Coupled-Channel Approach to Proton Scattering on Molecular Hydrogen Using an Effective One-Electron Model

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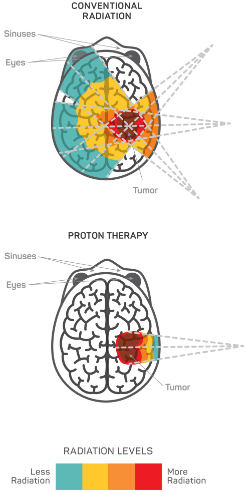
Introduction

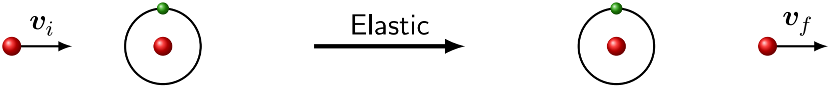
What is the motivation to study $\mathrm{p} + \mathrm{H}_2$ collisions?

- Challenging theoretical problem
- Current theory inconsistent with experiment
- Pathway to more complex targets
- Applications
  - Monte-Carlo simulations for Hadron therapy treatment planning
  - Nuclear fusion plasma projects
  - Astrophysical charge-exchange

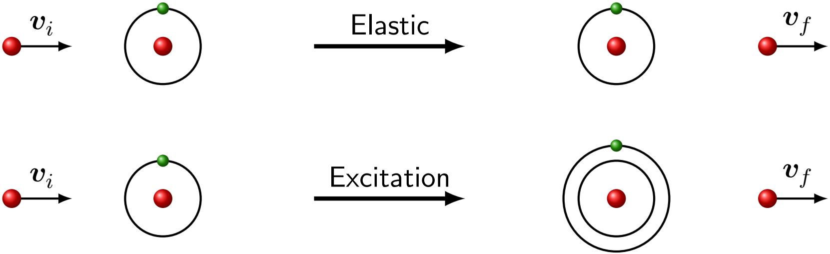


https://www.seattlecca.org/treatments/proton-therapy/what-is-proton-therapy

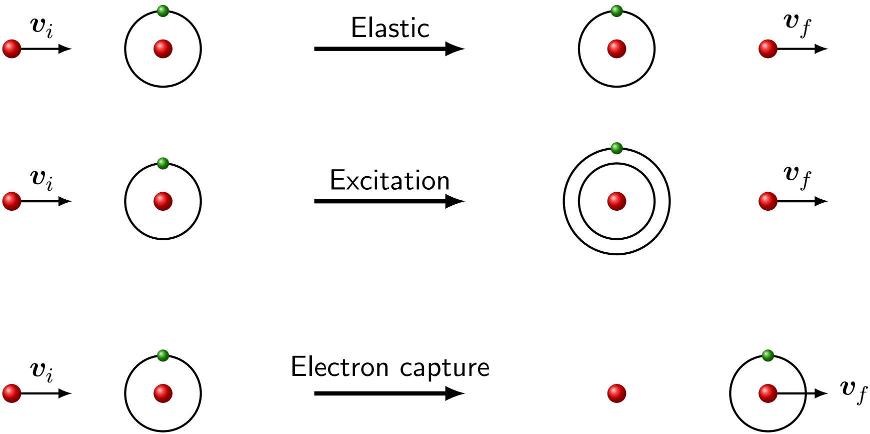
Scattering outcomes



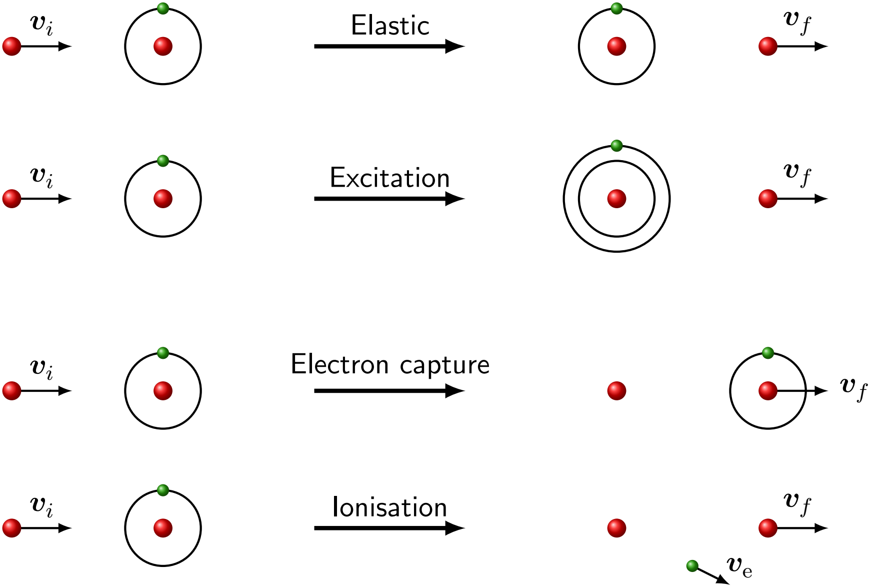
Scattering outcomes



Scattering outcomes



Scattering outcomes



Literature review

	TCS (direct)	TCS (electron loss)	TCS (capture)	TCS (ionisation)
FBA				
CDW				
1c-CC				
AOCC				
MOCC				
CTMC				

Literature review

	TCS (direct)	TCS (electron loss)	TCS (capture)	TCS (ionisation)
FBA			✓	
CDW			✓	✓
1c-CC		✓		
AOCC			✓	
MOCC		✓		
CTMC	✓	✓	✓	✓

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CTMC	✓	✓	✓	✓

	SDCS (direct)	SDCS (capture)	SDCS (ion E_{e})	SDCS (ion θ_{e})	SDCS (ion θ_f)
FBA					
CDW					
Eikonal					
1c-CC					
CTMC					
Gryzińksi					

Literature review

