Ionization, total and state selective charge exchange cross sections in fusion related collision systems

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The aim

BES diagnostics

- **Active** plasma diagnostics procedure
- Use of H-type of atoms such as D,Li,Na. (which posses **one valence electron**)
  - Heating beams (H, D)
  - Diagnostic beams (Li, Na)
- Purpose: **density** and **fluctuation** meas.
  - Fluct. timescale: 10 – 200kHz
  - Fluct. spatial scale: 1 – 4 cm
Outlook

Basic idea – Classical treatments

Theory
Classical Trajectory Monte Carlo (CTMC) model
Quasi-Classical Trajectory Monte Carlo (QCTMC) model

Results
1. Data for Atomic Processes of Neutral Beams in Fusion Plasma
   Be\(^{4+}\) + H(1s) collisions
   H + H type collisions
2. Injected Impurities
   Li\(^+\) + He, Li\(^+\) N

Summary
Approximations: CTMC simulations

Flow diagram for a MC simulation:

- **Initial distribution**
  - randomly select representative ensemble of "test particles"

- Propagate particles according to Newton eq. (or Langevin eq)

- Analyze the end points of trajectories

- **Final distribution**
Ionization in ion-atom collisions

Description:

Distorted wave approximations

Non-perturbative models:
Classical Trajectory Monte Carlo (CTMC) method
3-body CTMC approach

- Classical nonperturbative method – „theoretical experiment”
- Treats the many-body interactions

Model potential:

\[ V(r) = -\frac{(Z-1)\Omega(r) + 1}{r}, \quad \text{where} \quad \Omega(r) = \left[Hd(e^{r/d} - 1) + 1\right]^{-1} \]

- Screened core potentials for both partners (analytic GSZ model pot.)
- Strategies for extracting the relevant information
  - a three-body balance is bound by \( E \) and \( p \) conservation;
  - final-state kinematics does not provide information about the mechanism
**CTMC approach**

- Classical nonperturbative method
  - „theoretical experiment“
- Treats the many-body interactions

\[
L = L_K - L_V
\]

\[
L_K = \frac{1}{2} m_p \hat{r}_p^2 + \frac{1}{2} m_e \hat{r}_e^2 + \frac{1}{2} m_T \hat{r}_T^2
\]

\[
L_V = \frac{Z_p (|\hat{r}_P - \hat{r}_e|) Z_e}{|\hat{r}_P - \hat{r}_e|} + \frac{Z_p (|\hat{r}_P - \hat{r}_T|) Z_T (|\hat{r}_P - \hat{r}_T|)}{|\hat{r}_P - \hat{r}_T|} + \frac{Z_e Z_T (|\hat{r}_e - \hat{r}_T|)}{|\hat{r}_e - \hat{r}_T|}
\]
The total cross sections

\[ \sigma = \frac{2\pi b_{\text{max}}}{T_N} \sum_j b_j^{(i)} \]

The statistical uncertainty

\[ \Delta \sigma = \sigma \left( \frac{T_N - \overline{T_N}^{(i)}}{T_N \overline{T_N}^{(i)}} \right)^{1/2} \]

\( T_N \): Total number of trajectories calculated for impact parameters less than \( b_{\text{max}} \)

\( T_N^{(i)} \): Number of trajectories that satisfy the criteria for a given channel

\( b_j^{(i)} \): Actual impact parameter for the trajectory corresponding to the channels.
Classical Limits - extension
Improvement of the classical description of the one electron atomic system by including a model potential in the Hamiltonian of the system mimicking quantum features.

**Quasi-Classical Trajectory Monte Carlo (QCTMC) Model**

\[ H_{QCTMC} = T + V_{coul} + V_H \]

\[ V_H = \sum_{n=a,b} \sum_{i=1}^{N} f(r_{ni}, p_{ni}; \xi_H, \alpha_H) \]

\[ f(r_{\lambda\nu}, p_{\lambda\nu}; \xi, \alpha) = \frac{\xi}{4\alpha r_{\lambda\nu}^2 \mu_{\lambda\nu}} \exp\left\{ \alpha \left[ 1 - \left( \frac{r_{\lambda\nu} p_{\lambda\nu}}{\xi} \right)^4 \right] \right\} \]
Hamiltonian of hydrogen atom is defined as follows:

\[ H = \frac{p^2}{2} - \frac{1}{r} + \left[ \frac{\xi_H^2}{4\alpha_H r^2} \right] \exp \left\{ \alpha_H \left[ 1 - \left( \frac{rp}{\xi_H} \right)^4 \right] \right\} \]

