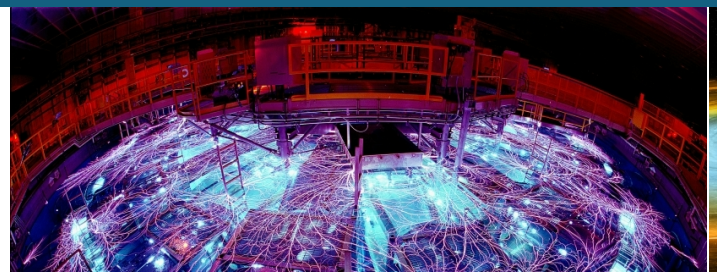
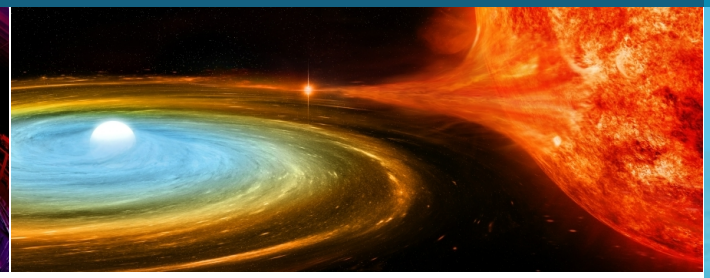
SAND2021-12775PE

Progress in Line-Shape Theory: the BALROG code





Thomas Gomez

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Common Approximations in Line-Shape Calculations

- Line shape theory is a multi-disciplinary field, requiring
  - Atomic Physics
  - Collision Physics
  - Plasma Physics
  - Statistical Mechanics
- Drawing from so many sources usually means that approximations have to be employed to keep calculations tractable

- Approximations include
  - Static Ion Approximation
  - No-Quenching Approximation
  - Dipole Approximation
  - 2^{nd}-Order Approximation
  - Classical Approximation
  - Factorized Density Matrix Approximation
  - Binary-Collision Approximation
  - Straight-Path & Screening Approximations

The Xenomorph Code

- The Xenomorph code was developed during my master's thesis and has been improved upon by P. Cho
  - P. Cho will discuss more after this
- Xenomorph easily removes some of these approximations
  - As a simulation, it easily tackles several approximations all at once

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- Xenomorph easily removes some of these approximations
  - As a simulation, it easily tackles several approximations all at once
- But, it is missing some important physics
  - Dipole approximation and Classical Approximation cannot be removed within the framework of Xenomorph
  - Removing these approximations requires a new approach

- Approximations include
  - ~~Static Ion Approximation~~
  - ~~No-Quenching Approximation~~
  - **Dipole Approximation***
  - ~~2nd-Order Approximation~~
  - **Classical Approximation**
  - Factorized Density Matrix Approximation
  - ~~Binary-Collision Approximation~~
  - Straight-Path & Screening Approximations

We Can Include Other Physics By using Different Approach

- By changing to an analytic approach, we can include different physics than simulations
- Analytic calculations are able to incorporate
  - Finite size of plasma electrons [1]
  - Penetration of plasma electrons into the radiator wavefunctions [2]
  - Include more general density matrix [3,4]
  - Include plasma electrons becoming bound to atom [5]

Xenomorph cannot capture any of these effects

- Approximations include
  - Static Ion Approximation
  - ~~No-Quenching Approximation~~
  - ~~Dipole Approximation~~
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[1] Smith & Hooper (1967); [2] Woltz & Hooper (1984); [3] Hussey et al. (1975); [4] Gomez et al. (2018);[5] Gomez et al. (2020)

Analytic Calculations have a Severe Problem…Until Now

- However, analytic codes so far have had difficulty removing the 2nd-Order Approximation

$$T(E) = \frac{1}{1 - V[E - H_0]^{-1}} V$$
$$\approx V + V[E - H_0]^{-1} V$$

The 2nd-order approximation poses a problem because it does not preserve unitarity

$$U^\dagger(t)U(t) = 1 \qquad |\langle\psi(t)|\psi(t)\rangle|^2 = 1$$

- Approximations include
  - Static Ion Approximation
  - ~~No-Quenching Approximation~~
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We Learned how to Remove the 2nd-order Approximation in Analytic Methods (Balrog Code)

