

# Production of cross sections for atomic collisions with Asymptotic Orbital Semiclassical Coupled Channel calculations

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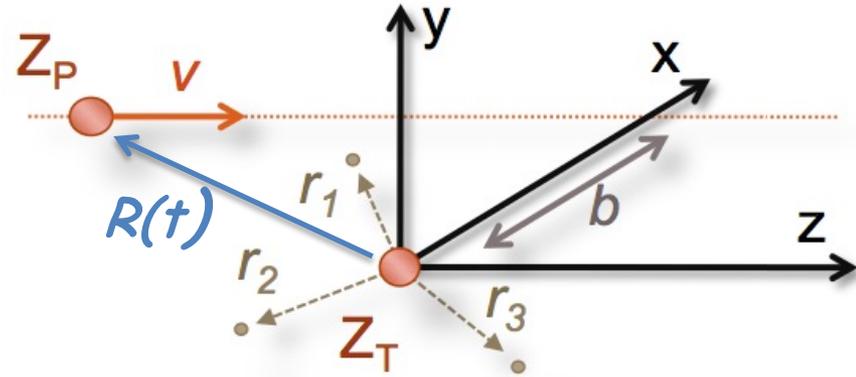
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# THEORETICAL TREATMENT:

- Semi-classical approach

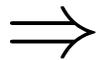
$$\vec{R}(t) = \vec{b} + \vec{v} t$$

*impact parameter approximation*



- Sudden approximation

(for molecular targets)



Eikonal equation

$$\left[ H_{el}(t) - i \frac{\partial}{\partial t} \right] \Psi(\{\vec{r}_i\}, t) = 0$$

with

$$H_{el}(t) = \sum_i \left[ -\frac{1}{2} \Delta_i - \frac{Z_t}{r_i} - \frac{Z_p}{|\vec{r}_i - \vec{R}(t)|} \right] + \sum_{i < j} \frac{1}{r_{ij}}$$

or model potentials

## THEORETICAL TREATMENT:

and 
$$\Psi(\{\vec{r}_i\}, t) = \sum_k a_k(t) \Phi_k^T(\{\vec{r}_{i'}\}, t) \Phi_k^P(\{\vec{r}_{j' \neq i'}\}, t)$$

expansion on a set of asymptotic **target** and **ETF-augmented projectile** states

$$\begin{aligned} \Phi_k^T(\{\vec{r}_{i'}\}, t) &= \phi_k^T(\{\vec{r}_{i'}\}) e^{-i\epsilon_k^T t} \\ \Phi_k^P(\{\vec{r}_{j'}\}, t) &= \phi_k^P(\{\vec{r}_{j'}\}) e^{-i\epsilon_k^P t} \prod_{j'} e^{i\vec{v} \cdot \vec{r}_{j'}} \downarrow e^{-i\frac{1}{2}v^2 t} \end{aligned}$$

*ETF*( $\{\vec{r}_i\}$ )

$\phi^{T/P}$  ( $\epsilon^{T/P}$ )  
eigenfunctions (eigenvalues)  
of the T/P Hamiltonians

- solve

$$\left[ H_{el}(t) - i \frac{\partial}{\partial t} \right] \Psi(\{\vec{r}_i\}, t) = 0 \implies i \dot{\bar{a}} = \bar{S}^{-1} \bar{M} \bar{a}$$

with evaluation of all matrix elements, e.g.  $\langle i^P j^P | \frac{1}{r_{12}} e^{-i\vec{v} \cdot (\vec{r}_1 + \vec{r}_2)} | k^T l^T \rangle$

- to compute probability and cross section

$$P_{ij}(v, b) = \lim_{t \rightarrow +\infty} |a_j(b, v, t)|^2 \quad \sigma_{ij}(v) = 2\pi \int_0^\infty P_{ij}(v, b) b db$$

and also differential cross sections ...

