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*)

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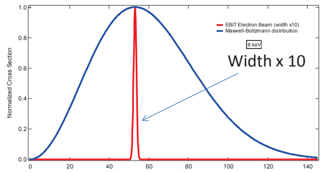
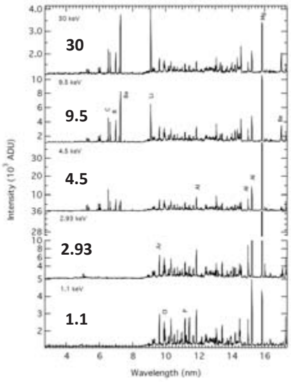
NIST EBIT: factory of highly-charged ions



- Many operate, a few under construction
- "Table-top" device
- Low electron density
  - **N_e ~ 10^{11}-10^{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

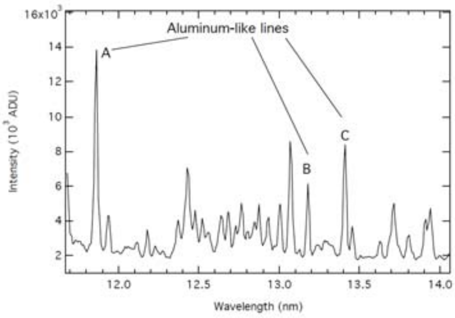
EBIT: Kr XXII-Kr XXXIV spectra

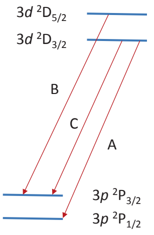


- Krypton is important for fusion
- E_{beam} = 1.1-30 keV
- Six new lines identified, accuracy improved for twelve lines
- Low- and high-charged ions are present
- 30 keV is not enough to reach H-like Kr with IP=18 keV (charge exchange!)
- And there's something else…

Y.A. Podpaly et al, J. Phys. B **47**, 095702 (2014)

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



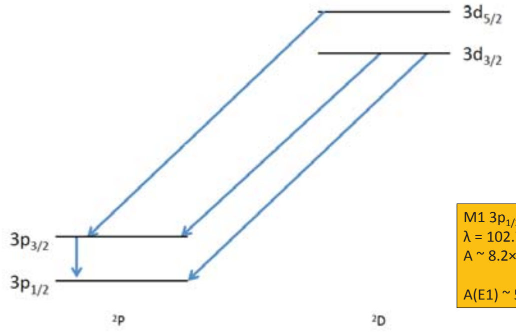


A_A = 6.2×10^{10} s^{-1}
A_B = 7.4×10^{10} s^{-1}
A_C = 3.2×10^{10} s^{-1}

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 Maron, 2001)
  - Universal non-Maxwellian time-dependent code
    - Ion distributions
    - Synthetic spectra
    - Radiative power losses
  - 7-8 ions, 10^3-10^4 states per ion, millions of transitions

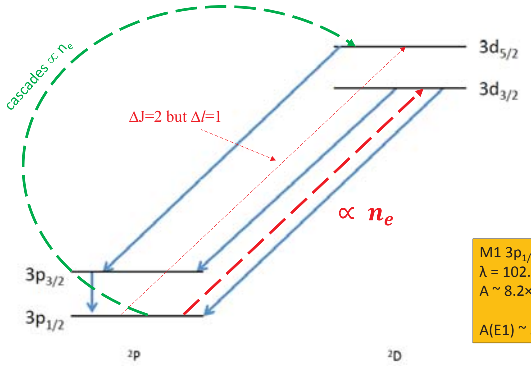
Population channels for 3d



M1 $3p_{1/2}$-$3p_{3/2}$
λ = 102.76 nm
A ~ 8.2×10^3 s^{-1}

A(E1) ~ 5×10^{10} s^{-1}

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



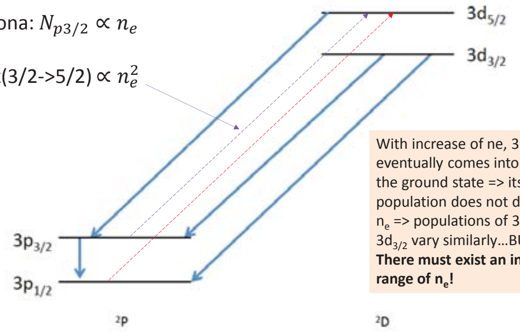
M1 $3p_{1/2}$-$3p_{3/2}$
λ = 102.76 nm
A ~ 8.2×10^3 s^{-1}