- Consultation with collision physicists gave us the tools to remove the 2nd-order approximation
- The technique involves re-arranging the problem to be Ax=b and use linear solver

$$T(E) = \frac{1}{1 - V[E - H_0]^{-1}} V$$

$$\left\{1 - V[E - H_0]^{-1}\right\} T(E) = V$$

- Balrog presents a significant update to the current state of line-shape models

- Approximations include
  - Static Ion Approximation
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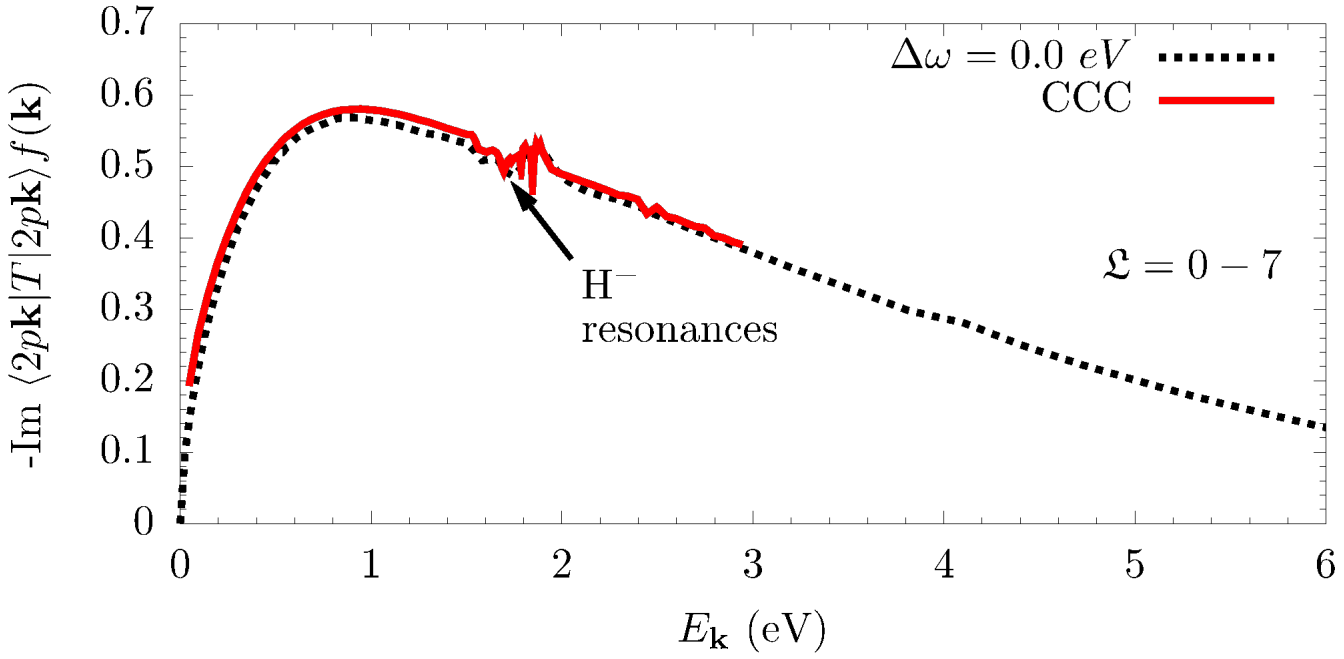
We Need to Confirm the Accuracy of Our Calculations by Comparing against CCC

- Before we start applying our T-matrices to line-shapes, we need to confirm that our code is accurate
- The CCC [1] code is a collision code that calculates T-matrices that treats the plasma particles quantum mechanically and uses the full-Coulomb treatment for the interaction (with Pauli exclusion/exchange)
- For these reasons, we choose to compare our T-matrices against those

We are now free to remove certain physics to test approximations



[1] Bray & Stelbovics (1992)

