Detailed Spectra Modeling in Low-Density Plasmas

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Plan

- Introduction
- EBIT modeling
  - M1 line in Kr XXIV and density diagnostics in tokamaks
  - Benchmarking Motional Stark Effect models in Alcator-C Mod
- Charge exchange stabilization modeling in zero-density plasmas
  - Single and double CX in O^6++H_2 and O^6++He
  - Monte-Carlo approach to multiple CX
- Conclusions

Low density plasmas: what’s so special for spectroscopy?..?

- Truly NLTE → quality of atomic data
- Non-statistical (non-Boltzmann) effects are very strong
- Forbidden transitions become prominent (especially in highly-charged ions)
- Effects of electromagnetic fields on populations and spectra are more distinct
- Other processes (e.g., charge exchange)

NIST EBIT: factory of highly-charged ions

- Many operate, a few under construction
- “Table-top” device
- Low electron density
  - N_e ~ 10^{11-12} cm^{-3}
- Monoenergetic electrons
  - E_{beam} = 0.1-30 keV
  - Width ~ 50 eV
- Localized volume
- Continuous operation
- (Almost) Any ion of any element
- Effective injection of metals and gases
- Spectroscopy: x-ray, EUV, UV, visible

EBIT: Kr XXII-Kr XXXIV spectra

- Krypton is important for fusion
- E_{beam} = 1.1-30 keV
- Six new lines identified, accuracy improved for twelve lines
- Low- and high-charged ions are present
- 30 keV is not enough to reach H-like Kr with IP=18 keV (charge exchange!)
- And there’s something else...

Al-like Kr: what’s wrong with the E1 lines?

A_a = 6.2\times10^{16} s^{-1}
A_b = 7.4\times10^{16} s^{-1}
A_c = 3.2\times10^{16} s^{-1}
Physical processes and modeling for EBIT

- Important
  - Radiative
  - Electron-impact excitation, sometimes deexcitation, ionization
  - Radiative recombination
  - Charge exchange
    - Relative velocity and density of neutrals are not well known
- Not so much...
  - Three-body recombination
  - Dielectronic recombination (may be accidentally important)

Atomic Data
- Relativistic Flexible Atomic Code (Gu, 2008)

Collisional-Radiative Model
- NOMAD (Ralchenko and Marot, 2001)
  - Universal non-Maxwellian time-dependent code
  - Ion distributions
  - Synthetic spectra
  - Radiative power losses
  - 7-8 ions, $10^9-10^{10}$ states per ion, millions of transitions

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Population channels for 3d: $n_e \to 0$

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Motional Stark effect and parabolic states

\[ \mathbf{E} = \hat{\mathbf{v}} \times \mathbf{B} \]

\[ \alpha = \pi/2 \text{ for MSE} \]

Classical excitation: $n_f/m_f \rightarrow n_i/m_i$

Only one axis: along projectile velocity

There is another axis: along the induced electric field $\mathbf{E}$

Cross sections for parabolic states

\[ \sigma(E) = \int |F(E, \Omega)|^2 \, d\Omega \]

\[ F_{\alpha\beta} = \sum_{a = \pm 1} C_{a m_f/m_i}^{n_f/m_f} \Phi_{a m_i} \]

Transformation 1:
- parabolic along $z$ into spherical along $z$

\[ \psi_{\alpha}\beta = \sum m_i \Phi_{a m_i} \Phi_{\beta m_i} \]

With increase of $n_e$, $3p_{3/2}$ eventually comes into LTE with the ground state $\Rightarrow$ its population does not depend on $n_e$ $\Rightarrow$ populations of $3d_{5/2}$ and $3d_{3/2}$ vary similarly...BUT: There must exist an interesting range of $n_e$!
Non-statistical populations and E-field ionization

Marchuk, Ralchenko, Schultz, PPCF (2012)

Benchmarking the parabolic CR model on Alcator C-Mod

<table>
<thead>
<tr>
<th>Parameter</th>
<th>ITER</th>
<th>Alcator C-Mod</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n_e), pedestal to core, cm(^{-3})</td>
<td>[0.9-1.35]\times10(^{14})</td>
<td>[0.6-1.36]\times10(^{14})</td>
</tr>
<tr>
<td>(E_{\text{beam}}), keV/u</td>
<td>100/1000.0</td>
<td>50.0</td>
</tr>
<tr>
<td>(T_e), pedestal to core, keV</td>
<td>2-15</td>
<td>0.4-2.5</td>
</tr>
<tr>
<td>(Z_{\text{eff}})</td>
<td>1.7-2.3 (He:1.7-2%, Be:2%, Ar:0.1-0.3%)</td>
<td>1.5-2.2 (B:1-2%, Ar:0.2%)</td>
</tr>
<tr>
<td>(B_{\text{tor}}), T</td>
<td>4.0 (outer edge)-5.37 (axis)</td>
<td>4.2 (outer edge)-5.57 (axis)</td>
</tr>
</tbody>
</table>