A(E1) ~ 5×10^{10} s^{-1}

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

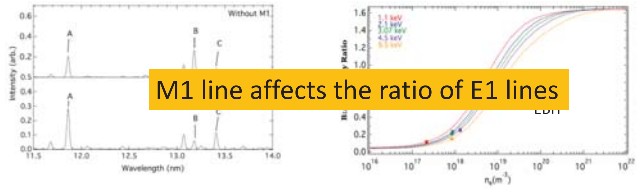
Corona: $N_{p3/2} \propto n_e$

Flux(3/2->5/2) ∝ n_e^2



With increase of ne, $3p_{3/2}$ eventually comes into LTE with the ground state => its population does not depend on n_e => populations of $3d_{5/2}$ and $3d_{3/2}$ vary similarly…BUT: **There must exist an interesting range of n_e!**

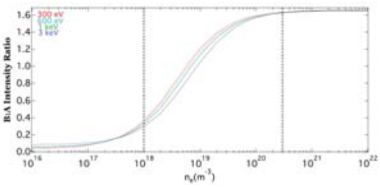
CR modeling: EBIT and tokamaks



M1 line affects the ratio of E1 lines

Maxwellian plasma, 10^{14} cm^{-3}

Good diagnostics of density



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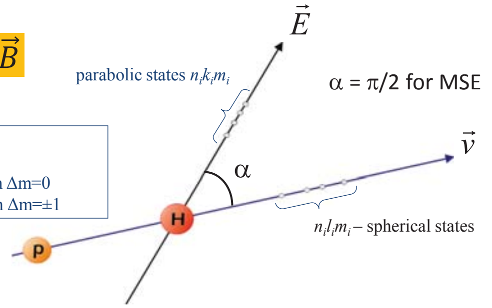
Motional Stark effect and parabolic states

$\vec{E} = \vec{v} \times \vec{B}$



Radiative channel
$n_ik_im_i \rightarrow n_jk_jm_j$
π – components with Δm=0
σ – components with Δm=±1

Classical excitation: $n_il_im_i \rightarrow n_jl_jm_j$

Only one axis: along projectile velocity

There is another axis: along the induced electric field **E**

Cross sections for parabolic states

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

Scattering amplitude between parabolic states a ≡ (nkm)

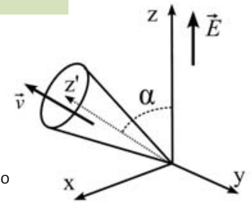
$$F_{ba} = \langle \psi_b | \hat{\Gamma} | \psi_a \rangle$$

Transformation 1:
parabolic along z into spherical along z

$$\psi_{nkm} = \sum_{l=|m|}^{n-1} C_{j_1\mu_1 j_2\mu_2}^{lm} \varphi_{nlm}$$

Transformation 2:
spherical along z into spherical along z’

$$\varphi_{nlm} = \sum_{m'=-l}^{l} D_{m'm}^{(l)}(\alpha) \varphi_{nlm'}$$

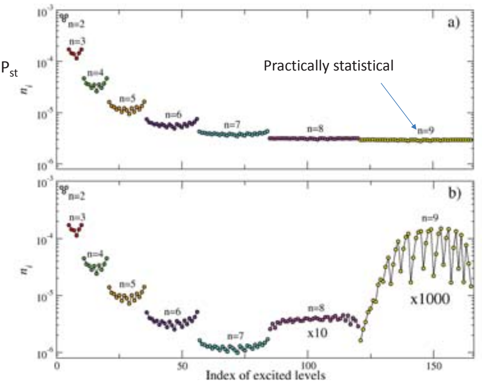


Use: ***nkm***-resolved (parabolic) CR model

Marchuk, Ralchenko, Janev, et al (2010)