	TCS (direct)	TCS (electron loss)	TCS (capture)	TCS (ionisation)
FBA			✓	
CDW			✓	✓
1c-CC		✓		
AOCC			✓	
MOCC		✓		
CTMC	✓	✓	✓	✓

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FBA		✓	✓		
CDW		✓			
Eikonal		✓			
1c-CC			✓		
CTMC	✓			✓	
Gryzińksi			✓		

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CTMC	✓	✓	✓	✓
WP-CCC	✓	✓	✓	✓

	SDCS (direct)	SDCS (capture)	SDCS (ion E_e)	SDCS (ion θ_e)	SDCS (ion θ_f)
FBA		✓	✓		
CDW		✓			
Eikonal		✓			
1c-CC			✓		
CTMC	✓			✓	
Gryzińksi			✓		
WP-CCC	✓	✓	✓	✓	✓

Wave-packet convergent close-coupling (WP-CCC)

Start with Schrödinger equation

$$(H - E)\Psi_i^+ = 0$$

and expand the scattering wave function in terms of orthogonal pseudostates and plane waves

$$\Psi_i^+ \approx \sum_{\alpha=1}^{N} F_\alpha(t, \boldsymbol{b})\psi_\alpha(\boldsymbol{r}_\mathrm{t})e^{i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}} + \sum_{\beta=1}^{M} G_\beta(t, \boldsymbol{b})\psi_\beta(\boldsymbol{r}_\mathrm{p})e^{i\boldsymbol{q}_\beta\cdot\boldsymbol{\sigma}}$$

obtain differential equations for expansion coefficients

$$i\begin{pmatrix} \boldsymbol{I} & \boldsymbol{\mathcal{K}} \\ \tilde{\boldsymbol{\mathcal{K}}} & \boldsymbol{I} \end{pmatrix}\begin{pmatrix} \dot{\boldsymbol{F}} \\ \dot{\boldsymbol{G}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathcal{D}} & \boldsymbol{\mathcal{Q}} \\ \tilde{\boldsymbol{\mathcal{Q}}} & \tilde{\boldsymbol{\mathcal{D}}} \end{pmatrix}$$