## OUR TWO IMPLEMENTATIONS:

Both based on the use of (multi-center) Gaussian Type Orbitals (GTO)

(and their products)

- implementation 1

- $G_\ell(\vec{r}) = N_\ell r^\ell e^{-\alpha r^2} Y_{\ell,m}(\theta, \varphi)$

- developed up to 4 active electrons (including all possible spin states)

- matrix element evaluations based on

$$I = \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz r^{m_1} r'^{m_2} r''^{m_3} x^{u_1} y^{v_1} z^{w_1} x'^{u_2} y'^{v_2} z'^{w_2} \frac{\exp(-\alpha_1 r^2 - \alpha_2 r'^2 - \alpha_3 r''^2 + i\mu\vec{v} \cdot \vec{r})}{(r'')^\lambda}$$

( $\lambda = 0, 1; \mu = 0, \pm 1$ ),

$$= \lim_{\vec{a} \rightarrow \mu\vec{v}} \lim_{\vec{b} \rightarrow \vec{0}} \left(-i \frac{\partial}{\partial a_x}\right)^{u_1} \left(-i \frac{\partial}{\partial a_y}\right)^{v_1} \left(-i \frac{\partial}{\partial a_z}\right)^{w_1} \left(-i \frac{\partial}{\partial b_x}\right)^{u_2} \left(-i \frac{\partial}{\partial b_y}\right)^{v_2} \left(-i \frac{\partial}{\partial b_z}\right)^{w_2} \left(-i \frac{\partial}{\partial \alpha_1}\right)^{\frac{m_1}{2}} \left(-i \frac{\partial}{\partial \alpha_2}\right)^{\frac{m_2}{2}} \left(-i \frac{\partial}{\partial \alpha_3}\right)^{\frac{m_3}{2}} J_\lambda,$$

with, e.g.

$$J_1 = \frac{2\pi^{3/2}}{B\sqrt{\alpha}} \exp(-\alpha_2 R^2 - \alpha_3 \rho^2 - i\vec{b} \cdot \vec{R}) e^{A^2/(4\alpha)} \operatorname{erf}\left(\frac{B}{2\sqrt{\alpha}}\right)$$

details in PRA 84 052722 (2011)

- implementation 2

- $G_\ell(x, y, z) = N x^i y^j z^k e^{-\alpha(x^2+y^2+z^2)}$  with  $i + j + k = \ell$

