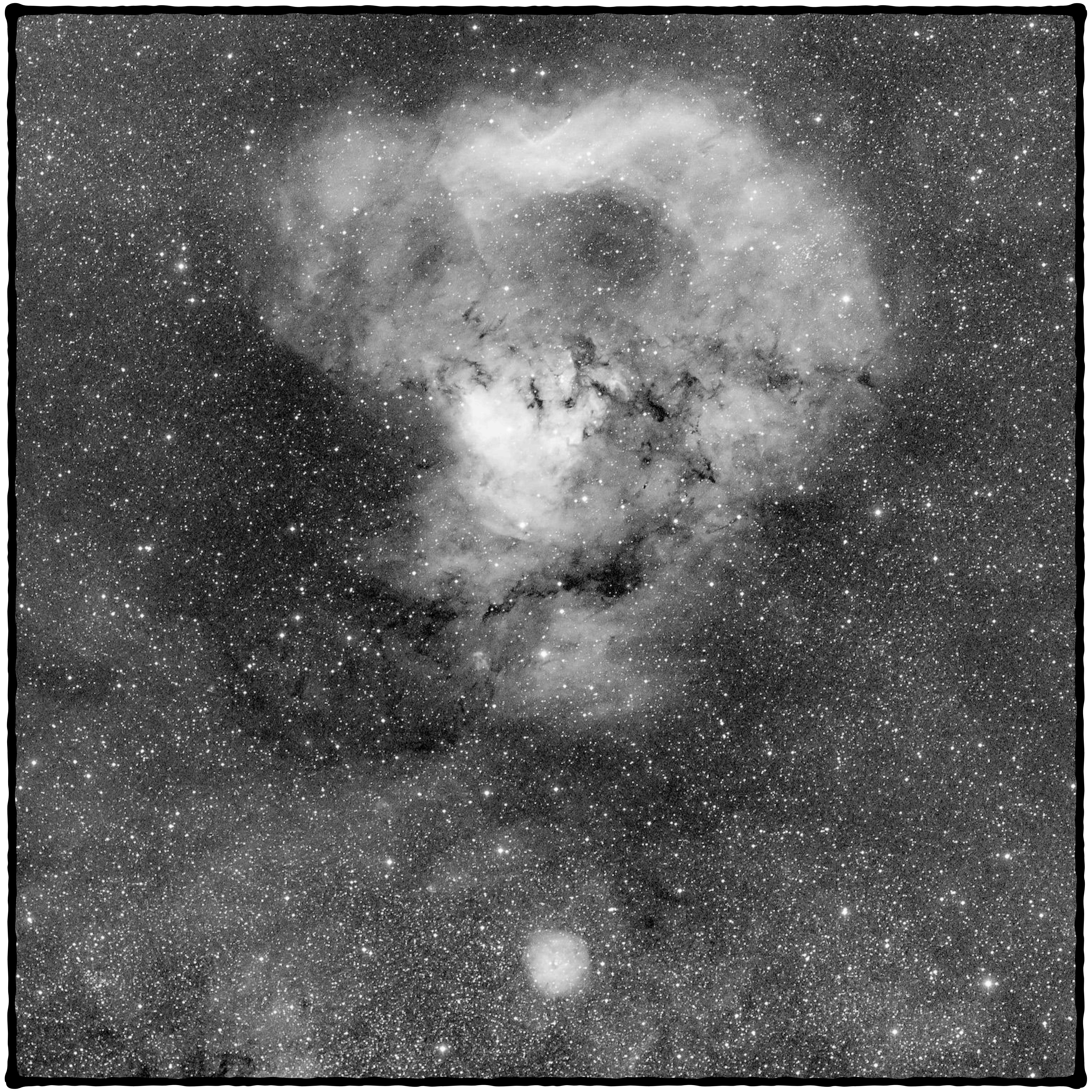
Non-LTE

Anish Amarsi (Uppsala University)

Tartu stellar spectroscopy workshop, 27 September 2023

Outline

- Motivation 15min
- Theory and methods 10min
- Typical non-LTE effects 20min
- Applying non-LTE corrections 5min
- **Questions** (at anytime…) 10min