Structure of atomic hydrogen

- Separate radial and angular parts $\psi_{n\ell m}(\boldsymbol{r}) = \phi_{n\ell}(r) Y_{\ell m}(\hat{\boldsymbol{r}})$
- for projectile atom use bound eigenstates of hydrogen atom, and
- wave packets made from the Coulomb wave

$$\phi_{n\ell}^{\mathrm{WP}} = \frac{1}{\sqrt{\kappa_n - \kappa_{n-1}}} \int_{\kappa_{n-1}}^{\kappa_n} d\kappa \; U_\ell(\kappa, r)$$

Target structure

- Model effective-potential

$$V_{\mathrm{mod}}(r) = \frac{1}{r}(1 + \mathrm{e}^{-\zeta r}), \qquad \zeta = 5.4824$$

- satisfies:
  - ionisation energy -0.5976 au
  - asymptotic form $1/r$ as $r \to \infty$

- Numerically solve target Schrödinger equation for wave functions of effective one-electron H_2 "atom"

- construct wave packets from positive-energy solutions

Calculation: total cross sections

Total cross sections are found from

$$\sigma_f = \int_0^\infty db\, b P_f(b)$$

and probabilities are given by expansion coefficients in the asymptotic state

$$P_f^{\mathrm{DS}}(b) = \left| F_f(+\infty, \boldsymbol{b}) - \delta_{fi} \right|^2$$

and

$$P_f^{\mathrm{EC}}(b) = \left| G_f(+\infty, \boldsymbol{b}) \right|^2$$

Scattering amplitudes

Momentum-space amplitudes found from expansion coefficients,

$$\begin{aligned} T_{fi}^{\mathrm{DS}}(\boldsymbol{q}_f, \boldsymbol{q}_i) &= \frac{1}{2\pi} \int d\boldsymbol{b}\, e^{i\boldsymbol{q}_\perp \cdot \boldsymbol{b}} \mathcal{T}_{fi}^{\mathrm{DS}}(\boldsymbol{b}) \\ &= 2\pi i v e^{im\phi_f} \int_0^\infty db\, b[\tilde{F}_f(+\infty, b) - \delta_{fi}] J_m(q_\perp b), \end{aligned}$$

and

$$\begin{aligned} T_{fi}^{\mathrm{EC}}(\boldsymbol{q}_f, \boldsymbol{q}_i) &= \frac{1}{2\pi} \int d\boldsymbol{b}\, e^{i\boldsymbol{q}_\perp \cdot \boldsymbol{b}} \mathcal{T}_{fi}^{\mathrm{EC}}(\boldsymbol{b}) \\ &= 2\pi i v e^{im\phi_f} \int_0^\infty db\, b\tilde{G}_f(+\infty, b) J_m(q_\perp b), \end{aligned}$$

Calculation: differential cross sections

Angular differential cross section is

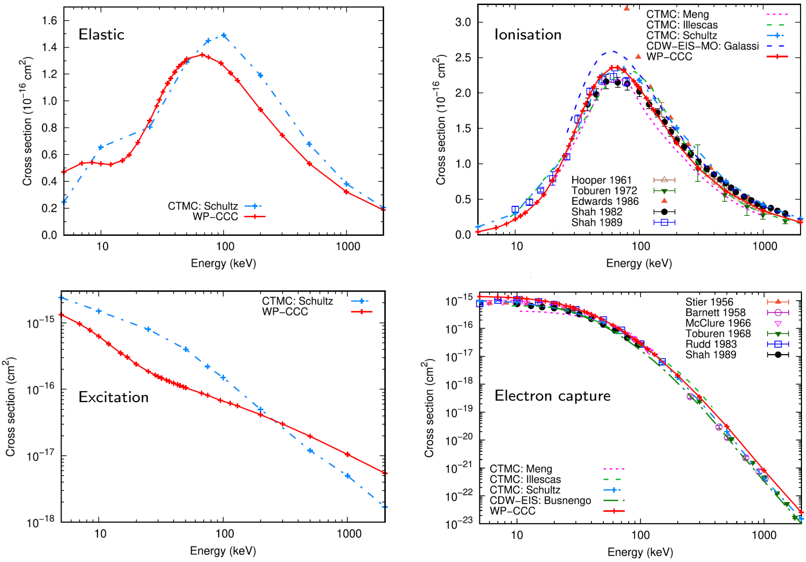
$$\frac{d\sigma_{fi}^{\mathrm{DS(EC)}}}{d\Omega_f} = \frac{\mu^2}{(2\pi)^2}\frac{q_f}{q_i}\left|T_{fi}^{\mathrm{DS(EC)}}(\boldsymbol{q}_f, \boldsymbol{q}_i)\right|^2,$$