Non-statistical populations and E-field ionization

POP/POP$_{st}$



w/o field

w/ field

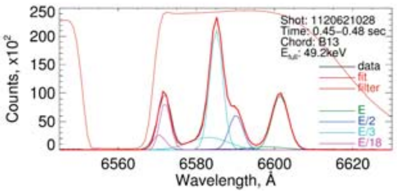
Marchuk, Ralchenko, Schultz, PPCF (2012)

Benchmarking the parabolic CR model on Alcator C-Mod

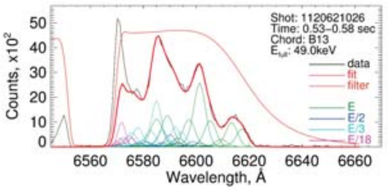
Parameter	ITER	Alcator C-Mod
n_e, pedestal to core, cm^{-3}	$[0.9\text{-}1.35]\times10^{14}$	$[0.6\text{-}1.36]\times10^{14}$
E_{beam}, keV/u	**100.0/1000.0**	**50.0**
T_e, pedestal to core, keV	**2-15**	**0.4-2.5**
Z_{eff}	1.7-2.3 (He:1.7-2%, Be:2%, Ar:0.1-0.3%)	1.5-2.2 (B:1-2%, Ar:0.2%)
B_{tor}, T	4.0(outer edge)-5.3T(axis)	4.2(outer edge)-5.57(axis)

I.O. Bespamyatnov, W.L. Rowan, K.T. Liao, O. Marchuk,
Yu. Ralchenko and R.S. Granetz, *Nucl. Fusion* **53**, 123010 (2013)

MSE spectra: Alcator C-Mod

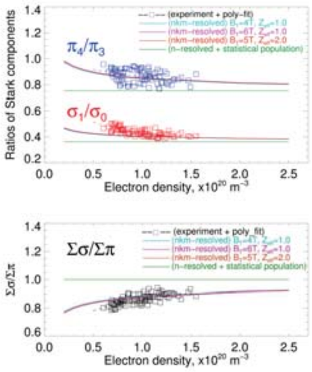


No plasma (gas)



Plasma injection

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:
  - $\lesssim 32\%\ for\ 100\frac{keV}{u}$
  - $\lesssim 43\%\ for\ 500\frac{keV}{u}$

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Charge exchange

- $A^{z+} + B \to A^{(z-k)+} + B^{k+}$
  - A: initial configuration + (n_1l_1,n_2l_2,…n_kl_k)
- 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 $n \sim Z^{3/4}$

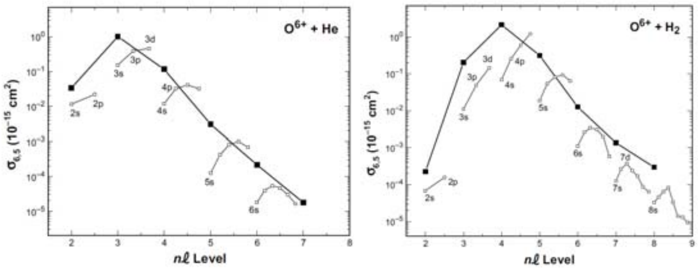
Experiment at JPL: O^{6+}+H_2,He

- 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)×10^{-3} Pa**
- No indication of metastables

J.R. Machacek, D.P. Mahapatra, D.R. Schultz, Yu. Ralchenko. A. Chutjian, J. Simcic, R.J. Mawhorter, Phys. Rev. A **90**, 052708 (2014)

