H- and He-like X-ray emission due to charge exchange

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PREVIOUSLY UNDER THE DIRECTION OF
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Outline

Charge eXchange (CX): The basics

Why do we care? (CX in astrophysics)

Producing a CX theoretical spectrum:
  ◦ Cross sections
  ◦ Radiative Cascade

Theoretical Spectra
  ◦ Interesting features: Energy & Neutral target

How do we trust the theory?
  ◦ Benchmarking to experiments

CX Model
  ◦ Applications

Summary
Charge Exchange Process

Ionized Plasma

 Ion

 v

Neutral

Neutral Gas

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Charge Exchange Process
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While single electron capture is significant for H-like and He-like system, multi electron capture (2 or more electrons are transferred) can be important for collision systems with more than one electron.
Astrophysical environments for CX

• Comae of comets (Bodewits et al. 2007, Mullen et al. 2017)
• Planetary atmospheres (Dennerl et al. 2006, Bhardwaj et al. 2007, +)
• Earth’s exosphere (Freyberg 1998, Snowden et al. 2004)
• Heliosphere (Cravens 2000, Cravens et al. 2001)

• Filaments in Perseus cluster? (Walker et al. 2015, Gu et al 2017)
• 3.5 keV line? (Gu et al. 2015)
• Rim of supernova remnants? (Katsuda et al. 2011, Cumbee et al. 2014)
• Starburst galaxies? (Zhang et al. 2014)
First X-ray image of Mars

Comet Hyakutake

From Dennerl, 2002

From Liu et al., 2012

From Cravens, 2002
CX Emission vs Thermal Emission

• X-ray emission from charge exchange produces a very distinct spectrum compared to thermal emission.
• With high resolution spectra, it is plausible to disentangle CX from thermal emission!

\[ Ne^{10+} + H \rightarrow Ne^{9+} + H^+ \]

\[ O^{7+} + H \rightarrow O^{6+} + H^+ \]
Charge Exchange Theory

Two steps are required to produce charge exchange X-ray emission spectrum:

1) Calculate cross-section (Not easy!)

2) Radiative cascade (easier!)
Charge Exchange Cross Section ($\sigma$)

The *probability* of an electron to transfer from the neutral atom into a specific excited state ($n, l, S$) of the ion.

For charge exchange calculations:
- $\sigma$ depends on the
  - $n$ (principle quantum number)
  - $l$ (orbital angular momentum quantum number)
  - $S$ (spin quantum number)
  - $v$ (collision velocity)
- $\sigma_{nls}(v)$ is required to produce reliable theoretical CX X-ray emission spectra

"Effective area" that quantifies the likelihood of a scattering event to occur.
Ne$^{10+}$ + H $\rightarrow$ Ne$^{9+}$+H +

Cross Sections

Recommended Cross-sections for the n=6 quantum levels

- Multi-channel Landau-Zener
  - Statistical $l$-distribution
  - Low energy $l$-distribution

Classical Trajectory Monte Carlo

Atomic Orbital Close Coupling

Quantum Mechanical Molecular orbital Close Coupling

All available cross-sections for H-like and He-like CX collisions are implemented in Kronos Database

Cumbee et al. 2016

Accuracy & difficulty:

Collisional Energy (eV/u)
Radiative Cascade

To produce theoretical CX X-ray emission spectra, these $n$ and $l$ levels are given an initial population that is directly proportional to the cross-section $\sigma_{nl}$ for that given state.

\[ \text{i.e. } \text{Population}_{2s} \propto \sigma_{2s} \]

The electron then transitions to a lower energy level, obeying quantum mechanical selection rules,

\[ \Delta l = \pm 1, \]

until it reaches the ground state

Photons are emitted
Radiative Cascade

\[
C^6 + H \rightarrow C^5 + H^+
\]

1 keV/u (435 km/s)

MCLZ Low-energy l-distribution

\[\text{Ly } \gamma\]

\[4p - 1s\]
Radiative Cascade

\[ C^{6+} + H \rightarrow C^{5+} + H^+ \]

1 keV/u (435 km/s)

MCLZ Low-energy l-distribution

\[ 3p - 1s \]

cascades of transitions
The $2p-1s$ transition is dominant due to the cascade from higher excited states (3s, 3d, 4s, 4d, 4f).
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CX as a diagnostic

CX is highly dependent on:
- Ion stage ($O^{8+}, O^{7+}$)
- Neutral target ($H, He, CO_2$)
- Velocity of the collision
CX as a diagnostic

