,k_i)=\int_{-\infty}^{\infty}dz\,\mathcal{V}_{fi}(z)\exp(i(k_i-k_f)z) \qquad T_{fi}(k_f,k_i)=\int_{-\infty}^{\infty}dz\,\mathcal{T}_{fi}(z)\exp(i(k_i-k_f)z)$$

$$\frac{k_i}{\pi}\sum_{n=1}^{N_A+N_B}\int_{-\infty}^{\infty}dk\,\frac{V_{fn}(k_f,k)T_{ni}(k,k_i)}{k_n^2-k^2+i0}$$

$$\int_{-\infty}^{\infty}dk\,\frac{e^{ik(z-z')}}{k_n^2-k^2+i0}=\begin{cases}-\dfrac{\pi i}{k_n}e^{ik_n(z-z')} & \text{if } z>z' \\ 0 & \text{if } z<z'\end{cases}$$

$$\frac{k_i}{\pi}\sum_{n=1}^{N_A+N_B}\int_{-\infty}^{\infty}dz\,e^{-ik_f z}\,\mathcal{V}_{fn}(z)\int_{-\infty}^{\infty}dz'\,e^{ik_i z'}\,\mathcal{T}_{ni}(z')\int_{-\infty}^{\infty}dk\,\frac{e^{ik(z-z')}}{k_n^2-k^2+i0}$$

$$-i\sum_{n=1}^{N_A+N_B}\frac{k_i}{k_n}\int_{-\infty}^{\infty}dz\,e^{i(k_n-k_f)z}\,\mathcal{V}_{fn}(z)\int_{-\infty}^{z}dz'\,e^{i(k_i-k_n)z'}\,\mathcal{T}_{ni}(z')$$

New scattering equations:

$$\mathcal{T}_{fi}(z) = \mathcal{V}_{fi}(z) - i \sum_{n=1}^{N_A+N_B} \frac{k_i}{k_n} e^{i(k_n-k_f)z} \mathcal{V}_{fn}(z) \int_{-\infty}^{z} dz' e^{i(k_i-k_n)z'} \mathcal{T}_{ni}(z')$$

Solving strategy:

Initialize using
$$\mathcal{V}_{fi}(-\infty) = 0$$
$$\mathcal{T}_{fi}(-\infty) = 0$$