ionisation differential cross sections found from

$$\frac{d^3\sigma_{\mathrm{ion}}}{dE_{\mathrm{e}}d\Omega_{\mathrm{e}}d\Omega_f} = \frac{\mu^2}{(2\pi)^2}\frac{q_f\kappa}{q_i}\left(\left|T_{fi}^{\mathrm{DI}}(\boldsymbol{\kappa}, \boldsymbol{q}_f, \boldsymbol{q}_i)\right|^2 + \left|T_{fi}^{\mathrm{ECC}}(\boldsymbol{\kappa} - \boldsymbol{v}, \boldsymbol{q}_f, \boldsymbol{q}_i)\right|^2\right),$$

integrate to obtain singly or doubly differential cross sections.

Results: total cross sections



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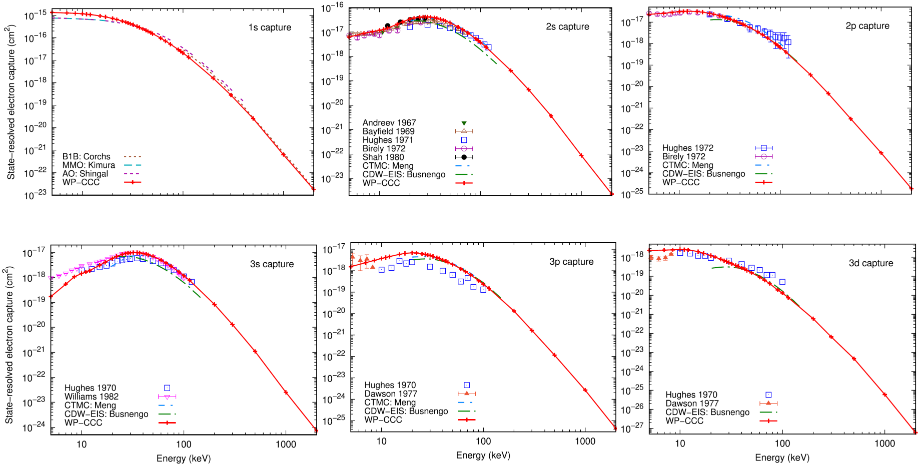
Results: state-resolved electron capture



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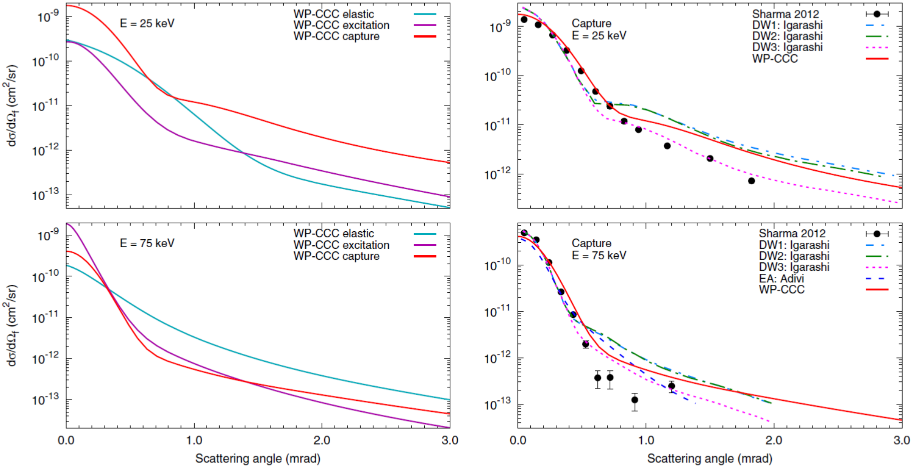
Results: SDCS, binary collisions