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EBIT: Electron beam ion trap (experiment) at LLNL

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CX as a diagnostic

CX is highly dependent on:

- Ion stage (O$^{8+}$, O$^{7+}$)
- Neutral target (H, He, CO$_2$)
- Velocity of the collision

EBIT: Electron beam ion trap (experiment) at LLNL
CX as a diagnostic: Ionization stage

CX is highly dependent on:
- Ion stage (O^{8+}, O^{7+})
- Neutral target (H, He, CO_2)
- Velocity of the collision

![Diagram showing photon energy distribution and relative intensity for Ne^{9+} + H and Ne^{10+} + H.](image-url)
CX as a diagnostic: Hardness Ratios ($H_2$)

CX is highly dependent on:
- Ion stage ($O^{8+}$, $O^{7+}$)
- Neutral target (H, He, CO$_2$)
- Velocity of the collision

$$H = \frac{Ly_\beta + Ly_\gamma + \cdots}{Ly_\alpha}$$

A. Miller, In Prep
Benchmarking Theory to Experiments

\[ \text{Ne}^{10+} + \text{He} \rightarrow \text{Ne}^{9+} + \text{He}^+ \]

\[ 4.5 \text{ KeV/u} \]

\[ \text{Ali et al. 2005} \]

\[ \text{C}_6^+ + \text{He} \rightarrow \text{C}_5^+ + \text{He}^+ \]

\[ \text{Defayet et al. (2013)} \]

\[ \text{C}_6^+ + \text{H}_2 \rightarrow \text{C}_5^+ + \text{H}_2^+ \]

\[ \text{Fogle et al. (2014)} \]
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Summary
Pure Charge eXchange Model: 8 collision velocities

Collision Energy: 200 eV/u

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Pure Charge eXchange Model: 8 collision velocities

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

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Pure Charge eXchange Model:
8 collision velocities

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Pure Charge eXchange Model: 8 collision velocities

Collision Energy: 700 eV/u

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Pure Charge eXchange Model: 8 collision velocities

Collision Energy: 1000 eV/u

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Pure Charge eXchange Model: 8 collision velocities

Methods:
- QMOCC
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- AOCC
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Neutrals:
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Collision Energy: 3000 eV/u

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- QMOCC
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- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Pure Charge eXchange Model: 8 collision velocities

Collision Energy: 5000 eV/u

Methods:
- QMOCC
- CTMC
- AOCC
- MCLZ

Neutrals:
- H
- He(10%)

Each spectrum is normalized to a relative intensity of 1

*relative abundance not considered
Charge eXchange Model: Cygnus Loop Supernova Remnant

XSPEC model of CX in Cygnus Loop

CX contribution in XSPEC model

$\chi^2 \approx 1.8 - 4$
CX Modeling

M82
Zhang et al. 2014

XMM-Newton
RGS

SPEX

Mullen et al., 2016

Liu et al. 2012

Line Ratio Direct Comparisons

\( \chi^2 \) vs Photon Energy (keV)

Counts s^{-1} keV^{-1}

Energy (keV)

Photon Energy (keV)
Limitations

- In comets, more ionization stages (other than H-like and He-like) are significant.
- Multi-electron capture, in which 2 or more electrons is transferred can be significant for collisions with neutrals with more than 1 electron.
- Current theory needs to be benchmarked to experiment for a variety of collision energies.
- MCLZ is relatively easy to calculate, but requires more approximations than QMOCC or AOCC.
Summary

Cross-sections are calculated for various ion-atom collisions

- H-like and He-like C, N, O, Ne, Mg, Al, and Si
- H and He targets
- 200-1000 km/s
- QMOCC, AOCC, CTMC, and MCLZ methods

CX model is applied to a region on the Northeast rim of the Cygnus Loop Supernova remnant

- Including all ions calculated and a fraction of 10% He
- For 8 energies

For a proper solar wind model

- More ionization stages (O$^{6+}$, etc)
  - In the works

All data available in Kronos Database

https://www.physast.uga.edu/research/stancil-group/atomic-molecular-databases/kronos

Google search: UGA Stancil Kronos

Zach Dorsey: Li-like CX
Liyi Gu: Astrophysical CX
Jason Terry: Double Electron Capture
Ruitan Zhang: Fully stripped ions
Mike Fogle: COLTRIMS measurements