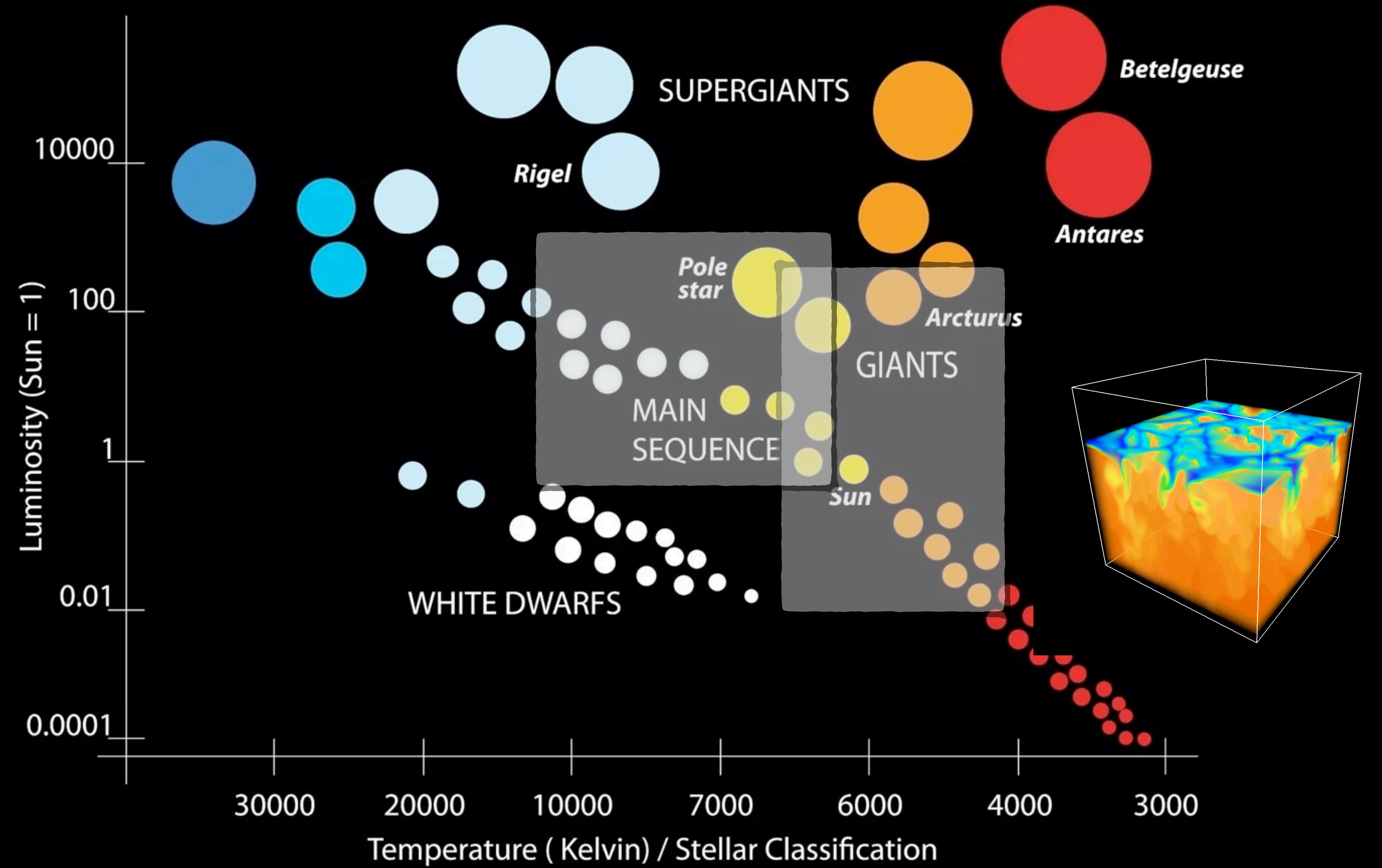
Motivation

Are LTE models good enough?


Macrophysics
Radiative transfer
Spectrum
Atmosphere models
Atom producing spectral line
Perturbations from fast electrons
slow hydrogen
Microphysics (e.g. Non-LTE)
Knowledge
Atoms, planets, stars, galaxies, cosmos...
Parameters
Teff, logg, abundances...

