Basis Generator Method Calculations for Ion-Atom Collisions of Indirect and Direct Relevance to Neutral Beams in Fusion Plasmas

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redefine THE POSSIBLE.

Two (not so) easy pieces

Lyman line ratios in charge-exchange collisions of C^{6+} and O^{8+} ions with hydrogen and krypton atoms

Phys. Rev. A **97**, *062705 (2018)*

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Target excitation, electron capture, and ionization in p-H($n = 2$) collisions

(work in progress)

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Outline

1. Intro ✓
2. Theory : brief recap of treatment of few-electron problem and two-center basis generator method (TC-BGM)
3. Study #1: collisions with hydrogen vs. krypton atoms
4. Study #2: collisions with excited hydrogen atoms
5. Summary and outlook

2. **Theory**: the few-electron problem and the TC-BGM

Few-electron problem I

- Explicit solution is hard
- Ansatz (independent electrons – IEM):

$$\hat{H}_e(t) \;\rightarrow\; \sum_{j=1}^{N} \hat{h}_j(t), \quad i\partial_t \psi_j(\boldsymbol{r},t) = \hat{h}(t)\psi_j(\boldsymbol{r},t)$$

$$\hat{h}(t) \;=\; -\frac{1}{2}\Delta - \frac{Z_T}{r} - \frac{Z_p}{|\boldsymbol{r} - \boldsymbol{R}(t)|} + v_{ee}(\boldsymbol{r},t)$$

- Choice of v_{ee} defines model
- Time-dependent density functional theory (TDDFT) provides foundation

Few-electron problem II

Choices:

$$\begin{aligned}
v_{ee}(\boldsymbol{r}, t) &= v_{ee}^{0}(r) && \text{no response} \\
v_{ee}(\boldsymbol{r}, t) &= f(t) v_{ee}^{0}(r) && \text{global target response}^{*} \\
(v_{ee}(\boldsymbol{r}, t) &= v_{ee}[\psi_j](\boldsymbol{r}, t) && \text{microscopic response})
\end{aligned}$$

- TC-BGM can be used within IEM
- Model uncertainties (IEM) $\leftrightarrow$ numerical uncertainties (convergence etc.)

[*] Kirchner *et al.*, PRA 2000

Few-electron problem III

Single-particle solutions → many-electron info

- Option 1: IEM (multinomial) analysis
  e.g. single and double capture for $N = 2$:

$$\begin{aligned} P_1 &= 2p_{\mathrm{cap}}(1 - p_{\mathrm{cap}}) \\ P_2 &= p_{\mathrm{cap}}^2 \end{aligned}$$

- Option 2: determinants (density matrices)*
- Further options: correlation integrals**, single-active electron model, ...

analysis = source of model uncertainties

*Lüdde and Dreizler, JPB 1985; **Baxter and TK, PRA 2016

Two-Center Basis Generator Method

Expansion (of single-particle solutions) in dynamically adapted model space

- Start with bound target and projectile states

$$\phi_v^0(\mathbf{r}) = \begin{cases} \phi_v(\mathbf{r}_t) \exp(i\mathbf{v}_t\mathbf{r}) & \textit{if } v \leq V_t \\ \phi_v(\mathbf{r}_p) \exp(i\mathbf{v}_p\mathbf{r}) & \text{else} \end{cases}$$

- Add pseudo states

$$\chi_v^\mu(\mathbf{r}, t) = [W_p(t)]^\mu \phi_v^0(\mathbf{r}) \quad v = 1, \ldots, V_t$$

- Expand

$$|\psi_i(t)\rangle = \sum_{v,\mu} c_{v,\mu}^i(t) |\chi_v^\mu(t)\rangle$$

- TC-BGM = TCAO + (special) pseudo states

3. Study #1: collisions with hydrogen vs. krypton atoms

Objective: Lyman-line emissions

- Radiative transitions of one electron in excited projectile state
- Consider pure single capture and autoionizating double capture[1]
- Solve rate equations

$$\frac{dN_p(t)}{dt} = \sum_{i=p+1}^{m} N_i(t) A_{i\to p} - N_p(t) \sum_{f=1}^{p-1} A_{p\to f}$$

- Total photon counts

$$(\mathrm{counts})_{nl\to n'l'} = A^{\mathrm{rad}}_{nl\to n'l'} \int_0^\infty N_{nl}(t)\,dt$$

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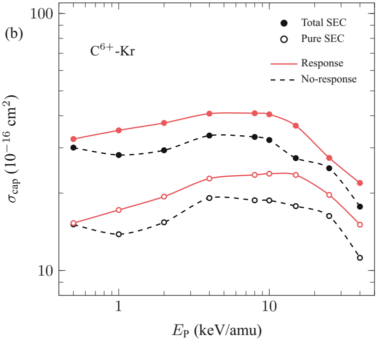
[1] Auger rates calculated with RATIP by S. Fritzsche (2001)