→

Propagate solution using some integration rule

→

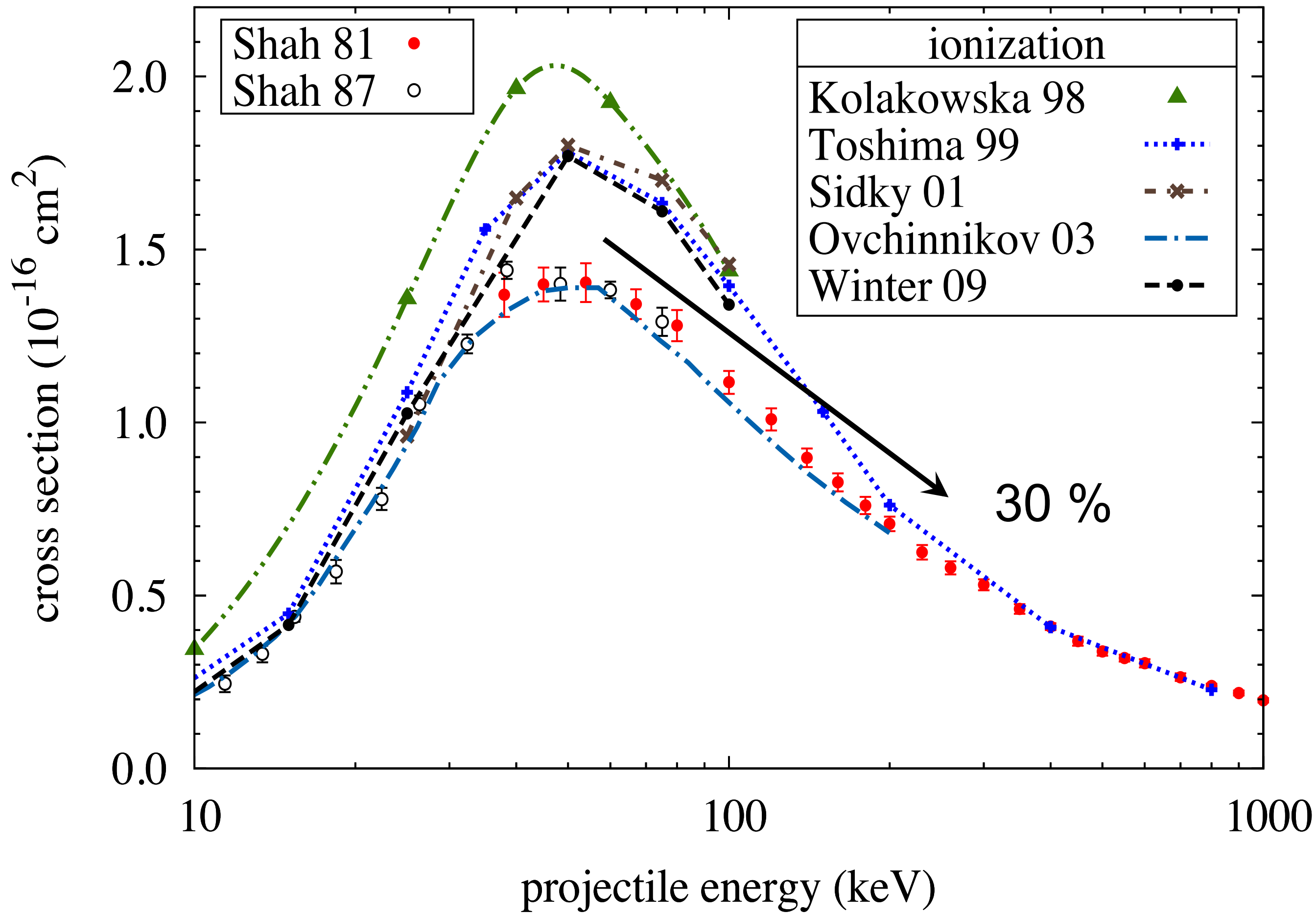
Finish at sufficiently large z

Cross sections:

$$\sigma_{fi} = \int_0^\infty dbb \left| \int_{-\infty}^{\infty} dz \mathcal{T}_{fi}(z,b) e^{i(k_i-k_f)z} \right|^2, \qquad \sigma_{\text{ion}} = \sum_{f \in [\varepsilon_f \geq 0]} \sigma_f$$

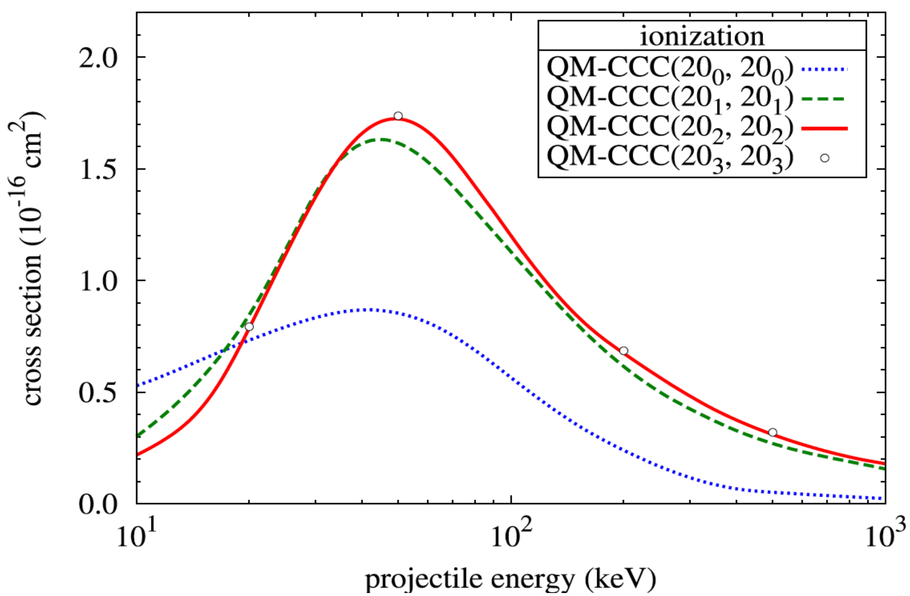
Details: Abdurakhmanov et al., J Phys B 49 (2016) 115203

p-H ionisation: which theory is correct?