CCC: Convergent Close Coupling

Balrog Preserves Unitarity to Machine Precision

- The S-matrix defined in terms of the T-matrix

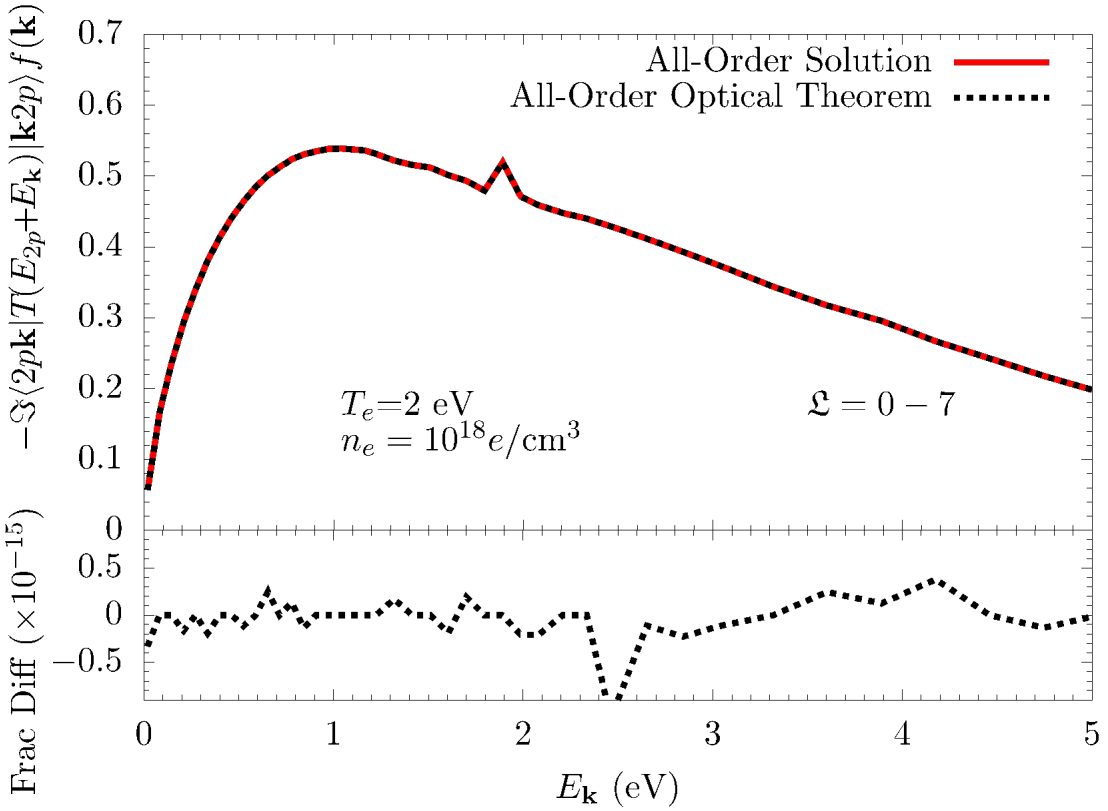
$$S = 1 - 2i\pi\delta(E - H_0)T(E)$$

- From the unitarity condition of the S-matrix, one can derive the optical theorem [1]