Motivation

- Elemental abundances (etc.) are inferred via comparison to **model spectra**
- Are LTE models good enough? Can we uncover **interesting astrophysics** when using more realistic (non-LTE) model spectra?

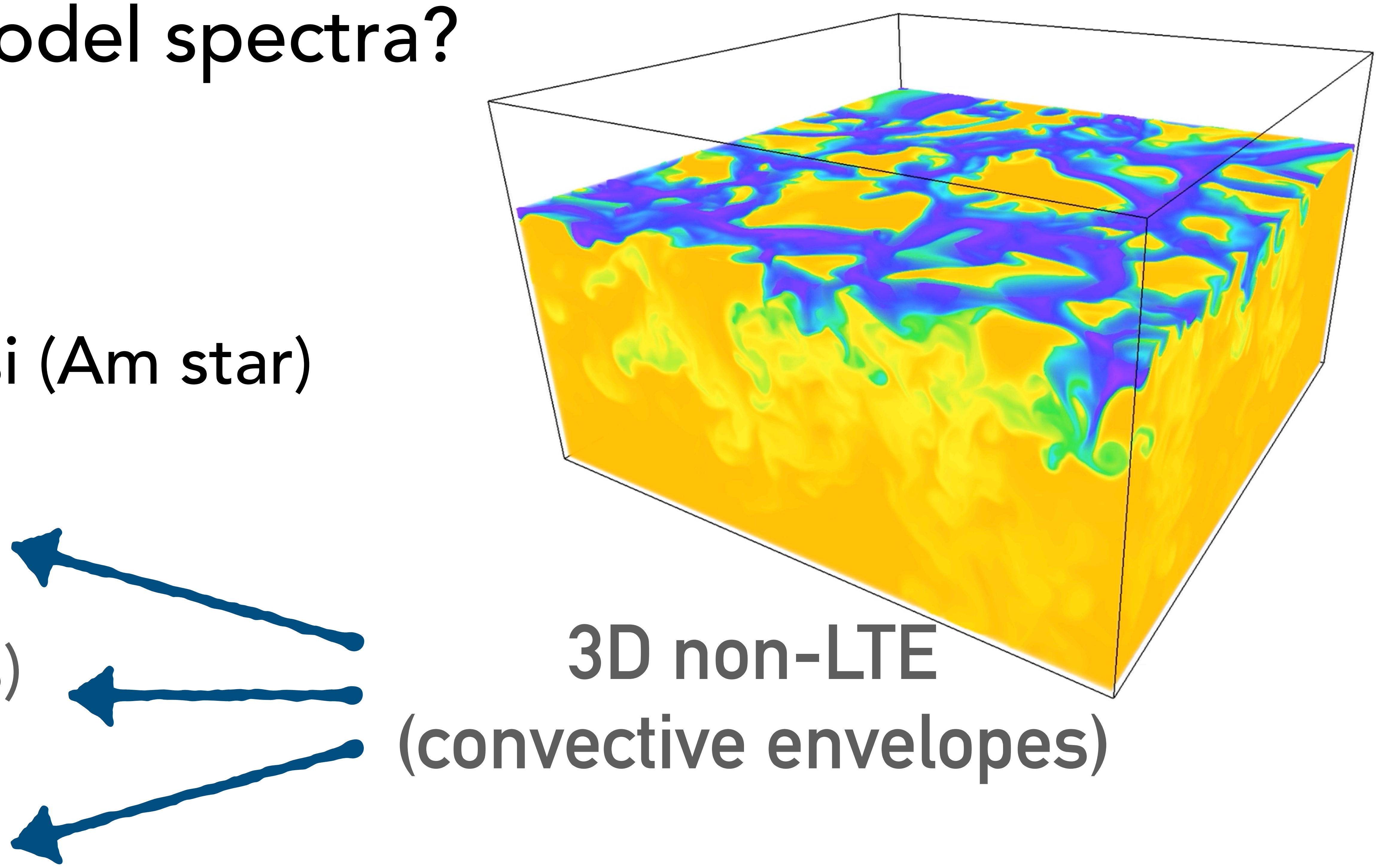


SUPERGIANTS
Betelgeuse
Rigel
Antares
Pole star
Arcturus
GIANTS
MAIN SEQUENCE
Sun
WHITE DWARFS
Luminosity (Sun = 1)
10000
100
1
0.01
0.0001
30000
20000
10000
7000
6000
4000
3000
Temperature (Kelvin) / Stellar Classification