Single CTMC CX cross sections at 7 keV q

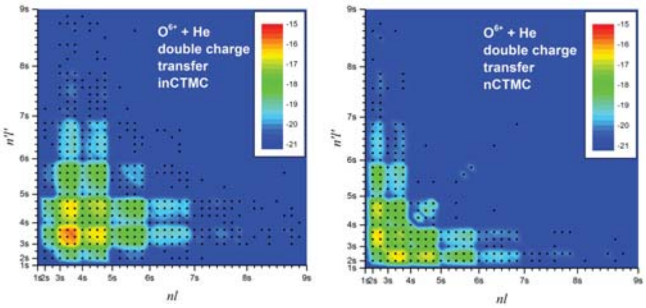
75% nCTMC + 25% inCTMC



inCTMC: independent electrons; nCTMC: correlated electrons

O^{6+}+ He (7 keV·q): Distribution over the final states

log(σ) vs (nl,$n'l'$)



Most of important states are autoionizing!!!

Rate (CR) equation solution

$$\frac{d\hat{N}(t)}{dt} = \hat{A} \cdot \hat{N}(t)$$

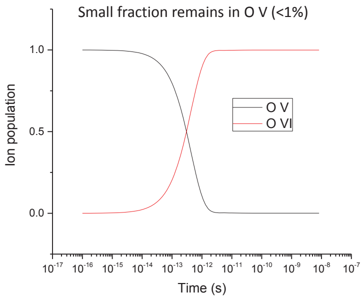
$$\hat{N}(0) = \hat{N}_{CTMC}$$

Integration until stabilization

Matrix size: ~ 4500 x 4500

Double charge exchange: CTMC

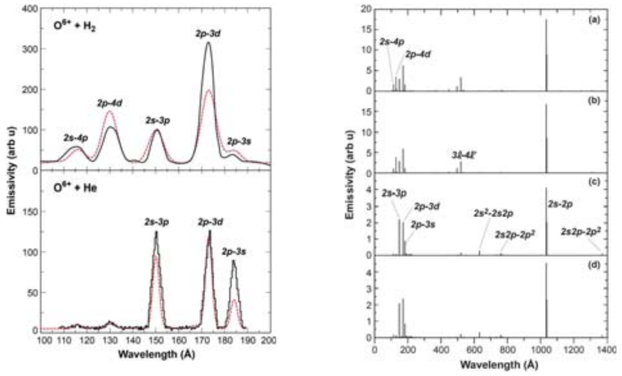
Atomic data: Flexible Atomic Code
- Energy levels
- Radiative rate
- **Autoionization** rates
- No collisional processes



Experiment (JPL) vs theory (CTMC+CR)

Cross Section (in 10^{-15} cm^2)		***He***		***H_2***	
		21.0 keV	***42.0 keV***	***21.0 keV***	***42.0 keV***
$\sigma_{6,5}$	**present experiment**	1.16 ± 0.08	1.34 ± 0.09	4.24 ± 0.29	4.24 ± 0.29
	present theory	1.32	1.39	4.64	4.37
$\sigma_{6,4}$	**present experiment**	0.116 ± 0.008	0.107 ± 0.008	0.118 ± 0.008	0.096 ± 0.007
	present theory	0.173	0.175	0.066	0.073

DCX+SCX spectra

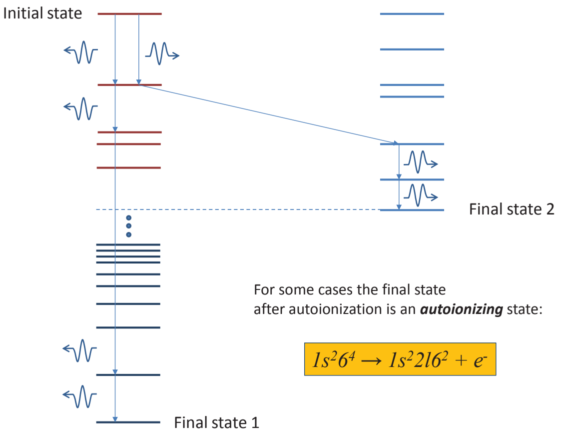


Multiple Charge Exchange (MCX)

- $A^{z+} + B \rightarrow A^{(z-k)+} + B^{k+}$
- 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
- Ali et al (1995): qualitative recommendations; no quantitative approach/modeling

MCX final states: which *nl*'s?..