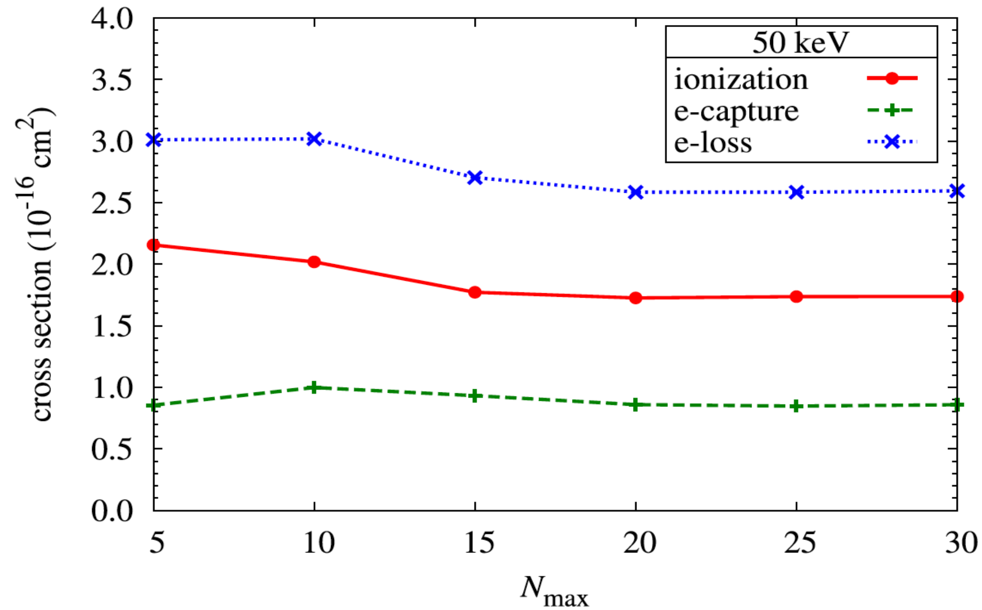


Electron capture and ionisation in p-H

Convergence in terms of ℓ_{max}



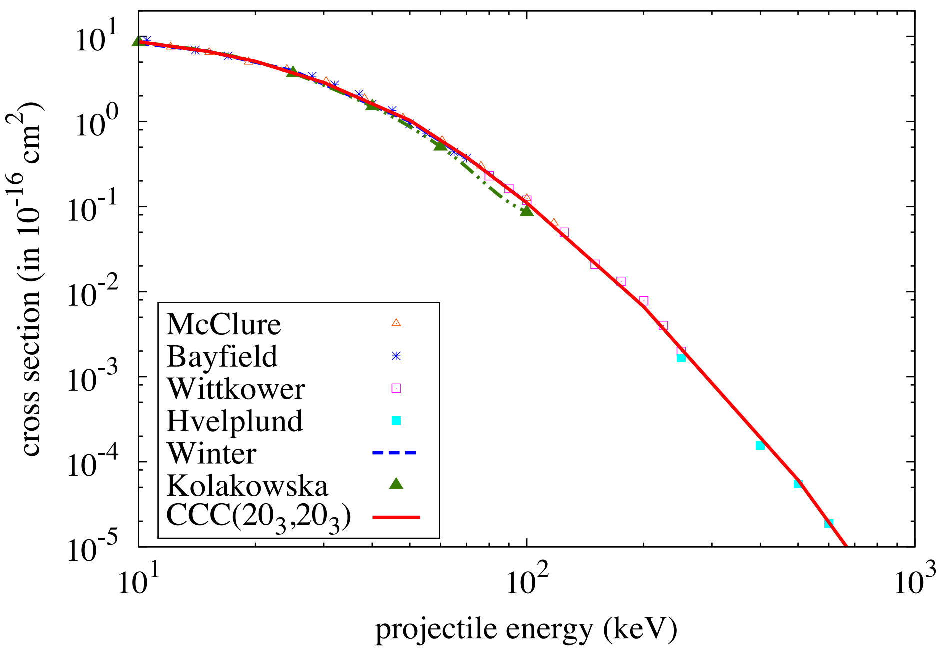
Convergence in terms of N_{max}

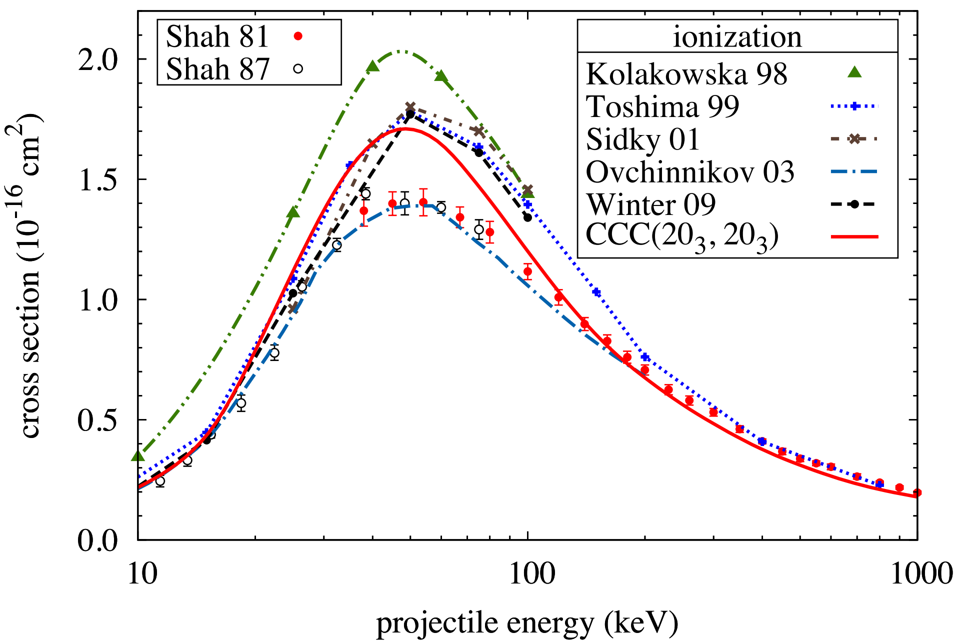


2-centre QM-CCC with Laguerre pseudostates:

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

Electron capture and ionisation in p-H

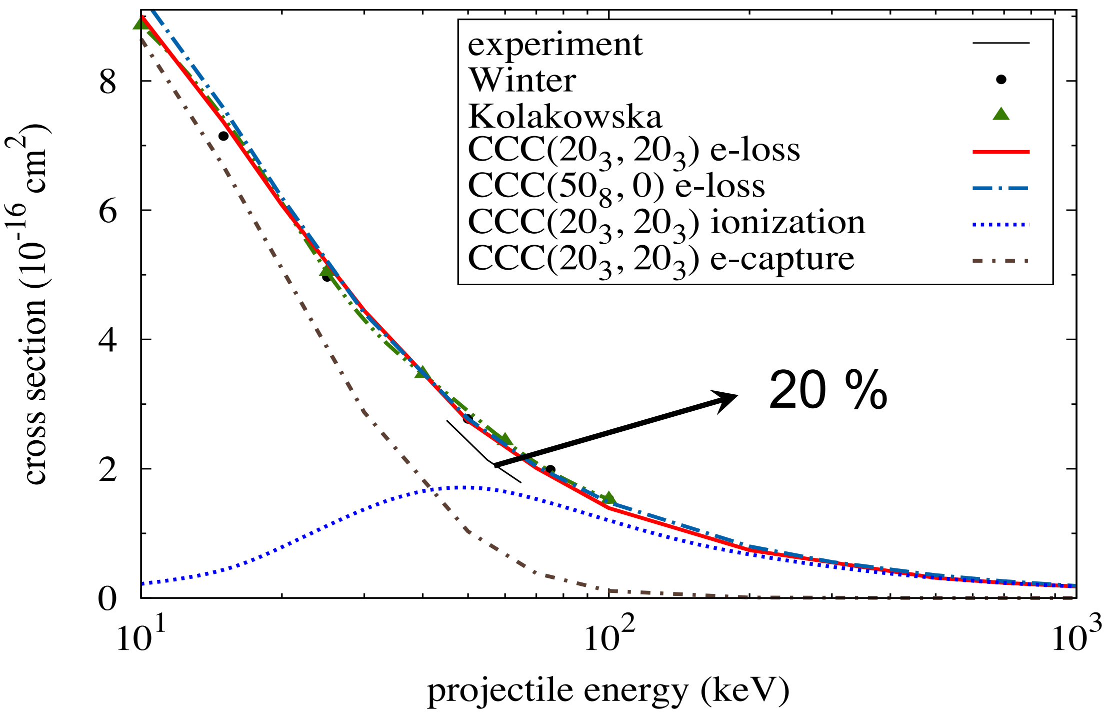




2-centre QM-CCC with Laguerre pseudostates:

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 %

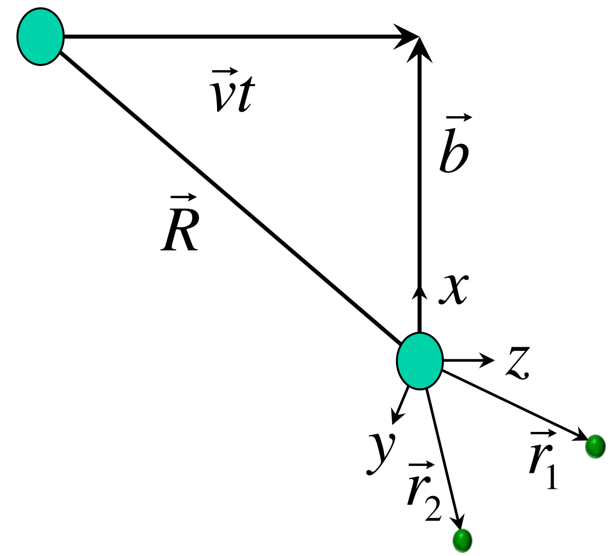
Net error < 0.5 %

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:

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

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

Wave-packet continuum discretisation

- Coulomb wave functions $\varphi_{\kappa l}(r)$:

no finite normalization → not suitable for scattering calculations

- Continuum is subdivided into non-overlapping intervals $[E_{i-1},E_i]_{i=1}^N$

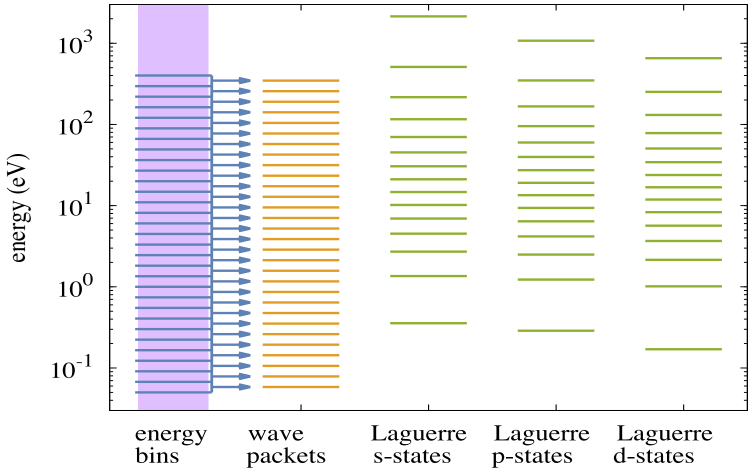
- Stationary wave packets:

$$\psi_{il}(r) = \frac{1}{\sqrt{w_i}} \int_{\kappa_{i-1}}^{\kappa_i} d\kappa \varphi_{\kappa l}(r)$$