$$SS^\dagger = 1$$

$$\Im T(E) = -\pi T(E)\delta(E - H_0)T^\dagger(E)$$

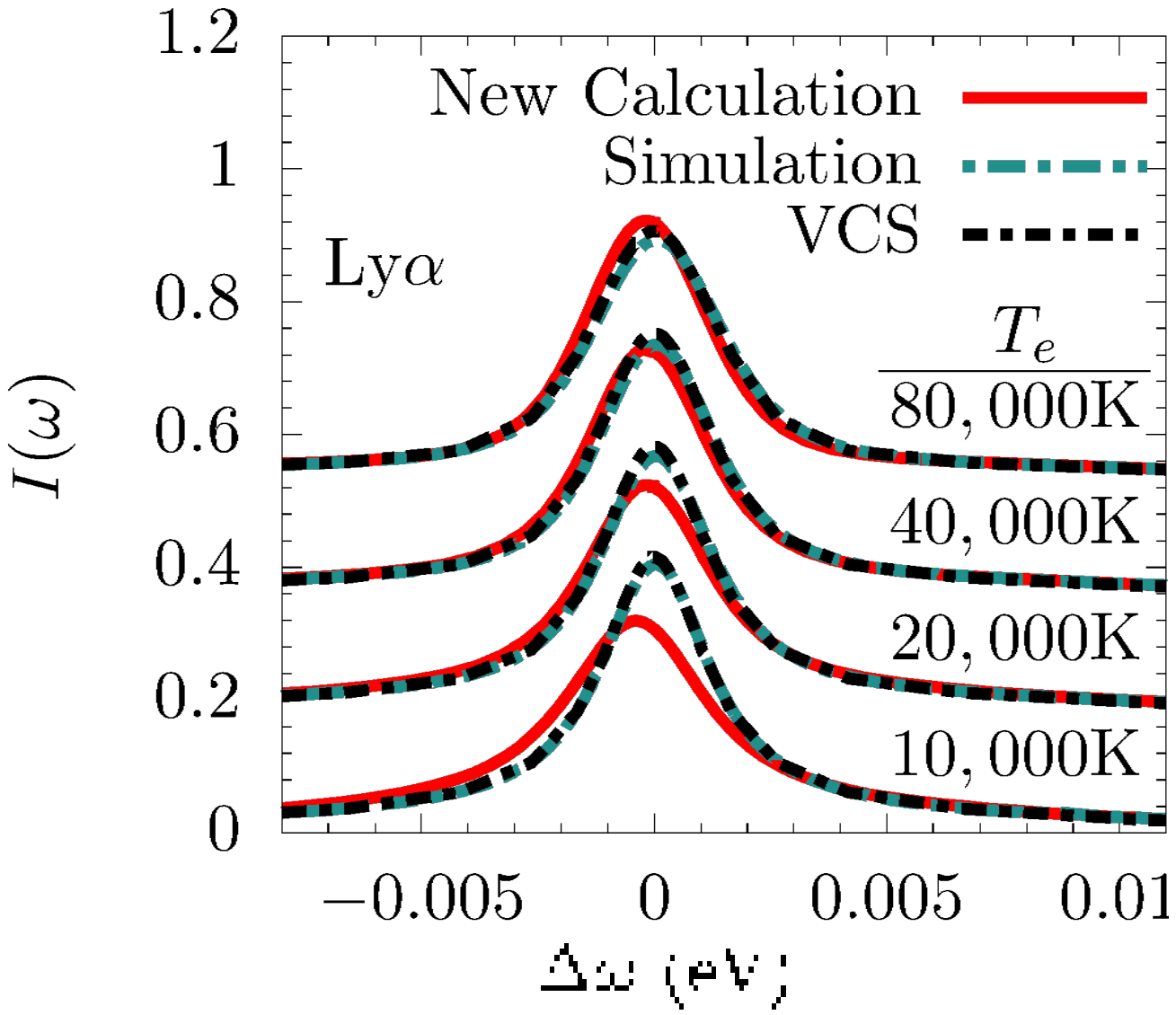
- Therefore, we know that if our T-matrix solution preserves the optical theorem that it preserves unitarity



Optical Theorem is Satisfied to one part in 10^{15}—which is the double precision limit

[1]Lippmann & Schwinger (1950)

Quantum Calculations Are Important For Some Transitions



- Lyα is the strongest line in stellar spectra
  - Dominant source of opacity
  - Changes in Lyα spectra can have wide ranging effects in stellar spectra
- Current line-broadening models are based on the Vidal-Cooper-Smith (VCS) model [1]
  - Classical Approximation
  - Dipole Approximation
  - *All-Order*
- New model is broader than VCS at low temperatures but is roughly equivalent at high temperatures