- MCX *nl*-distribution is given by, e.g., CTMC calculation
- 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 10^5x10^5 rate equation…



Initial state

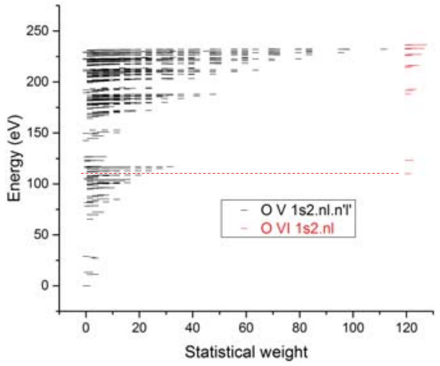
Final state 2

Final state 1

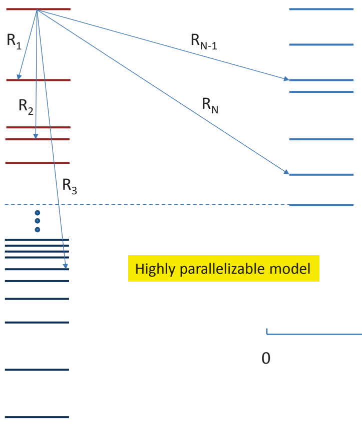
For some cases the final state after autoionization is an ***autoionizing*** state:

$1s^2 6^4 \rightarrow 1s^2 2l 6^2 + e^-$

Energy scheme for OV and OVI



Monte Carlo approach to MCX stabilization

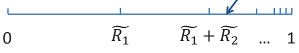


1. Normalize
2. Sort
3. Random pick
4. Proceed until stabilized
5. Repeat **999,999** times

$$\widetilde{R_i} = \frac{R_i}{\sum_k R_k}$$

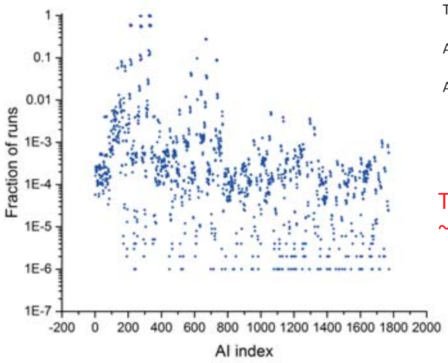
$$\widetilde{R_1} \le \widetilde{R_2} \le \widetilde{R_3} \dots$$

Highly parallelizable model



Ralchenko & Schultz, to be published

DCX stabilized fraction in O^{4+}



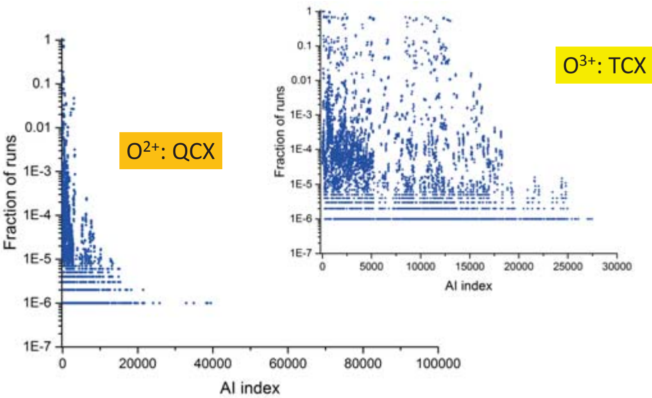
Typical radiative and AI rates:

A_r ~ 10^{11} s-1

A_a ~ 10^{13}-10^{14} s^{-1}

Time improvement: ~**320**!

TCX and QCX stabilized fractions



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