Some basis parameters

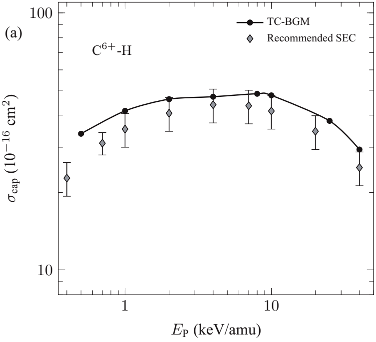
- Projectile states: $n = 1, \ldots, 7$ $(\sum = 84)$
- Target states
  - hydrogen: *KLMN* shell states $(\sum = 20)$
  - krypton: *MNO* shell states $(\sum = 31)$
- BGM pseudo states
  - hydrogen: up to 52
  - krypton: up to 66

C^{6+}-impact: total capture

krypton



hydrogen

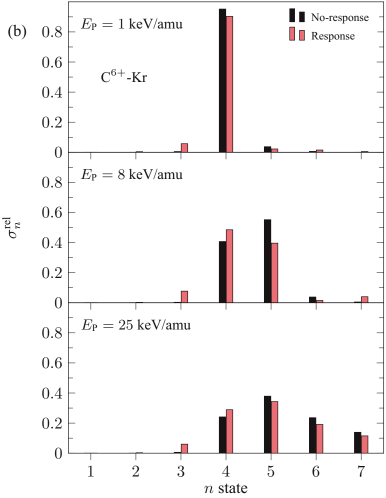


Recommended values: Janev *et al.*, ADNDT 1988

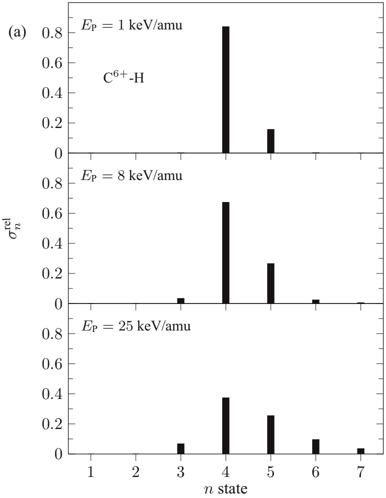
Leung and Kirchner, PRA **97**, 062705 (2018)

C^{6+}-impact: n-state distributions

krypton



hydrogen



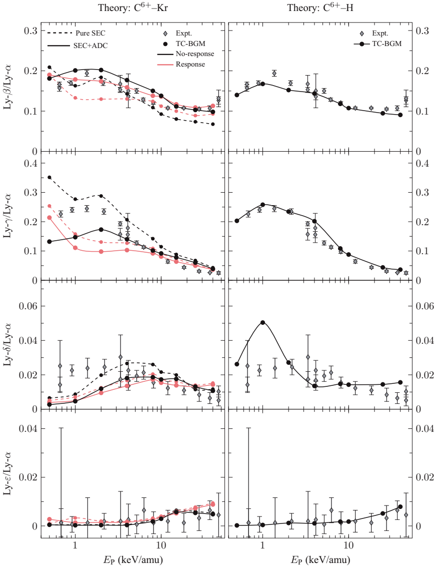
C^{6+}-impact: Lyman-emission ratios

$\frac{3p \rightarrow 1s}{2p \rightarrow 1s}$

$\frac{4p \rightarrow 1s}{2p \rightarrow 1s}$

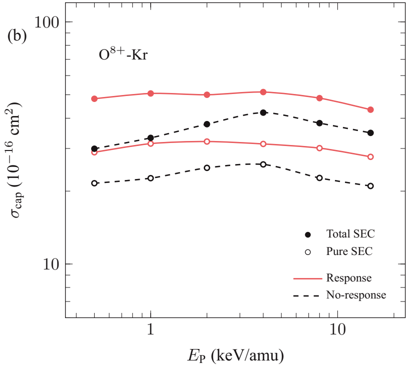
$\frac{5p \rightarrow 1s}{2p \rightarrow 1s}$