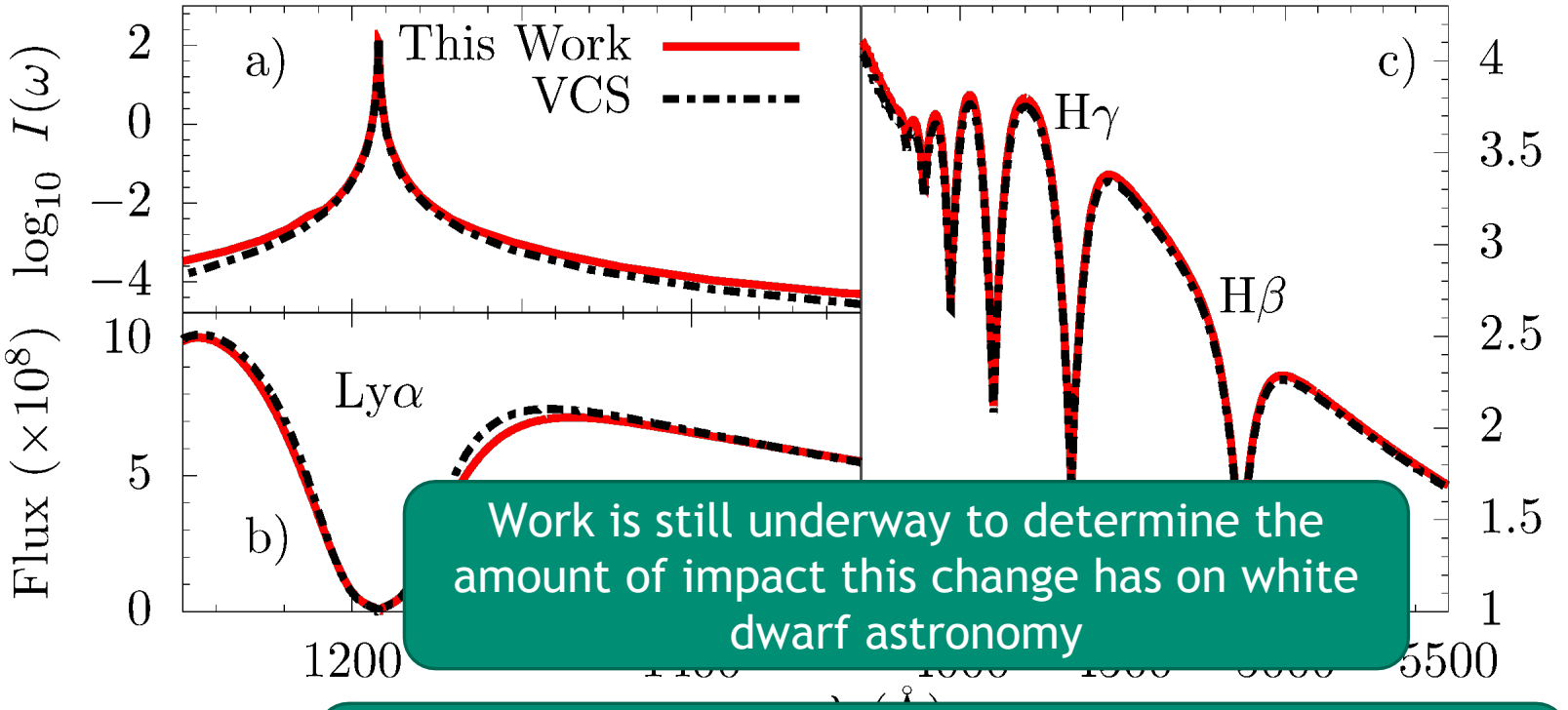
[1] Vidal, Cooper, and Smith (1973)

These Difference in Lyα Result in Increases in the White Dwarf Visible Spectrum

- The calculation with additional physics resulted in broader line shapes
- This raised the opacity in the area where most of the flux comes out of the star
  - The radiation has to get out elsewhere, so it comes out in the UV and visible
  - Thus raising the continuum flux by a few percent

(Larger than the <1% error estimates of WD fluxes [1,2])

Typical White Dwarf Conditions: T = 20,000K; log g = 8.0



Work is still underway to determine the amount of impact this change has on white dwarf astronomy