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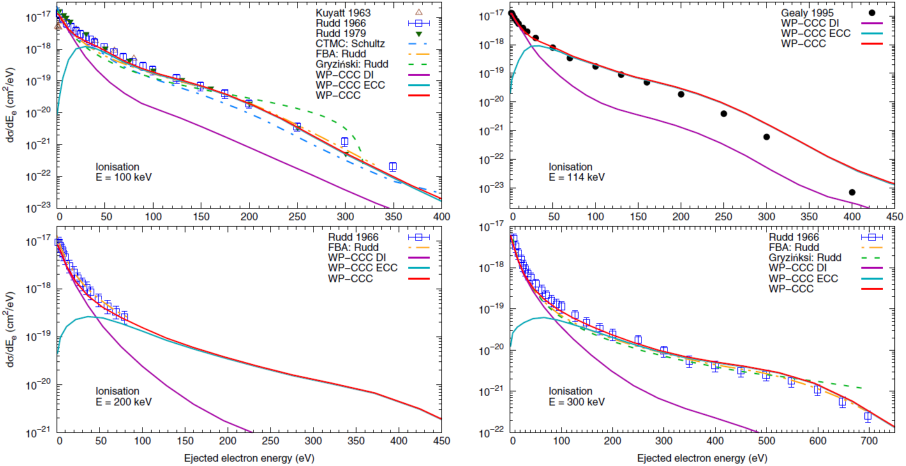
Results: SDCS, ionisation vs electron energy



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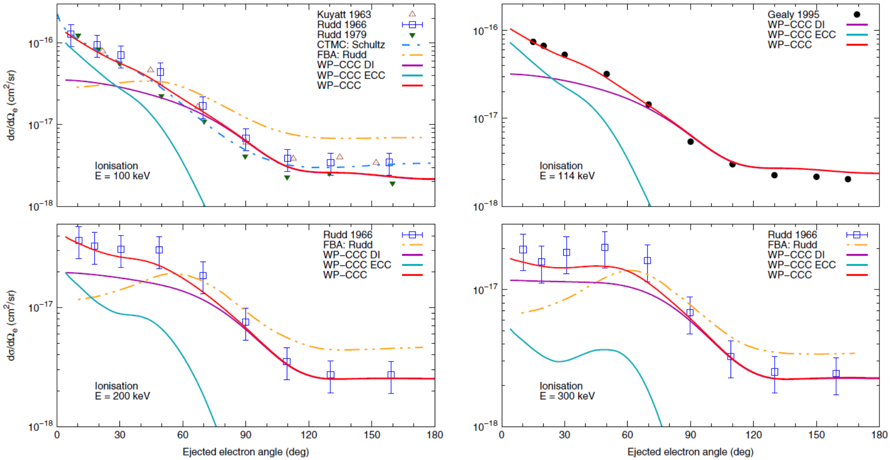
Results: SDCS, ionisation vs emission angle