$\frac{6p \rightarrow 1s}{2p \rightarrow 1s}$

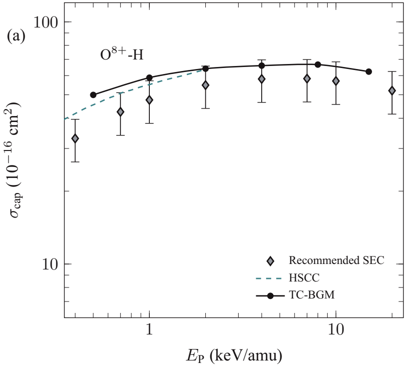


O^{8+}-impact: total capture

krypton



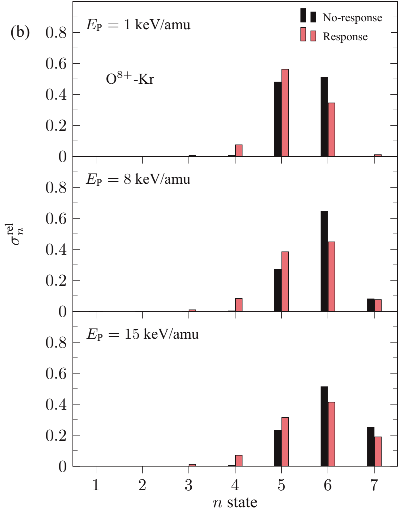
hydrogen



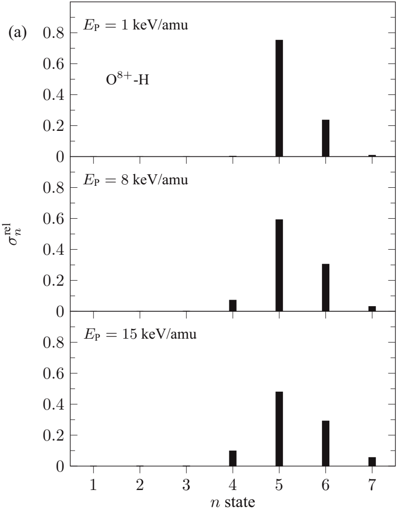
Rec.: Janev *et al.*, ADNDT 1988; HSCC: Lee *et al.*, PRA 2004
Leung and Kirchner, PRA **97**, 062705 (2018)

O^{8+}-impact: n-state distributions

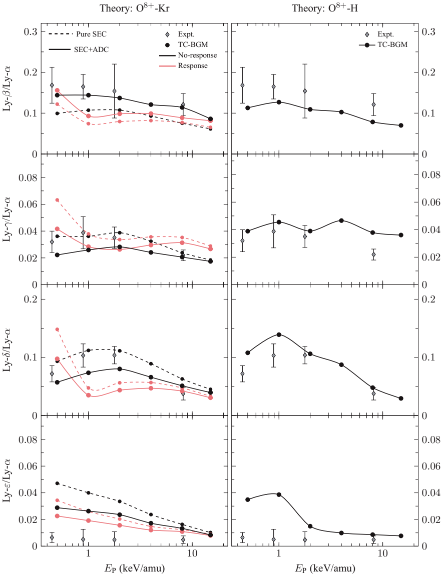
krypton



hydrogen



O^{8+}-impact: Lyman-emission ratios



3p -> 1s
2p -> 1s

4p -> 1s
2p -> 1s

5p -> 1s
2p -> 1s

6p -> 1s
2p -> 1s

4. **Study #2**: collisions with excited hydrogen atoms

Some basis parameters

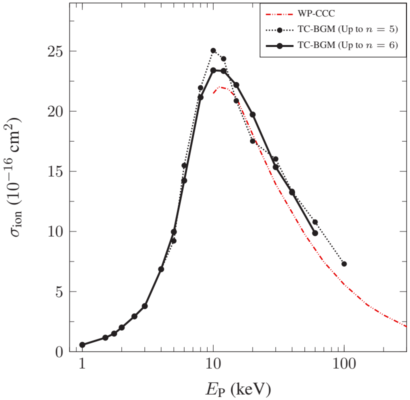
- Projectile states: $n = 1, \ldots, 6$ ($\sum = 56$)
- Target states
    - n=5 basis: *KLMNO* shell states ($\sum = 35$)
    - n=6 basis: *KLMNOP* shell states ($\sum = 56$)
- BGM pseudo states
    - n=5 basis: up to 94
    - n=6 basis: up to 106

Compare results for p-H(2s) with:

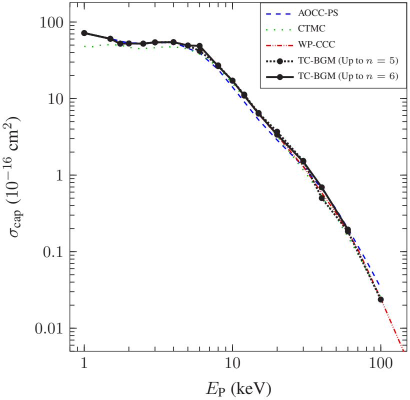
Abdurakhmanov *et al.*, Plasma Phys. Control. Fusion **60**, 095009 (2018)
Pindzola *et al.*, Phys. Rev. A **72**, 062703 (2005)
(see also Taouitioui et al., J. Phys. B 51, 235202 (2018))

p-H(2s): total ionization and capture

ionization



capture



WP-CCC: Abdurakhmanov *et al.*, Plasma Phys. Control. Fusion 2018

AOCC-PS and CTMC: Pindzola *et al.*, Phys. Rev. A 2005

Summary and outlook

(TC)-BGM: coupled-channel method within semiclassical approximation

Hydrogen vs krypton targets

- Krypton is not a good surrogate for hydrogen
- Need a better response model for more reliable/accurate Kr calculations

Excited hydrogen targets

- Higher demands on basis sets and sizes
- Overall good agreement with WP-CCC
- Move on to H($2p$)