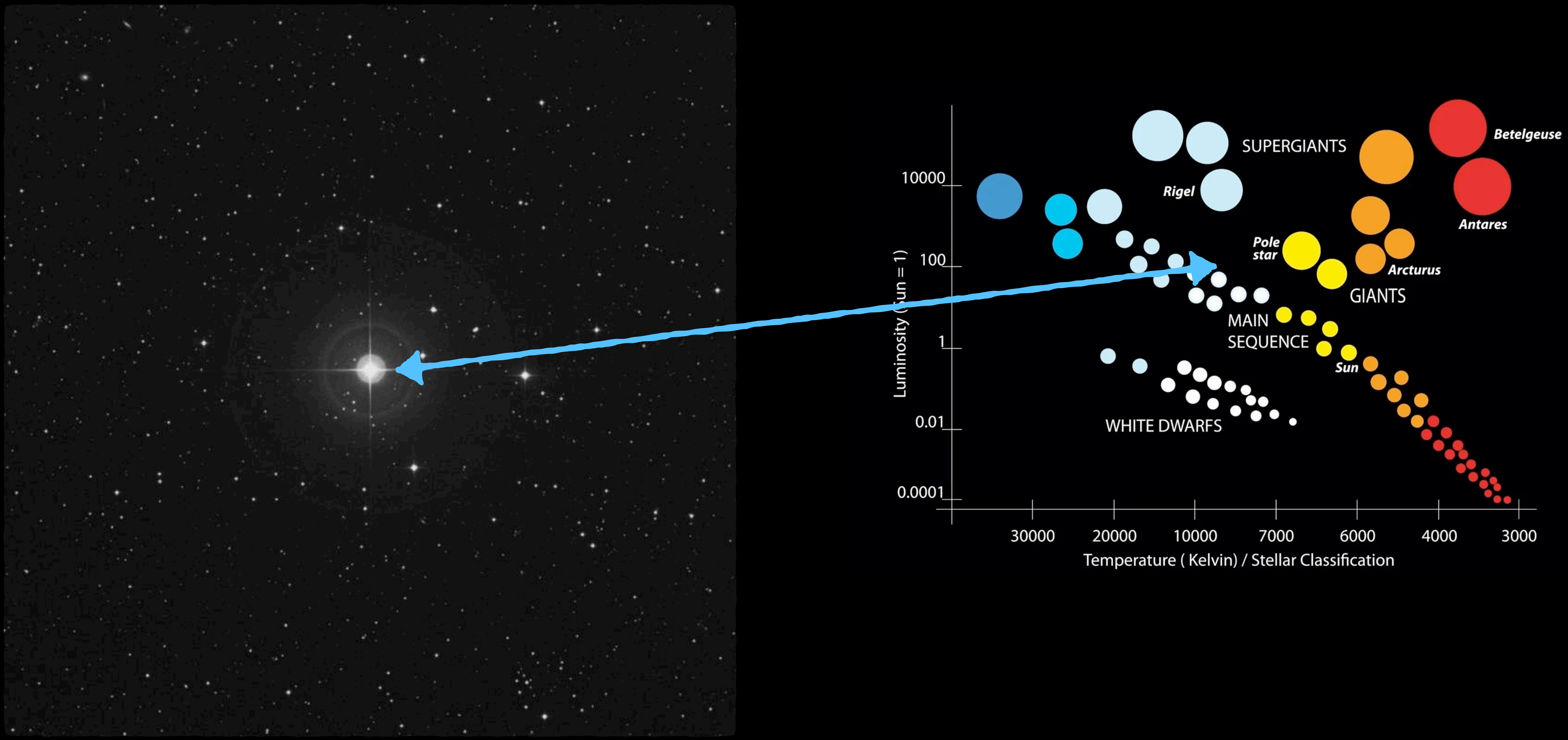
Motivation

- Elemental abundances (etc.) are inferred via comparison to **model spectra**
- Are LTE models good enough? Can we uncover **interesting astrophysics** when using more realistic (non-LTE) model spectra?
- Four examples