e.g., for d-states, 6 cartesian GTOs  $x^2, y^2, z^2, xy, xz, yz$

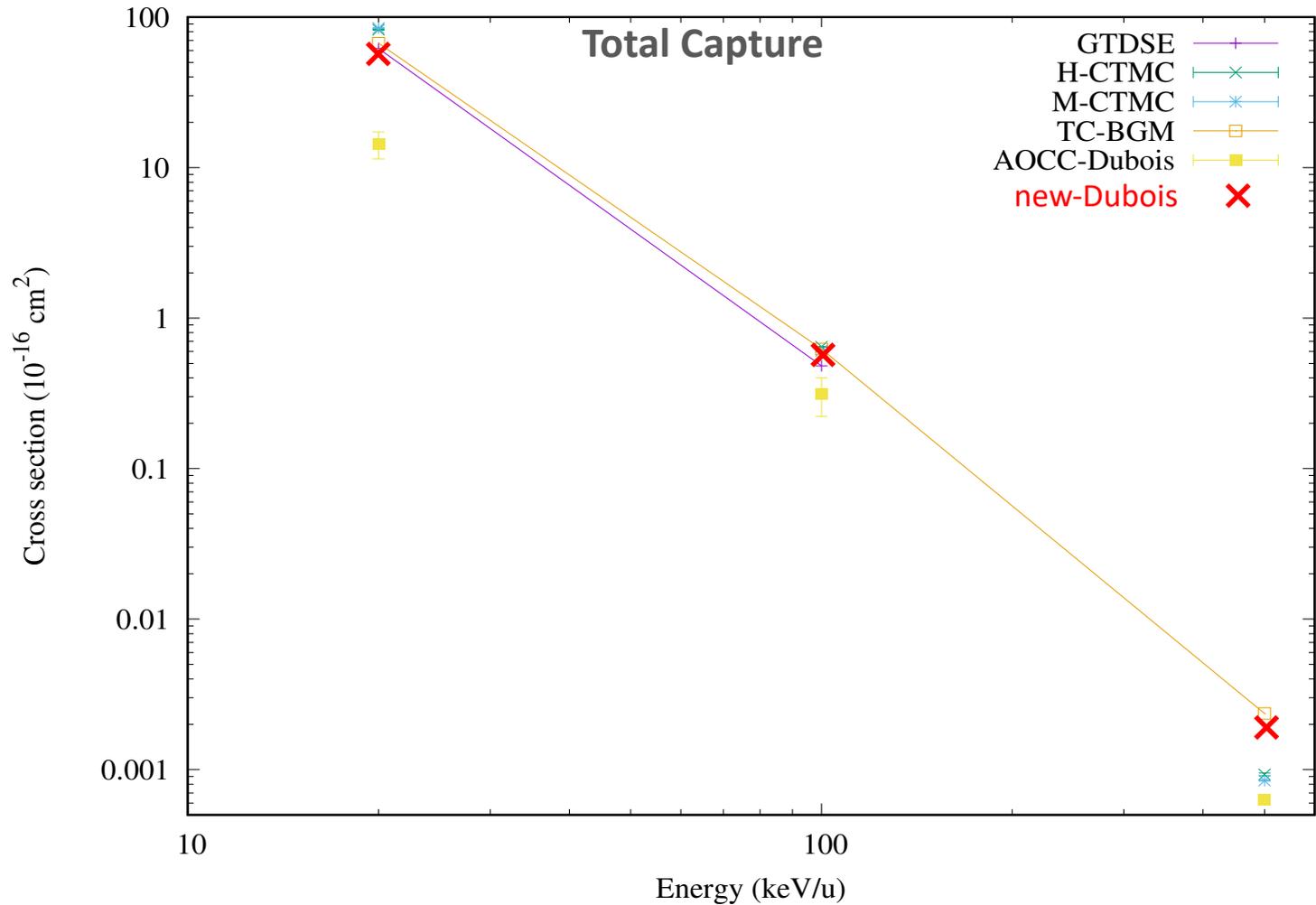
- developed up to 2 active electrons

- matrix element evaluations based on the same approach, except for