Benchmarking the \(nkm\) CR model

Conclusions:
- The difference between the experiment and \(nkm\)-model is mostly within 10%
- The difference from statistical model is larger, reaching 27%
- Expected differences from statistical model for ITER beams:
  - \(\leq 3.2\%\) for \(100\) keV/u
  - \(\leq 4.3\%\) for \(500\) keV/u

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Charge exchange

- \(A^{2+} + B \rightarrow A^{(2-k)+} + B^{k+}\)
  - A: initial configuration + \((n_j l_j, n_{j' l_{j'}}, \cdots n_{j' l_{j'}})\)
- Important in magnetic fusion (CXRS), astrophysics (e.g., x-rays from comets and other objects), EBITs...
- Several theoretical methods developed
  - Classical trajectory Monte Carlo (CTMC)
  - Close-coupling methods (e.g., AOCC)
- Capture into high \(n \sim Z^{3/4}\)

Experiment at JPL: \(O^6++H_2, He\)

- ECR source for production of \(^{18}O^6+\)
- Collisions with \(H_2\) and \(He\) (gas cell)
- Ion energies:
  - 3.5 keV·q (21 keV=1.17 keV/u)
  - 7 keV·q (42 keV=2.33 keV/u)
- Velocities: 464 km/s and 671 km/s
- Current: 5-20 nA
- Gas pressure: \((6.5-12)\times10^{-3}\) Pa
- No indication of metastables

Single CTMC CX cross sections at 7 keV q

75% nCTMC + 25% inCTMC

inCTMC: independent electrons; nCTMC: correlated electrons

log(σ) vs (nl\textprime l\textprime)

Most of important states are autoionizing!!!

Experiment (JPL) vs theory (CTMC+CR)

<table>
<thead>
<tr>
<th>Cross Section (in 10^{-15} cm^2)</th>
<th>He</th>
<th>Ne</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textit{present experiment}</td>
<td>1.16 ± 0.08</td>
<td>1.34 ± 0.09</td>
</tr>
<tr>
<td>\textit{theory}</td>
<td>1.32</td>
<td>1.39</td>
</tr>
<tr>
<td>\textit{present experiment}</td>
<td>0.116 ± 0.008</td>
<td>0.107 ± 0.008</td>
</tr>
<tr>
<td>\textit{theory}</td>
<td>0.173</td>
<td>0.175</td>
</tr>
</tbody>
</table>

Multiple Charge Exchange (MCX)

- \textit{A}^{z+} + B \rightarrow A^{(z-k)+} + B^{K+}
- Final distribution of electrons on the target: (n_1l_1, n_2l_2, ..., n_kl_k)
- The final states are (mostly) autoionizing
- Elementary act of MCX is (mostly) followed by autoionization with characteristic rates on the order of 10^{13} - 10^{14} s^{-1}
- Post-collision stabilization modeling should be an integral component of the MCX analysis

MCX final states: which nl's?..

- MCX nl-distribution is given by, e.g., CTMC calculation
- \textit{O}^{6+} + molecule (relativistic configurations)
  - Double CX: n_1 \leq 7, n_2 \leq 8 (108 and 1788 AI)
  - Triple CX: n_1 \leq 6, n_2 \leq 6, n_3 \leq 10 (130 and 28,434 AI)
  - Quadruple CX: n_1 \leq 6, n_2 \leq 6, n_3 \leq 6, n_4 \leq 7 (97 and 97,574 AI)
- It is hopeless today to try to solve a time-dependent 10^5 x 10^5 rate equation...

Energy scheme for OV and OVI
Monte Carlo approach to MCX stabilization

1. Normalize
2. Sort
3. Random pick
4. Proceed until stabilized
5. Repeat 999,999 times.

Highly parallelizable model

DCX stabilized fraction in O^{4+}

Typical radiative and AI rates:

- $A_\text{r} \sim 10^{11} \text{ s}^{-1}$
- $A_\text{a} \sim 10^{13-10^{14}} \text{ s}^{-1}$

Time improvement: $\sim 320$

Final steps

- Weight from CTMC calculations
- Count the emitted photons (easy in MC approach)
- Produce spectra
- Prepare a paper

Conclusions

- Low-density plasmas offer a wide range challenges that are fun to address

TCX and QCX stabilized fractions

TCX: O^{3+}  

QCX: O^{4+}

O^{3+}: TCX

O^{4+}: QCX