1. S I magnetic field diagnostic in o Pegasi (Am star)
2. C/O planet signature (FG dwarfs)
3. [Mg/Fe] accretion signature (FG dwarfs)
4. [C/O] Pop III signature (FG dwarfs)



1. S I magnetic field diagnostic in o Peg.



1. S I magnetic field diagnostic in o Peg.

Interesting differential diagnostic of magnetic fields
(Fine-structure components with different sensitivities)

[Kochukhov et al. 2024]

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LTE: possible false detection of magnetic field

Interesting differential diagnostic of magnetic fields
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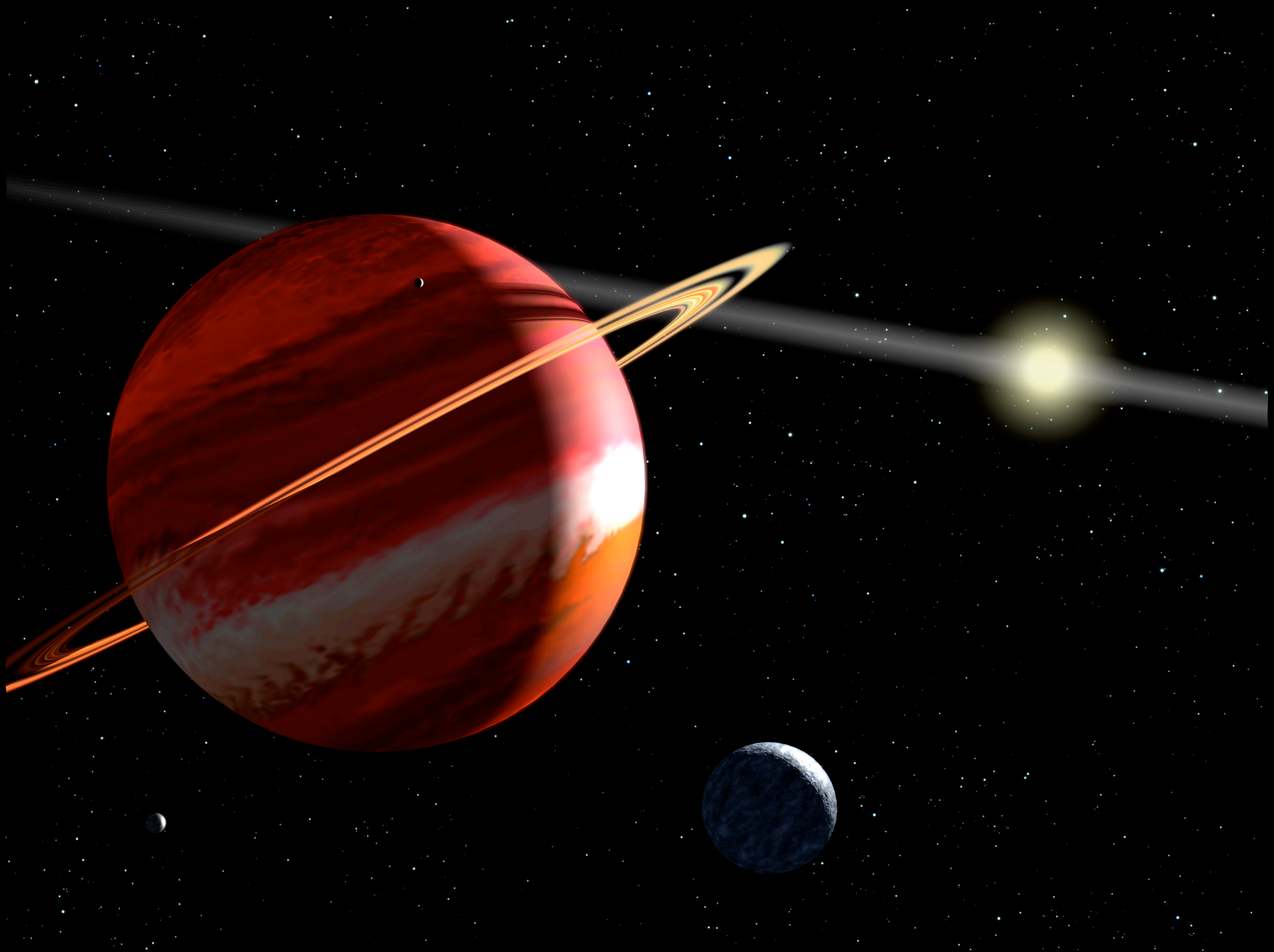
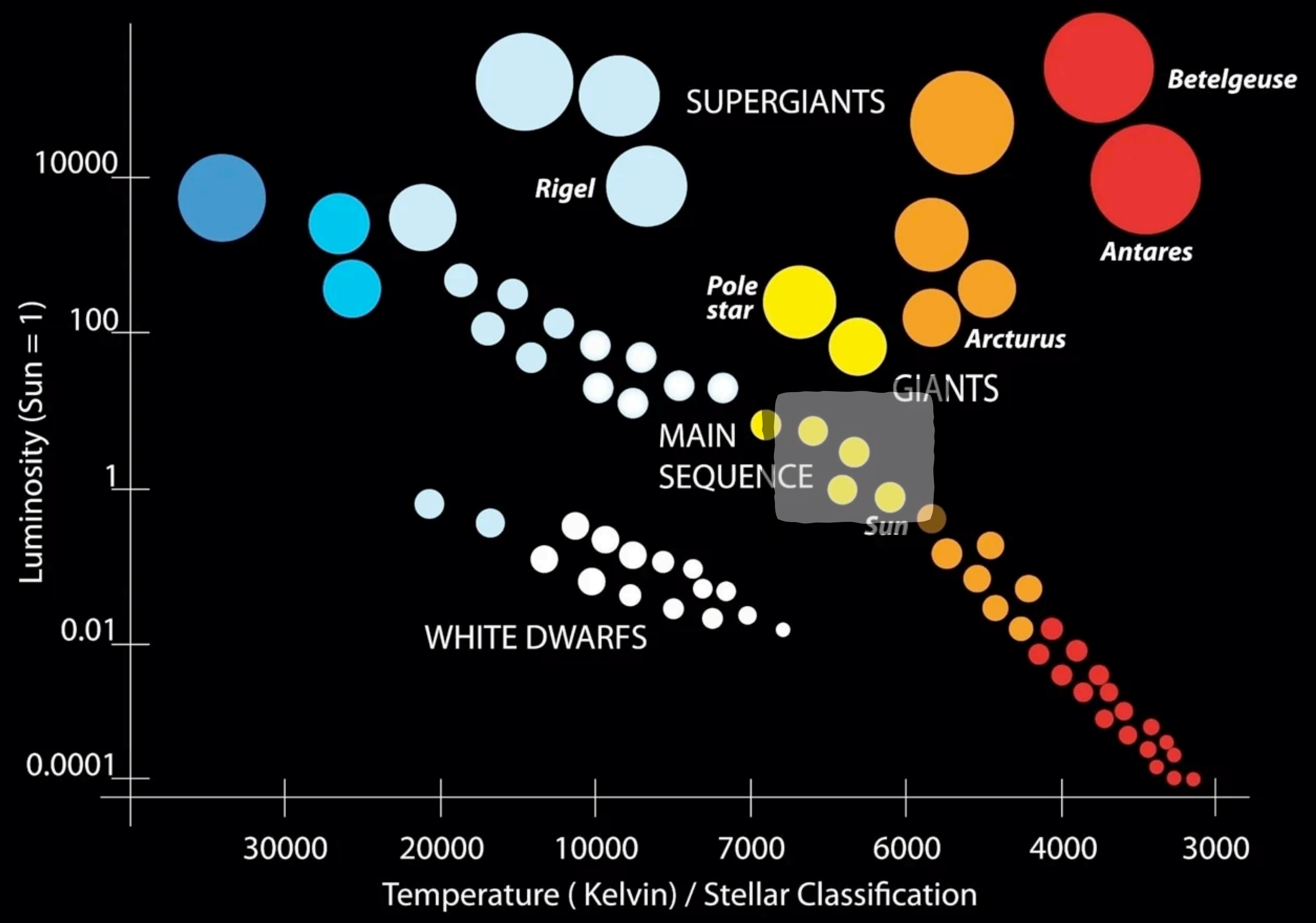
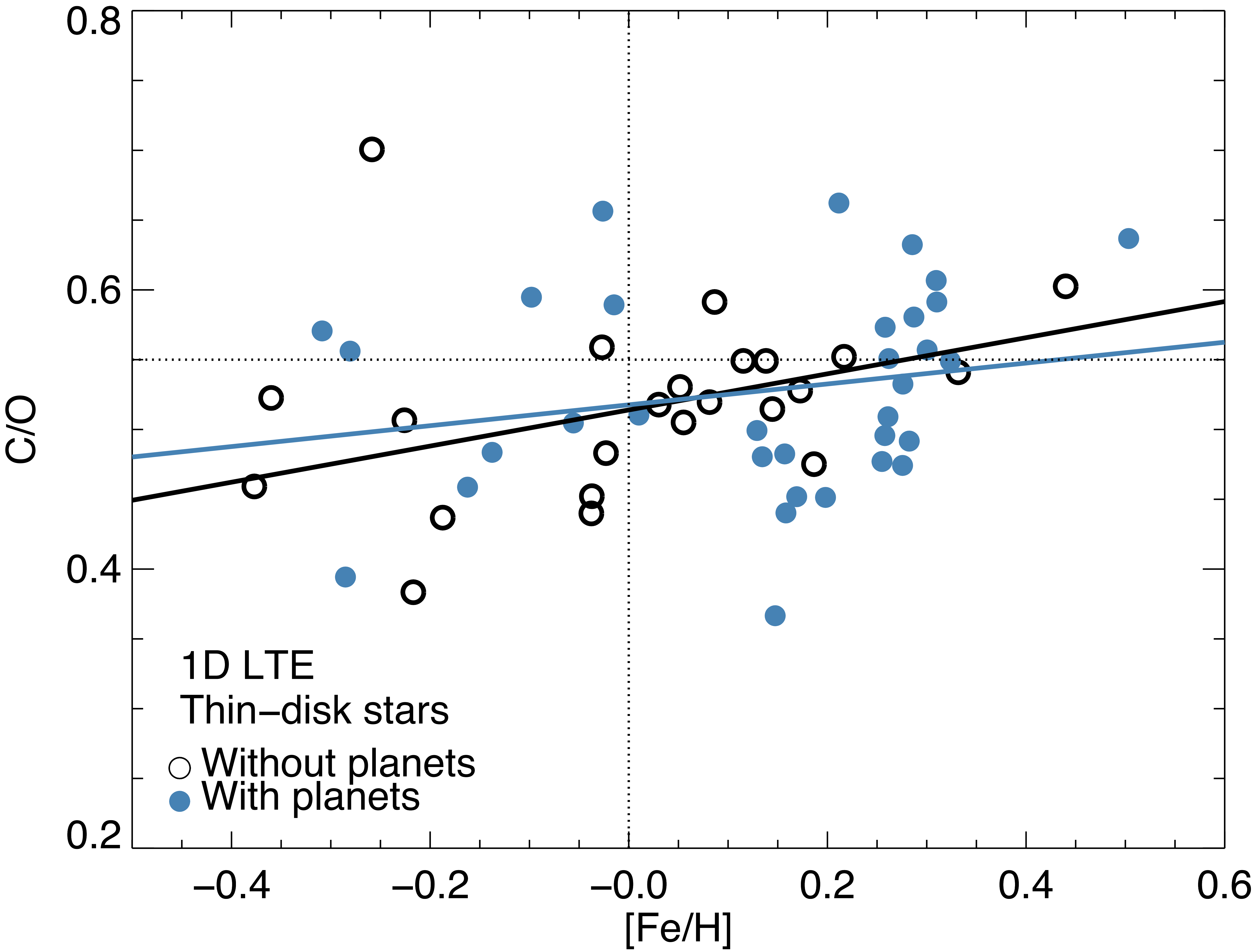
2. C/O planet signature