May impact mass determinations and spectroscopic calibrations

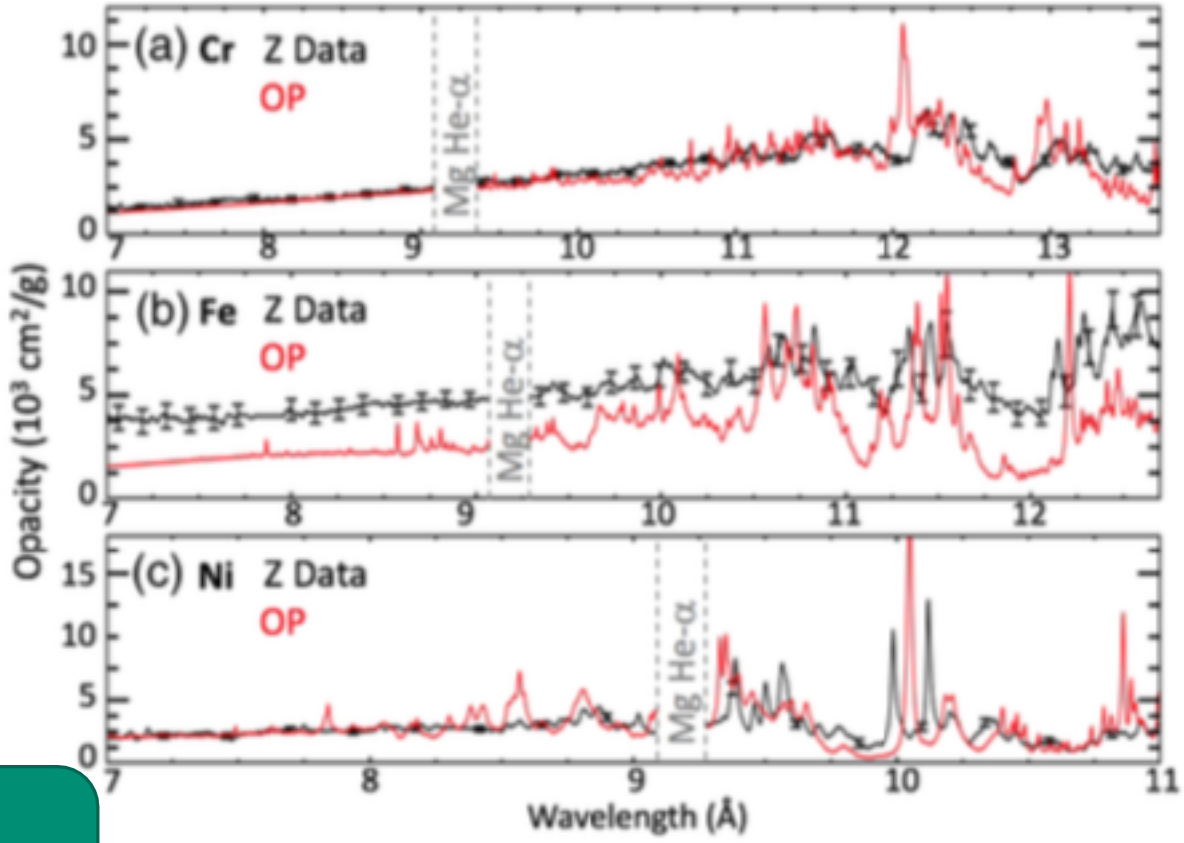
[1] Narayan et al. (2019); [2] Brohlin et al. (2020)

TLUSTY model atmosphere; Hubeny & Lanz (1995)

The Fe opacity experiment at Sandia National Laboratories

- At the Z-machine at Sandia, we are trying to measure the opacity of Fe at solar interior conditions
  - Opacity of Fe is substantially greater than predicted by models [1,2]

- One of the tools used to determine the plasma conditions is fitting line shapes of K-shell transitions of Mg
  - Mg Lyβ
  - Mg Heγ