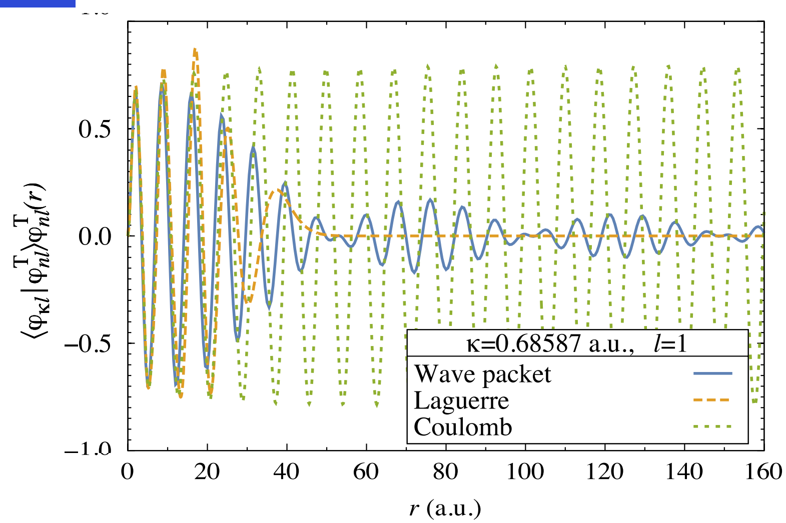
- They are orthonormal: $\langle \psi_{il} | \psi_{jl} \rangle = \delta_{ij}$

- The state energy is the middle point of the bin: $\langle \psi_{il} | H | \psi_{jl} \rangle = \varepsilon_i \delta_{ij}, \quad \varepsilon_i = \frac{E_{i-1} + E_i}{2}$

Wave-packet continuum discretization



Continuum energy levels



Pros:

- Aligned energy levels
- Full control over continuum range $[0{:}E_{\max}]$
- Overlap with Coulomb is just:

$$\int_0^\infty dr\varphi_{\kappa l}(r)\varphi_{nl}^{\mathrm{WP}}(r) = \frac{1}{\sqrt{w_n}}$$

Cons:

- Larger radial grid required

Breakup amplitude including ECC

- Ionization amplitude can be written as

$$T_{fi}(\boldsymbol{q}_f, \boldsymbol{q}_i) = \langle \Phi_f^- | \overleftarrow{H} - E | \Psi_i^+ \rangle$$

Details:
Kadyrov etal, Phys Rev Lett 101 (2008) 230405
Kadyrov et al., Ann Phys 324 (2009) 1516

Φ_f^- is a three-body Coulomb asymptotic state.

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

$$I_N^T = \sum_{n=1}^{N} \left| \phi_n^T \right\rangle \left\langle \phi_n^T \right|$$

$$I_M^P = \sum_{m=1}^{M} \left| \phi_m^P \right\rangle \left\langle \phi_m^P \right|$$

Thus the breakup amplitude splits into two:
direct ionisation (DI) and electron capture to continuum (ECC)

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

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

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

Coherent or Incoherent?

- With wavepacket pseudostates it reduces to:

$$T_\kappa(\mathbf{q}_f,\mathbf{q}_i)=\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}\frac{(-i)^l e^{i\sigma_l}Y_{lm}(\hat{\kappa})T_{nlm}(\mathbf{q}_f,\mathbf{q}_i)}{2\pi\kappa\sqrt{w_n}},$$

where $$T_{nlm}(\mathbf{q}_f,\mathbf{q}_i)=e^{im(\varphi_f+\frac{\pi}{2})}\int_0^\infty dbba_{nlm}(\infty,b)J_m(p_\perp b).$$