the rewriting of the integrations into recurrence formula for efficient calculations of matrix involving GTOs of high angular momenta

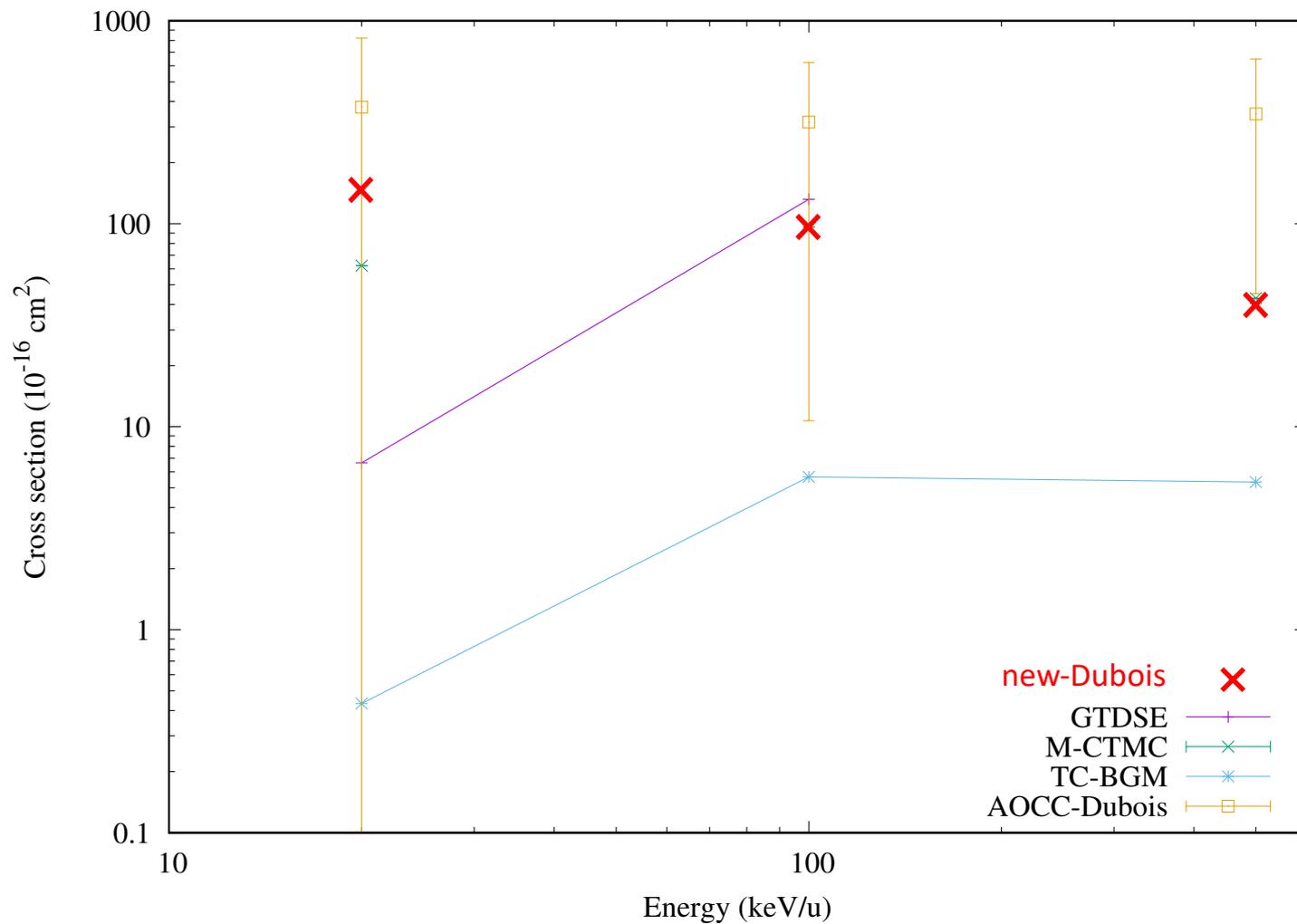
details in JPB **49**, 085202 (2016)