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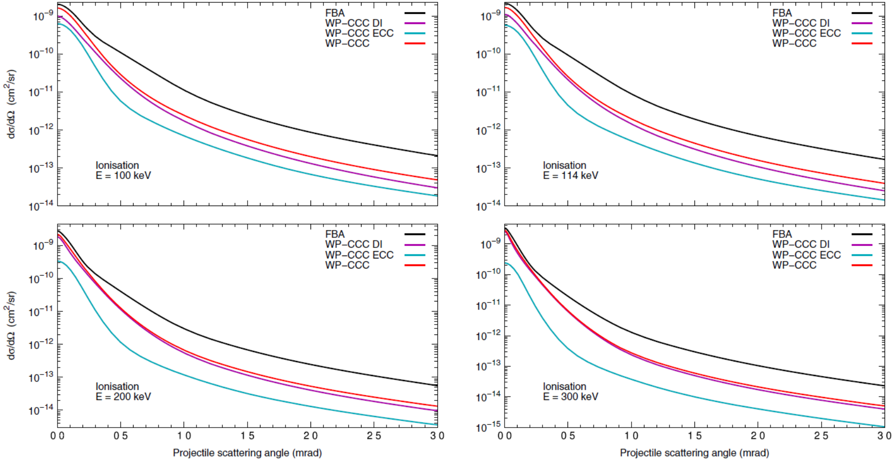
Results: SDCS, ionisation vs scattering angle



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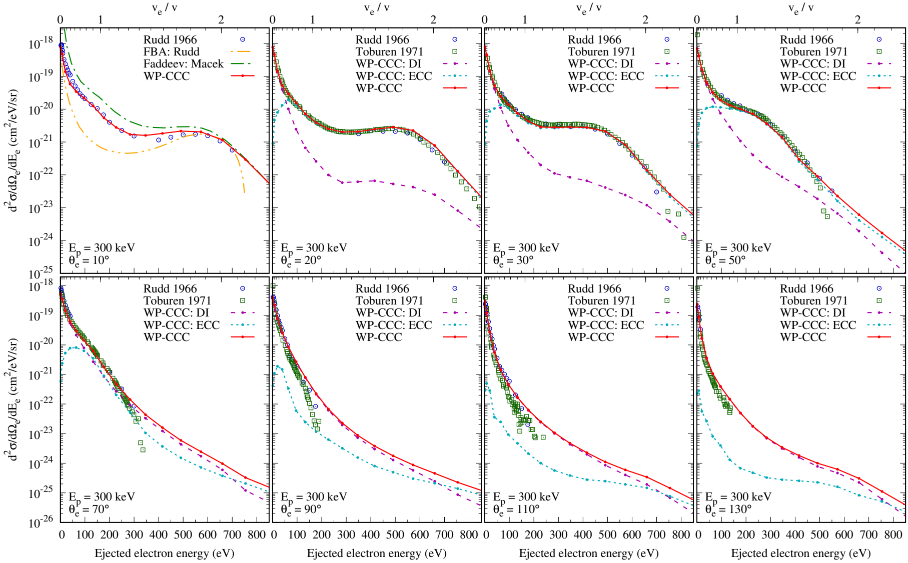
Results: DDCS, ionisation vs electron energy and angle



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Conclusion

- First two-centre close-coupling calculations for $\mathrm{p} + \mathrm{H}_2$ collsions
- Excellent agreement with experimental data
- Significant improvement over previously available calculations of differential cross sections
- Next we will apply the WP-CCC method to fully differential cross sections

Supplementary: coupled differential equations

Schrödinger equation becomes,

$$\begin{cases} i\dot{F}_{\alpha'} + i\sum_{\beta=1}^{M} \dot{G}_\beta \tilde{K}_{\alpha'\beta} = \sum_{\alpha=1}^{N} F_\alpha D_{\alpha'\alpha} + \sum_{\beta=1}^{M} G_\beta \tilde{Q}_{\alpha'\beta}, \\ i\sum_{\alpha=1}^{N} \dot{F}_\alpha K_{\beta'\alpha} + i\dot{G}_{\beta'} = \sum_{\alpha=1}^{N} F_\alpha Q_{\beta'\alpha} + \sum_{\beta=1}^{M} G_\beta \tilde{D}_{\beta'\beta}, \\ \alpha' = 1, 2, \ldots, N, \quad \beta' = 1, 2, \ldots, M \end{cases}$$