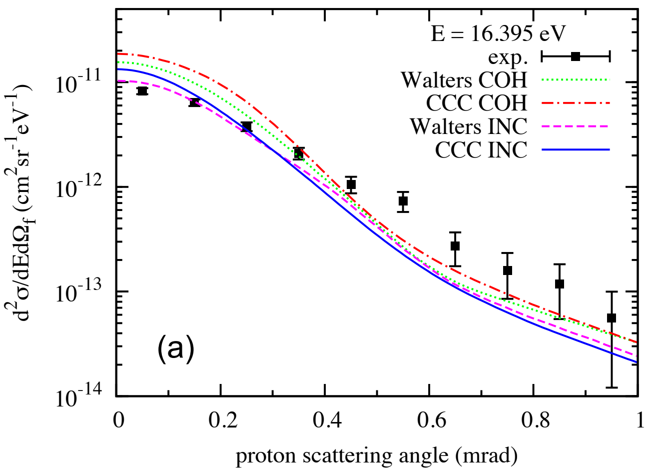
Ejected electron energy

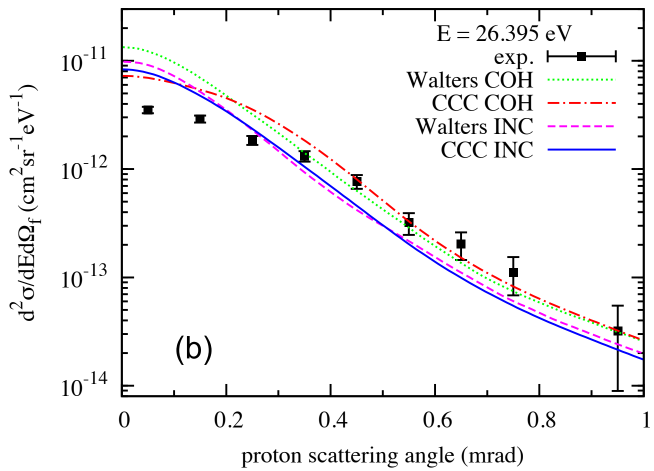
$$\frac{d^2\sigma^{\mathrm{COH}}(\kappa,\boldsymbol{q}_f,q_i)}{dEd\Omega_f}\sim\sum_l\sum_m\overbrace{\left|T_{fi}^{N,T}(\boldsymbol{q}_f,q_i)+T_{fi}^{N,P}(\boldsymbol{q}_f,q_i)\right|^2}^{\text{coherent combination of amplitudes}}$$

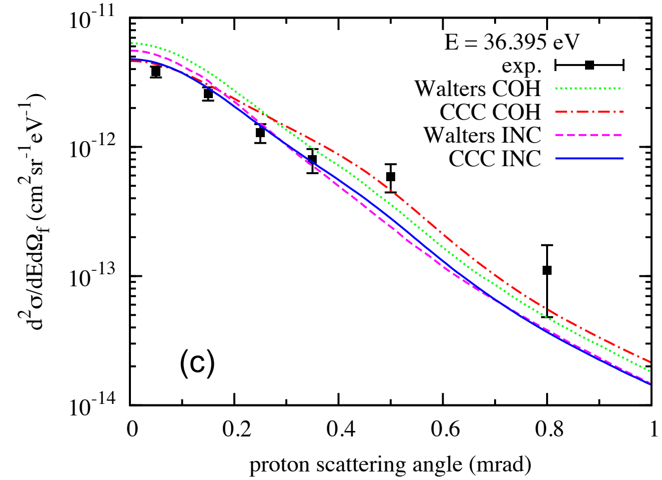
$$\frac{d^2\sigma^{\mathrm{INC}}(\kappa,\boldsymbol{q}_f,q_i)}{dEd\Omega_f}\sim\sum_l\sum_m\underbrace{\left|T_{fi}^{N,T}(\boldsymbol{q}_f,q_i)\right|^2+\left|T_{fi}^{N,P}(\boldsymbol{q}_f,q_i)\right|^2}_{\text{incoherent combination of amplitudes}}$$

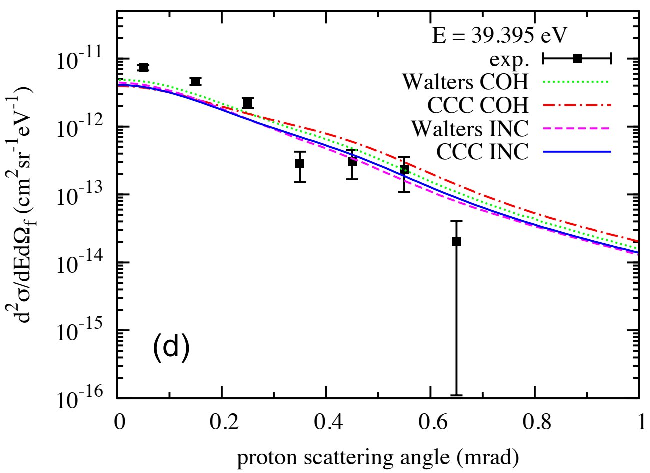
proton scattering angle

p-H double differential ionization:



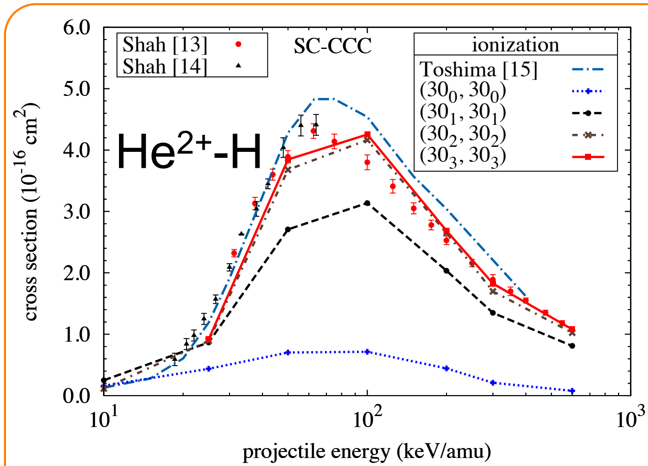


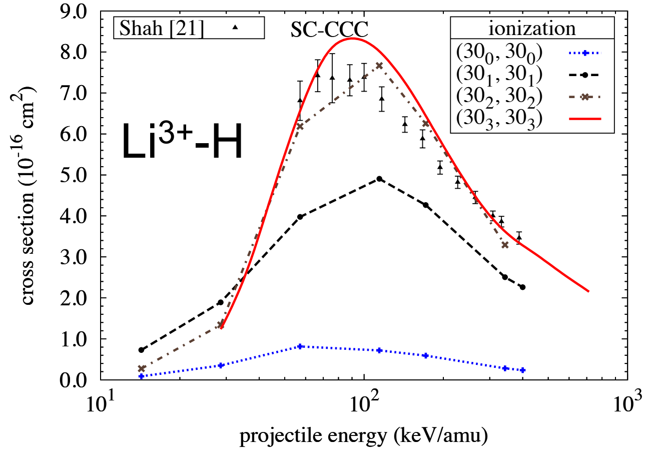


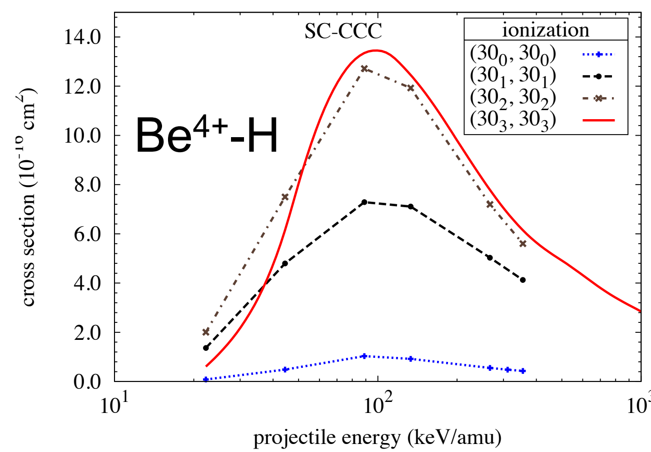


Double differential cross section for electrons ejected with energy of (a) 16.4 eV, (b) 26.4 eV, (c) 36.4 eV, and (d) 39.4 eV as a function of proton scattering angle. CCC calculations compared to theory of Walters and Whelan and experiment by Schultz et al.

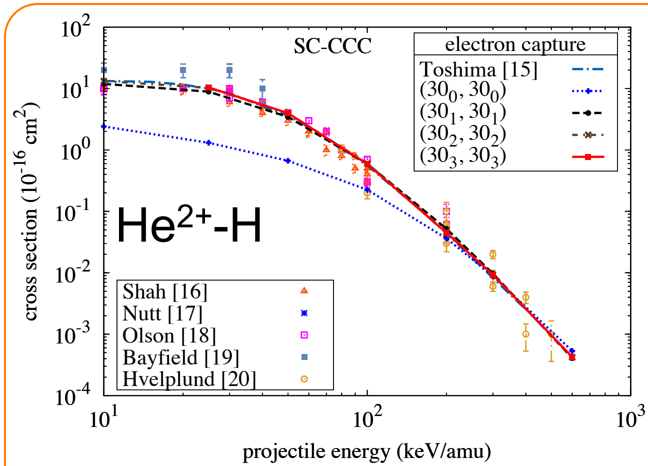
Preliminary results: MCI + H

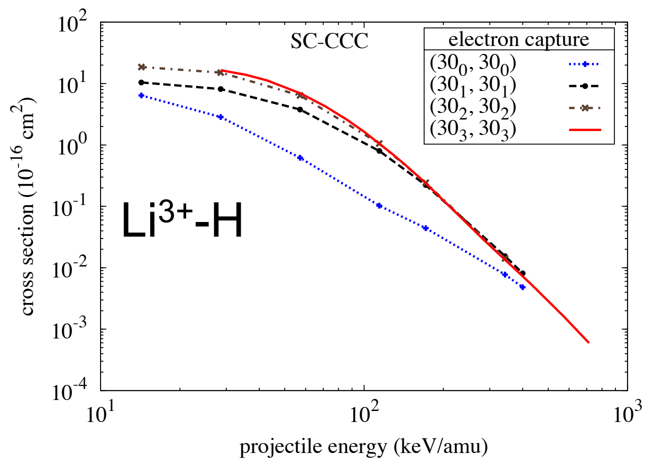


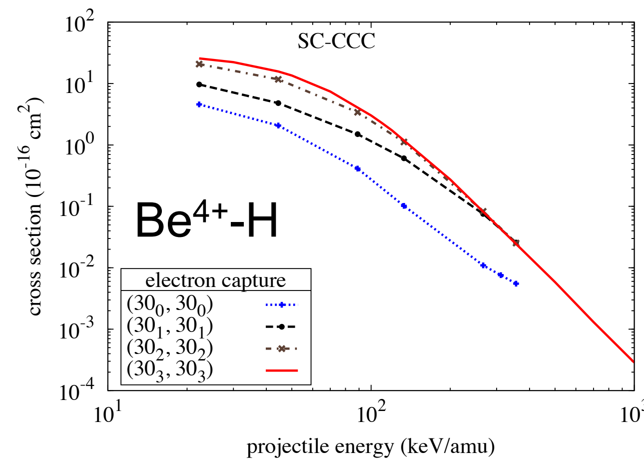




Ionization







Electron capture

WP approach to He

First attempt: frozen core approximation

$$\psi_\alpha(\boldsymbol{r}_1,\boldsymbol{r}_2) = \phi_{1s}^{\mathrm{He}^+}(\boldsymbol{r}_2)\varphi_\alpha(\boldsymbol{r}_1) + \phi_{1s}^{\mathrm{He}^+}(\boldsymbol{r}_1)\varphi_\alpha(\boldsymbol{r}_2)$$