In the ground or lowest-energy configuration, we require \( \frac{\partial H}{\partial p} = 0 \) and \( \frac{\partial H}{\partial r} = 0 \)

\[ E = -\frac{1}{2\xi_H^2 \left( 1 + \frac{1}{2\alpha_H} \right)} \]

Electron binding energy = 0.5
Initial conditions for $r$ and $p$

- In CTMC model, the initial conditions in $r$ and $p$:

A microcanonical ensemble characterizes the initial state of the target constrained to an initial binding energy of the given shell:

$$
\rho_{E_0}(\tilde{A}, \dot{\tilde{A}}) = K_1 \delta(E_0 - E) = \delta\left( E_0 - \frac{1}{2} \mu_{te} \dot{\tilde{A}}^2 - V(\tilde{A}) \right)
$$

$$
\begin{align*}
  r_0 &= \frac{|Z_e Z_T|}{2E_b} \\
  p_0 &= \sqrt{2|E_b| \mu_{te}}
\end{align*}
$$

- In QCTMC model, we considered two conditions that $r$ and $p$ have to satisfy them as follows:

$$
\begin{align*}
  \frac{|Z_e Z_T|}{2r} + f_H(r, p) &< 0.5 \\
  \frac{p^2}{2\mu_{Te}} - \frac{1}{r} + f_H(r, p) &\approx -0.5
\end{align*}
$$
\[ F(r, p) = \frac{p^2}{2\mu_T e} - \frac{1}{r} + f_H(r, p) + 0.5 \]
Projectile-centered Scheme

\[ \text{Be}^{3+} \]

Attractive Coulomb Force

Repulsive Heisenberg Force

\begin{align*}
\sigma (\text{cm}^2) \\
1 \times 10^{-22} & \quad 1 \times 10^{-21} & \quad 1 \times 10^{-20} & \quad 1 \times 10^{-19} & \quad 1 \times 10^{-18} & \quad 1 \times 10^{-17} & \quad 1 \times 10^{-16} \\
\text{Energy (keV/amu)} & \quad 1 & \quad 10 & \quad 100 & \quad 1000
\end{align*}

Present CTMC results
Present QCTMC results
Target-centered scheme

$\text{Be}^{3+}$

Attractive Coulomb Force

H$^+$

Repulsive Heisenberg Force

$\sigma \text{ (cm}^2\text{)}$

Energy (keV/amu)

$nl = 48$

Present CTMC results

Present QCTMC results


Combined one; i.e., target and projectile-centered scheme
Finding Best Combination of $\alpha$, $\xi$

Interaction between $H^+$ and Hydrogen atom

Total Electron Capture
$H^+ + H(1s) \rightarrow H + H^+$

- QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$)
- QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$)
- QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$)
- QCTMC ($\alpha_H = 4.5$, $\xi_H = 0.9486$)
- QCTMC ($\alpha_H = 5$, $\xi_H = 0.9534$)
- CTMC
- QTMC-EB
- Exp: McClure
Ionization
\[ \text{H}^+ + \text{H}(1s) \rightarrow \text{H}^+ + \text{H}^+ + e^- \]

Exitation
\[ \text{H}^+ + \text{H}(1s) \rightarrow \text{H}^+ + \text{H}(2p)^* \]
QCTMC Radial & Momentum Distribution

(a) Radial Distribution

(b) Momentum Distribution

CTMC Distribution
Quantum Distribution
Data for Atomic Processes of Neutral Beams in Fusion Plasma
Ionization

\[ \text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{4+} + \text{H}^+ + e^- \]

Total Electron Capture

\[ \text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{3+}(nl) + \text{H}^+ \]
Excitation
Be$^{4+}$ + H(1s) $\rightarrow$ Be$^{4+}$ + H(2s)*