⇒ these 2 different and independent codes covering about the same impact energy range and having different numerical features, extremely efficient to test accuracy and possible numerical instabilities and compare results.

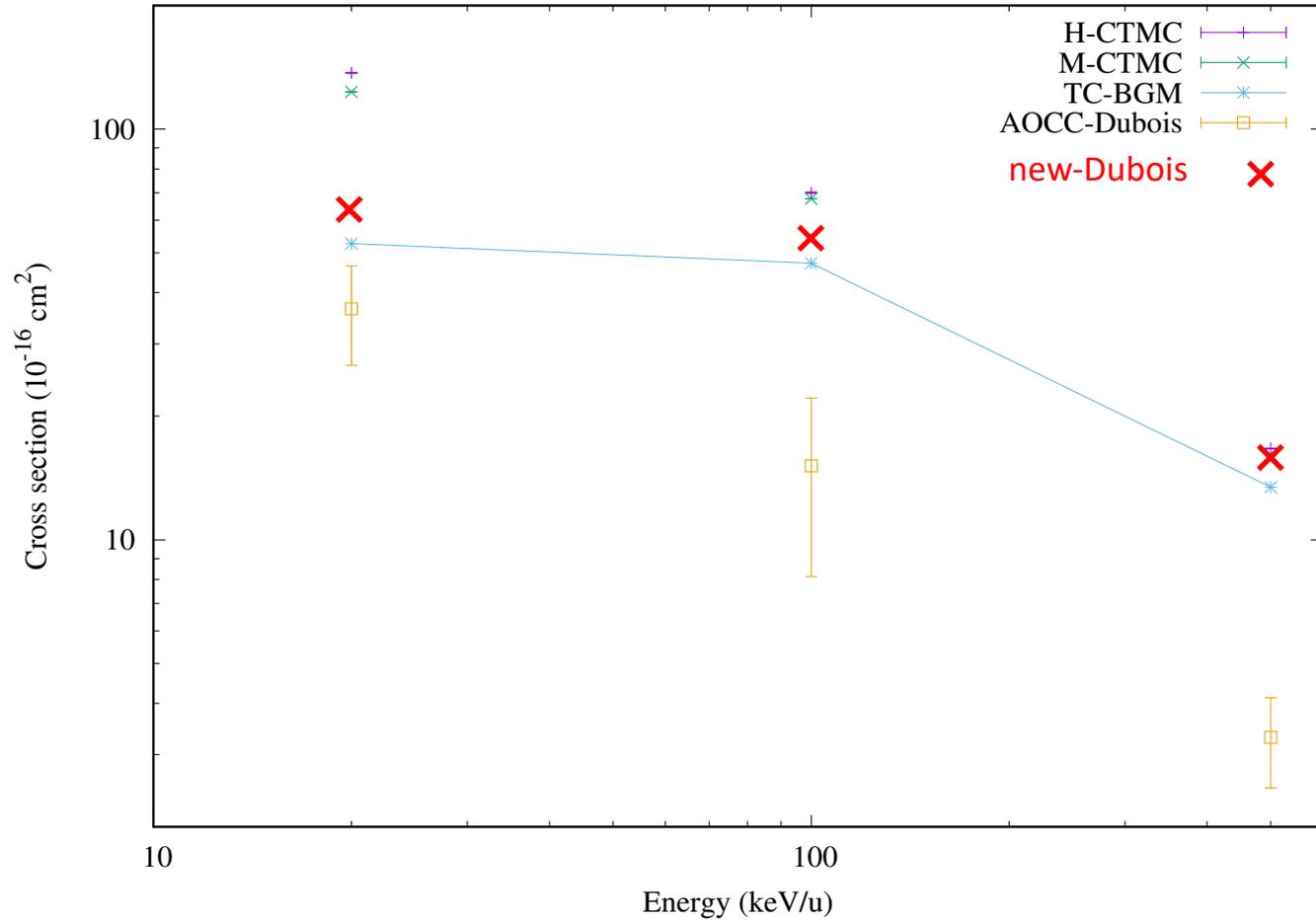
# Capture



# Excitation



# Ionisation



# About convergence ... from calculations using 5 basis sets

- S : 102 GTOs (20 s + 14\*3 p + 8\*5 d) on each center  
38+32 (0<E<4) = 70 states on T  
53+9 (0<E<4) = 62 states on P
- Sf : 144 GTOs (as S + 6\*7 f) on each center  
55+60 (0<E<4) = 105 states on T  
81+23 (0<E<4) = 104 states on P
- B : 153 GTOs (30 s + 21\*3 p + 12\*5 d) on each center  
48+49 (0<E<4) = 97 states on T  
63+27 (0<E<4) = 90 states on P
- Bf : 216 GTOs (as B + 9\*7 f) on each center  
62+84 (0<E<4) = 146 states on T  
98+48 (0<E<4) = 146 states on P
- Ng : 207 GTOs (24 s + 18\*3 p + 12\*5 d + 6\*7 f + 3\*9 g) on each center  
89+75 (0<E<3) = 164 states on T  
69+34 (0<E<4) = 123 states on P

e.g. energies on H

1s=	-0.50000	-0.5
2s=	-0.12500	-0.125
2p=	-0.12499	-0.125
3s=	-0.05553	-0.05555
3p=	-0.05552	-0.05555
3d=	-0.05555	-0.05555
4s=	-0.03108	-0.03125
4p=	-0.03110	-0.03125
4d=	-0.03105	-0.03125
4f=	-0.03124	-0.03125
5s=	-0.01853	-0.02
5p=	-0.01956	-0.02
5d=	-0.01906	-0.02
5f=	-0.01996	-0.02
5g=	-0.01990	-0.02

# Total cross section (in $10^{-16} \text{ cm}^2$ ) comparison

E (keV/u)		CAPTURE	EXCITATION	IONISATION
20	S	1.74E+01	1.80E+02	2.52E+01
	Sf	3.39E+01	1.74E+02	5.53E+01
	B	1.38E+01	4.70E+01	3.86E+01
	Bf	2.45E+01	5.05E+01	4.97E+01
	Ng	5.62E+01	1.51E+02	6.44E+01
100	S	3.97E-01	1.10E+02	3.63E+01
	Sf	6.07E-01	9.15E+01	6.06E+01
	B	2.63E-01	5.50E+01	2.78E+01
	Bf	4.26E-01	4.43E+01	4.20E+01
	Ng	5.64E-01	9.89E+01	5.51E+01
500	S	8.50E-04	3.99E+01	1.42E+01
	Sf	9.26E-04	3.83E+01	1.84E+01
	B	7.13E-04	2.26E+01	9.55E+00
	Bf	7.16E-04	2.25E+01	1.21E+01
	Ng	1.94E-03	4.09E+01	1.59E+01

The study of collisions involving initial excited states is a challenge:

- creation of large basis sets with very diffuse states,
- long calculations, even for 1-electron systems,
- convergence check is a real issue

Therefore to extend these calculations to very excited states (e.g.  $n=5-10$ ) would be very complex but scalings can be created using the comparison between "easy » classical (CTMC) and semiclassical close coupling calculations, see for example JPB 51, 235202 (2018) and also ADND Tables 129, 101281 (2019)