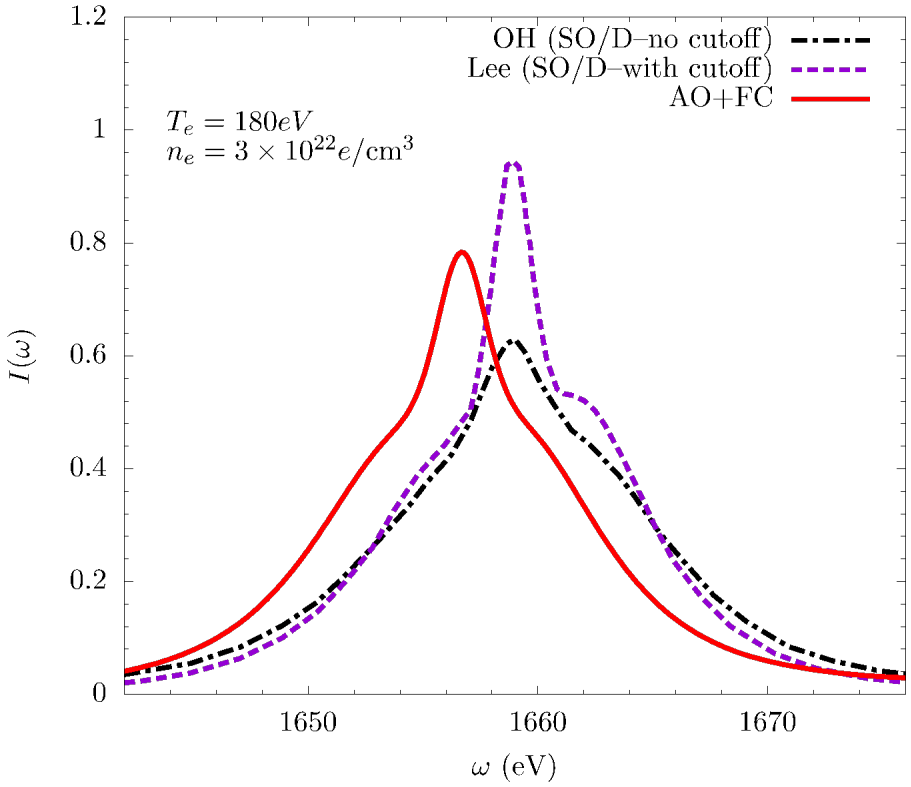


Improving line-shape model will help determine true discrepancies between data and model

[1] Bailey et al. (2015); [2] Nagayama et al. (2019)

New Mg Heγ Line Shape Calculations are Between Two Commonly-Used Models

- Nagayama [2] and Iglesias [3] showed how two commonly-used models (O'Brien & Hooper [4] and Lee [5]) differ in inferred electron density by more than 50%
  - Both use second-order and dipole approximations
  - Lee uses a strong collision treatment, OH does not
- New calculation is between OH and Lee and has additional shift