Matrix elements are

$$D_{\alpha'\alpha}(\boldsymbol{R}) = \left\langle \psi_{\alpha'} \middle| \overline{V}_\alpha \middle| \psi_\alpha \right\rangle \mathrm{e}^{i(\varepsilon_{\alpha'} - \varepsilon_\alpha)t} \qquad K_{\beta'\alpha} = \left\langle \psi_{\beta'} \middle| \mathrm{e}^{-i\boldsymbol{v}\cdot\boldsymbol{r}_\mathrm{P}} \middle| \psi_\alpha \right\rangle \mathrm{e}^{iv^2 t/2 + i(\varepsilon_{\beta'} - \varepsilon_\alpha)t}$$

$$\tilde{D}_{\beta'\beta}(\boldsymbol{R}) = \left\langle \psi_{\beta'} \middle| \overline{V}_\beta \middle| \psi_\beta \right\rangle \mathrm{e}^{i(\varepsilon_{\beta'} - \varepsilon_\beta)t} \qquad \tilde{K}_{\alpha'\beta} = \left\langle \psi_{\alpha'} \middle| \mathrm{e}^{i\boldsymbol{v}\cdot\boldsymbol{r}_\mathrm{T}} \middle| \psi_\beta \right\rangle \mathrm{e}^{iv^2 t/2 + i(\varepsilon_{\alpha'} - \varepsilon_\beta)t}$$

$$Q_{\beta'\alpha} = \left\langle \psi_{\beta'} \middle| \mathrm{e}^{-i\boldsymbol{v}\cdot\boldsymbol{r}_\mathrm{P}} (H_\alpha + \overline{V}_\alpha - \varepsilon_\alpha) \middle| \psi_\alpha \right\rangle \mathrm{e}^{iv^2 t/2 + i(\varepsilon_{\beta'} - \varepsilon_\alpha)t}$$

$$\tilde{Q}_{\alpha'\beta} = \left\langle \psi_{\alpha'} \middle| \mathrm{e}^{i\boldsymbol{v}\cdot\boldsymbol{r}_\mathrm{T}} (H_\beta + \overline{V}_\beta - \varepsilon_\beta) \middle| \psi_\beta \right\rangle \mathrm{e}^{iv^2 t/2 + i(\varepsilon_{\alpha'} - \varepsilon_\beta)t}$$

Supplementary: doubly differential cross section

Differential cross section for ionisation has two parts,

$$\frac{\mathrm{d}^2\sigma_n^{\mathrm{ion}}}{\mathrm{d}E_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{e}} = \frac{\mathrm{d}^2\sigma_n^{\mathrm{DI}}}{\mathrm{d}E_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{e}} + \frac{\mathrm{d}^2\sigma_n^{\mathrm{ECC}}}{\mathrm{d}E_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{e}}.$$

DI part is

$$\frac{\mathrm{d}^2\sigma_n^{\mathrm{DI}}}{\mathrm{d}E_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{e}} = \frac{2\pi}{\kappa w_n} \sum_{\ell=0}^{\ell_{\max}} \sum_{\ell'=0}^{\ell'_{\max}} \sum_{m=-\ell}^{\ell} \Bigg[Y_{\ell m}^*(\hat{\boldsymbol{\kappa}}) Y_{\ell' m}(\hat{\boldsymbol{\kappa}}) (-i)^{\ell'-\ell} \mathrm{e}^{i(\sigma_{\ell'}-\sigma_\ell)} \times \int_0^\infty \mathrm{d}b\, b \tilde{F}_{n\ell m}^*(\infty, b) \tilde{F}_{n\ell' m}(\infty, b) \Bigg],$$

substitute $\boldsymbol{\kappa} \to \boldsymbol{\kappa} - \boldsymbol{v}$ and $\boldsymbol{q}_\perp \to (\boldsymbol{q} - \boldsymbol{\kappa})_\perp$ for ECC part.