Then it is inserted into SE for helium atom:

$$H_{\mathrm{t}}\psi_\alpha(\boldsymbol{r}_1,\boldsymbol{r}_2) = (\varepsilon_\alpha + \varepsilon_{1s}^{\mathrm{He}^+})\psi_\alpha(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

state	present	LPS [36]	Moore [37]
1s	-23.7416	-23.74139	-24.5862
2s	-3.9035	-3.90343	-3.97155
3s	-1.6483	-1.64828	-1.66705
2p	-3.3307	-3.33198	-3.36931
3p	-1.48847	-1.48950	-1.50035
3d	-1.51024	-1.51150	-1.51329

After some algebra this becomes:

$$\frac{d^2R_\alpha(r)}{dr^2} - \left[\frac{l(l+1)}{r^2} - \frac{4}{r} + 2W_0[R_{1s}^{\mathrm{He}^+}, R_{1s}^{\mathrm{He}^+}] - 2\varepsilon_\alpha\right]R_\alpha(r)$$
$$= \left[\frac{2}{2l+1}W_l[R_{1s}^{\mathrm{He}^+}, R_\alpha] - 2\int_0^\infty R_{1s}^{\mathrm{He}^+}(t)W_0[R_{1s}^{\mathrm{He}^+}, R_{1s}^{\mathrm{He}^+}]R_\alpha(t)dt\right]R_{1s}^{\mathrm{He}^+}(r)$$

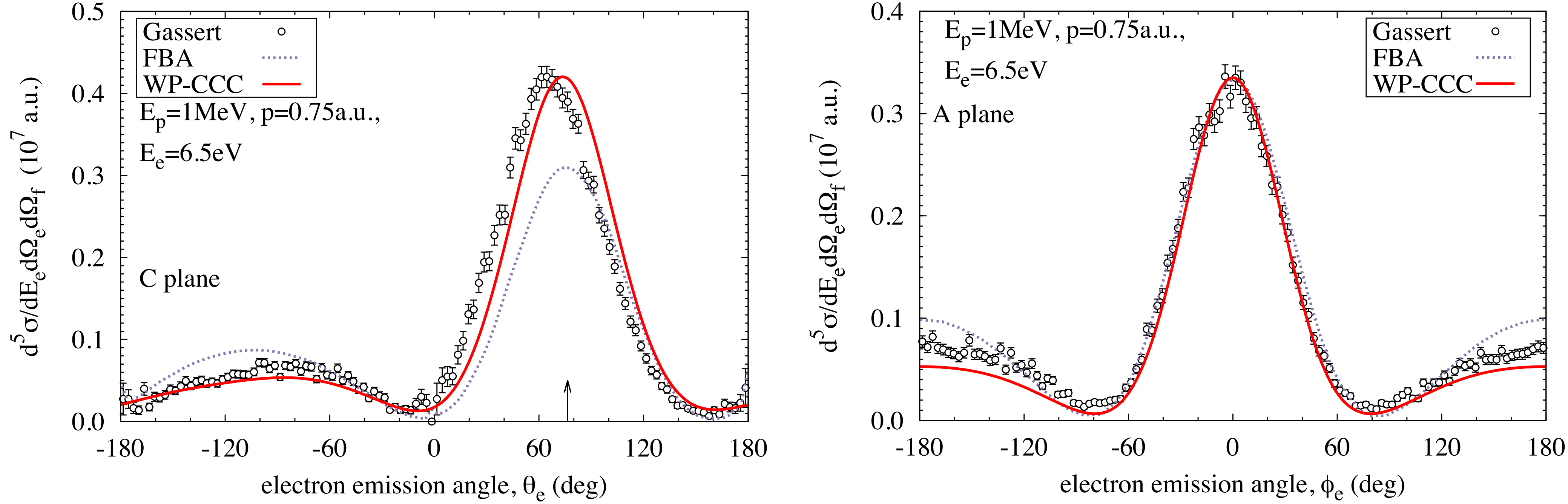
Solved by iterative Numerov.

For continuum states

$$R_{il}^{\mathrm{WP}}(r) = \nu_{il}\int_{\kappa_{i-1}}^{\kappa_i} d\kappa R_{\kappa l}(r)$$

Again, energies can be chosen arbitrarily.

He single ionization by 1 MeV protons



Electron capture is negligible at 1 MeV.
1-center CCC is used

Details:
Abdurakhmanov et al, Phys Rev A, 2017, *accepted*

Conclusions and future directions

- 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+}, Li^{3+} and Be^{4+}
- We can provide
  - fully *nlm*-resolved cross sections for excitation and electron capture
- data for any initial state H(nml)
- Currently working on:
  - multicore treatment of He, 2-electron processes etc
  - inclusion of electron capture channels into p-He problem

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Thank you