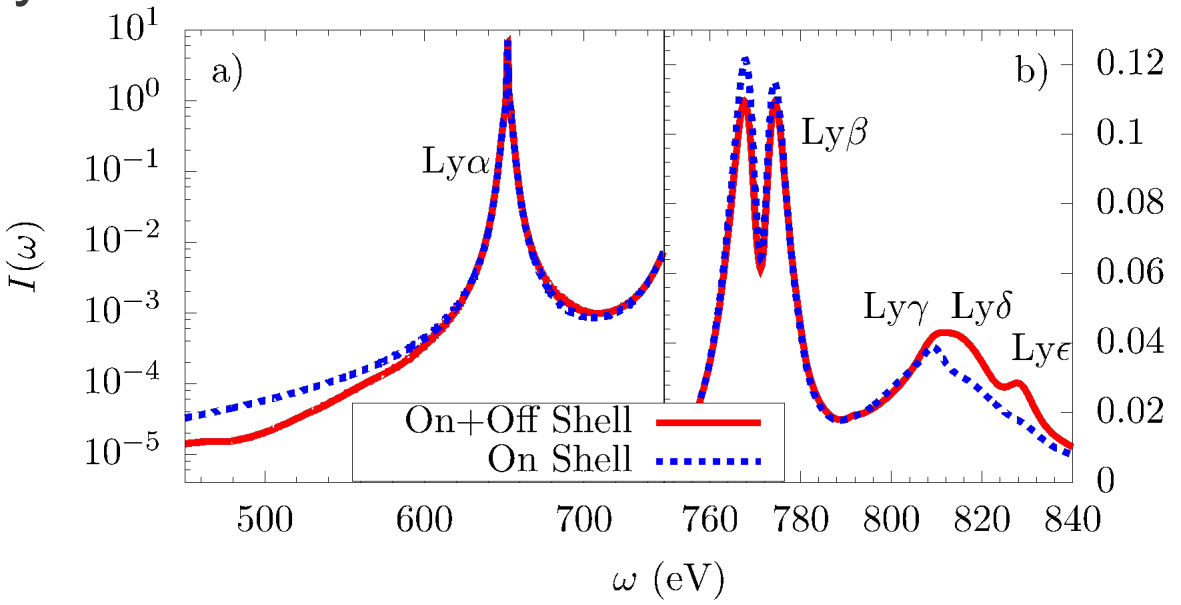


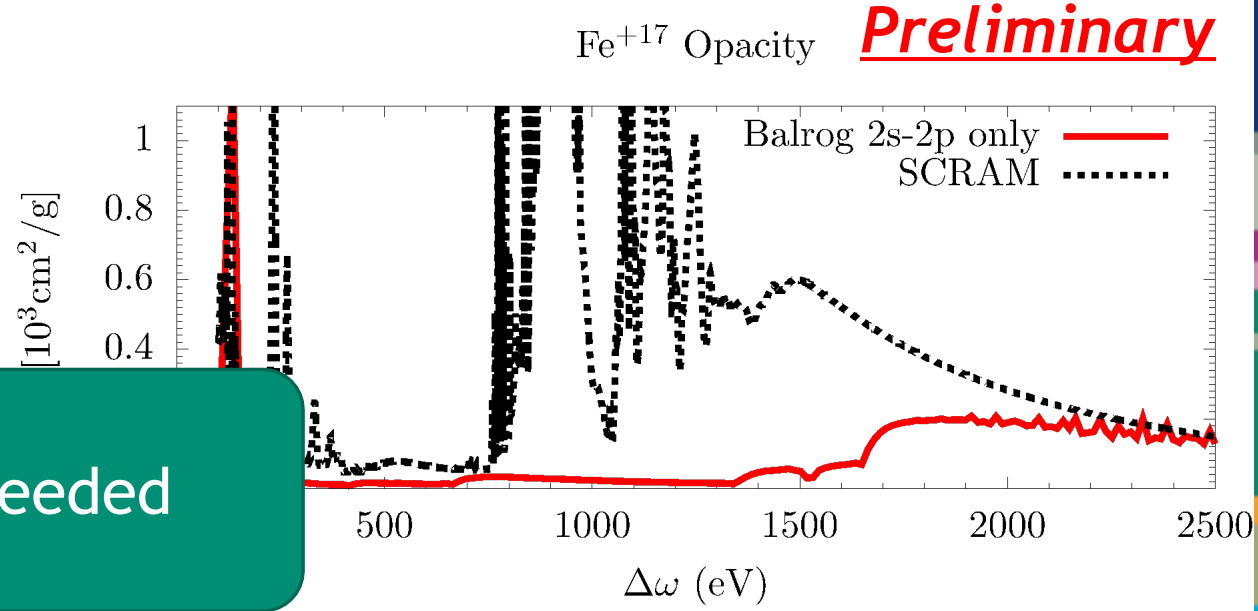
Preliminary fits to data indicate 30% higher density than estimated by OH

[1] Bailey et al. (2015); [2] Nagayama et al. (2016); [3] Iglesias (2016); [4] O'Brien & Hooper (1974); [5] Lee (1988)

Using Balrog to Calculate Fe opacity

- Balrog can also be used to calculate opacities at solar interior conditions
- The full Balrog treatment of the O spectra
  - Modifies line intensities
  - Raises opacity between Lyα and Lyβ
  - Gives structure to the wings of Lyα
- It's always been assumed that line shapes are area normalized
- However, this doesn't seem to be the case in balrog, where the oscillator strength is increased with plasma effects
  - i.e. may violate the TRK f-sum rule for H-like oxygen
- This raises [illegible] plasma broa[illegible]
- May have [illegible]





More Work in This Area is Needed