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

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Two (not so) easy pieces

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


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

(work in progress)
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):

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

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

- Choice of \( v_{ee} \) defines model
- Time-dependent density functional theory (TDDFT) provides foundation
Few-electron problem II

Choices:

\[ v_{ee}(r, t) = v_{ee}^0(r) \] no response
\[ v_{ee}(r, t) = f(t)v_{ee}^0(r) \] global target response
\[ v_{ee}(r, t) = v_{ee}[\psi_j](r, t) \] microscopic response

- TC-BGM can be used within IEM
- Model uncertainties (IEM) ↔ 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 $N = 2$:
  \[
  P_1 = 2p_{\text{cap}}(1 - p_{\text{cap}}) \\
  P_2 = p_{\text{cap}}^2
  \]

- **Option 2**: determinants (density matrices)*

- **Further options**: correlation integrals**, single-active electron model, ...

  analysis = source of model uncertainties

* Lüdде 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
  \[ \phi^0_v(r) = \begin{cases} \phi_v(r_t) \exp(i v t r) & \text{if } v \leq V_t \\ \phi_v(r_p) \exp(i v p r) & \text{else} \end{cases} \]
- Add pseudo states
  \[ \chi^\mu_v(r, t) = [W_p(t)]^\mu \phi^0_v(r) \quad \nu = 1, \ldots, V_t \]
- Expand
  \[ |\psi_i(t)\rangle = \sum_{\nu, \mu} c^i_{\nu, \mu}(t) |\chi^\mu_v(t)\rangle \]
- 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

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

- Total photon counts

\[
\text{(counts)}_{nl\rightarrow n'l'} = A_{nl\rightarrow n'l'}^{\text{rad}} \int_{0}^{\infty} N_{nl}(t)dt
\]

\(^1\)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
$^{6+}$-impact: total capture

krypton

hydrogen

Recommended values: Janev et al., ADNDT 1988
Leung and Kirchner, PRA 97, 062705 (2018)
$\text{C}^{6+}$-impact: n-state distributions

**Krypton**

- $E_p = 1\text{ keV/amu}$
- $E_p = 8\text{ keV/amu}$
- $E_p = 25\text{ keV/amu}$

**Hydrogen**

- $E_p = 1\text{ keV/amu}$
- $E_p = 8\text{ keV/amu}$
- $E_p = 25\text{ keV/amu}$
$C^6+ -$impact: Lyman-emission ratios

$3p \rightarrow 1s$

$2p \rightarrow 1s$

$4p \rightarrow 1s$

$2p \rightarrow 1s$

$5p \rightarrow 1s$

$2p \rightarrow 1s$

$6p \rightarrow 1s$

$2p \rightarrow 1s$
**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)
\( {\text{O}}^{8+} \)-impact: \( n \)-state distributions

**krypton**

\[ E_p = 1 \text{ keV/amu} \]

\[ E_p = 8 \text{ keV/amu} \]

\[ E_p = 15 \text{ keV/amu} \]

**hydrogen**

\[ E_p = 1 \text{ keV/amu} \]

\[ E_p = 8 \text{ keV/amu} \]

\[ E_p = 15 \text{ keV/amu} \]
**O$^{8+}$-impact: Lyman-emission ratios**

\[
\begin{align*}
\frac{3\,p \rightarrow 1\,s}{2\,p \rightarrow 1\,s} \\
\frac{4\,p \rightarrow 1\,s}{2\,p \rightarrow 1\,s} \\
\frac{5\,p \rightarrow 1\,s}{2\,p \rightarrow 1\,s} \\
\frac{6\,p \rightarrow 1\,s}{2\,p \rightarrow 1\,s}
\end{align*}
\]
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:

(see also Taouitiani 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
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 $\text{H}(2p)$