Excitation
Be$^{4+}$ + H(1s) $\rightarrow$ Be$^{4+}$ + H(2p)*
Electron capture cross sections into $n = 3, 4, 5, 6, 8, 10$ and $nl = 3l, 4l, 5l$ states of the projectile in Be$^{4+} + H(1s)$ using CTMC and QCTMC models.
State-selective Electron Capture
Be$^{4+}$ + H(1s) \rightarrow Be^{3+}(n) + H^+$

$\sigma$ (cm$^2$)

Energy (keV/amu)

$n = 3$

$n = 4$

$n = 5$
State-selective Electron Capture

$\text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{3+}(3l) + \text{H}^+$

![Graphs showing cross-sections for different states](image_url)
State-selective Electron Capture

$\text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{3+}(4l) + \text{H}^+$

$\sigma$ (cm$^2$) vs. Energy (keV/amu)

Present CTMC results
Present QCTMC results
AOCC (Fritsch)
MOCC (Harel)
QEDM (Errea)
BCCIS (Das)
$\text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{3+}(5l) + \text{H}^+$
C^{6+} + H(1s) → C^{5+}(n) + H^+

N^{7+} + H(1s) → N^{6+}(n) + H^+

Present CTMC results

Present QCTMC results


Two ground-state Hydrogen collision System
QCTMC Result: Projectile Ionization cross section

\[ H(1s)_P + H(1s)_T \rightarrow H_P^+ + H(1s)_T + e^- \]

The first possible one the *direct ionization of the projectile* channel. This channel originates from a one-step process

\[ (H^+_p, e^-_p) + (H^+_T, e^-_T) \rightarrow H^+_p + (H^+_T, e^-_T) + e^-_p \]

The second possible originates from the multi-electron interaction in a two-step process producing the same final particles.

\[ (H^+_p, e^-_p) + (H^+_T, e^-_T) \rightarrow H^+_p + (H^+_T, e^-_p) + e^-_T \]
Projectile ionization cross sections

\[ \sigma (\text{cm}^2) \]

- 2.0e-17
- 4.0e-17
- 6.0e-17
- 8.0e-17
- 1.0e-16
- 1.2e-16
- 1.4e-16

4-body QCTMC

Exp.data “McClure”

4-body CTMC

Exp.data “Wittkower et al”
Carbon ions \((c^{5+})\) with Hydrogen atom collision system

- Target ionization cross section

\[
c^{5+} + H \rightarrow c^{5+} + H^+ + e^- \quad (1)
\]

- Electron capture cross section

\[
c^{5+} + H \rightarrow c^{4+} + H^+ \quad (2)
\]
Target Ionization cross-section

(a) 4-body QCTMC

(b) Reduced 4-body QCTMC

3-body CTMC “R K Janev et al”

4-body CTMC

Reduced 4-body CTMC
Electron Capture Cross-Section of the Projectile

Energy (eV/amu)

$\sigma$ (cm$^2$)

- 3-body CTMC
- "R.K. Janev et al"

- Perturbed stationary-state (PSS) “E. J. Shipsey et al”

- Exp.data
- “Crandall et al”

- 4-body CTMC

- 4-body QCTMC
Publications

Be-H


H+H type

Atomic Data
for Injected Impurities in Fusion Plasmas
Total cross sections of the single-electron capture from $He(1s)$ by $Li^+$
Total cross sections of the single-electron capture from $N(2p)$ by $Li^+$
Total cross sections of the single-electron ionisation from $^{4}\text{He}(1s)$ by $^{6}\text{Li}^+$

Total cross sections of the single-electron ionisation from $^{14}\text{N}(2p)$ by $^{6}\text{Li}^+$
Conclusions

• Classical method (CTMC) reproduce different experiments for collisions between charged particles and atoms
• gives accurate cross sections for ionization, capture, excitation
• valid in wide projectile energy range
• can describe partial cross sections
• QCTMC model, represents one step further towards a better description of the classical atomic collisions. This model with simplicity can time efficiently carry out simulations where maybe the quantum mechanical ones become complicated, therefore, our model should be an alternative way to calculate accurate cross sections and maybe can replace the quantum-mechanical methods.
Thanks for your attention!