Basis Generator Method Calculations for Ion-Atom Collisions of Relevance to Neutral Beams in Fusion Plasmas: Short Summary (May 2022)

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Outline

1. The two-center basis generator method (TC-BGM) for orbital propagation in ion-atom collision systems

2. Stuff we have done

3. Things we have learned

4. What's next?

Two-Center Basis Generator Method

Solve (effective) one-electron collision problem within semiclassical approximation with straight-line trajectory $\mathbf{R}(t) = (b, 0, vt)$

$$i\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

$$\hat{H}(t) = -\frac{1}{2}\nabla^2 + V_t(r_t) + V_p(r_p = |\mathbf{r}_t - \mathbf{R}|)$$

with standard basis-expansion ansatz

$$|\psi(t)\rangle = \sum_{k=0}^{K} c_k(t)|\chi_k\rangle$$

and non-standard set of states $\{|\chi_k\rangle\}$

Two-Center Basis Generator Method

Idea: use dynamically adapted states

- Start with bound target and projectile states

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

- Add pseudo states

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

- TC-BGM = TCAO + (special) pseudo states for quasimolecular couplings and transitions into continuum

Zapukhlyak et al. J. Phys. B 2005

2. Problems we have addressed

Systems studied

- p-H(1s,2s,2p) at 1–300 keV/amu

  Leung and Kirchner, Eur. Phys. J. D **73**, 246 (2019)
- C^{6+}, O^{8+}-H (Kr) at a few keV/amu

  Leung and Kirchner, Phys. Rev. A **97**, 062705 (2018)
- Ne^{8+}-He, H_2 at a few keV/amu

  Leung and Kirchner, Atoms **7**, 15 (2019)
- Be^{4+}-H(1s,2s,2p) at 20, 100, 500 keV/amu

  (CCW activity, unpublished)
- Li^{3+}, C^{3+}, O^{3+}-H at 1–100 keV/amu

  Leung and Kirchner, Atoms **10**, 11 (2022)

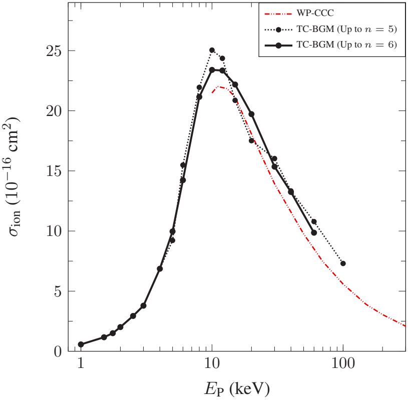
Processes calculated

- Capture, excitation, and ionization (total) cross sections
- In some cases: Lyman-line emissions (after capture) $\rightarrow$ solve rate equations

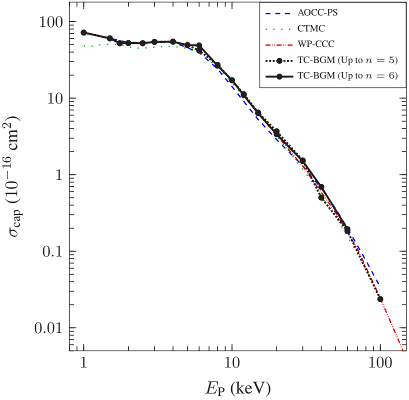
3. Things we have learned

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

ionization



capture

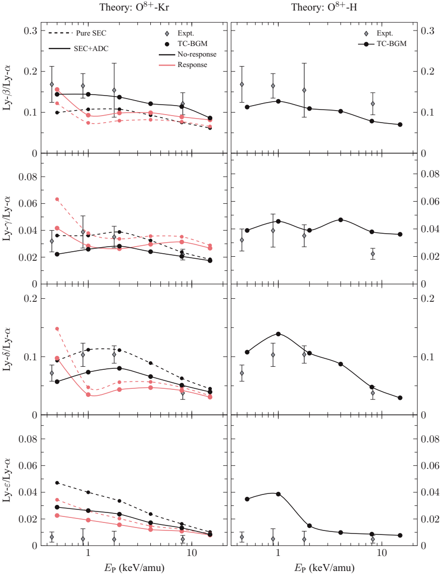


WP-CCC: Abdurakhmanov *et al.*, Plasma Phys. Control. Fusion 2018
AOCC-PS and CTMC: Pindzola *et al.*, Phys. Rev. A 2005

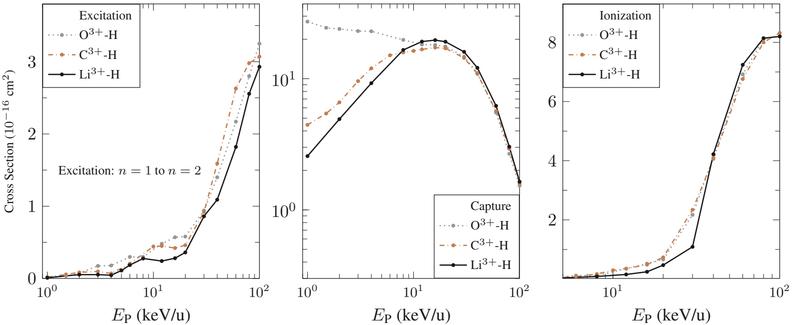
Be^{4+}-H

- Set-up straightforward, but achieving convergence challenging
- Some success for $H(1s)$ and $H(2s)$ initial states
- Basis parameters:
  - Projectile states: $n = 1, \ldots, 10$
  - Target states: $n = 1, \ldots, 5$
  - ~ 50 BGM pseudo states
- Higher n projectile states required for $H(2p)$ initial states

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



Ion^{3+}-H: comparisons



4. What’s next?

Let’s discuss ...