2. C/O planet signature

- C and O abundances for stars in the thin disk **with** and **without** confirmed planets
- LTE analysis: two populations overlap



[Amarsi, Nissen and Skúladóttir 2019]

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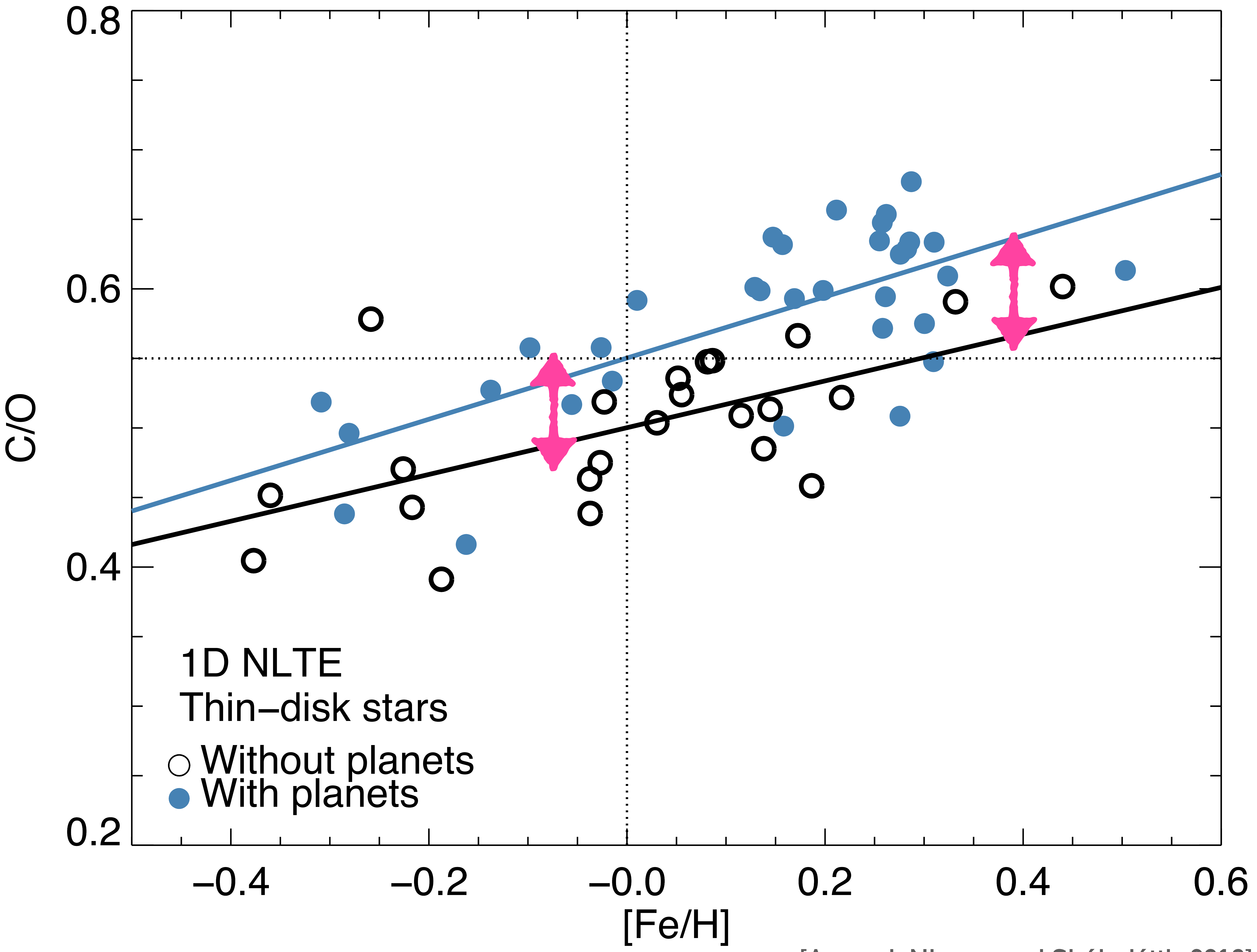

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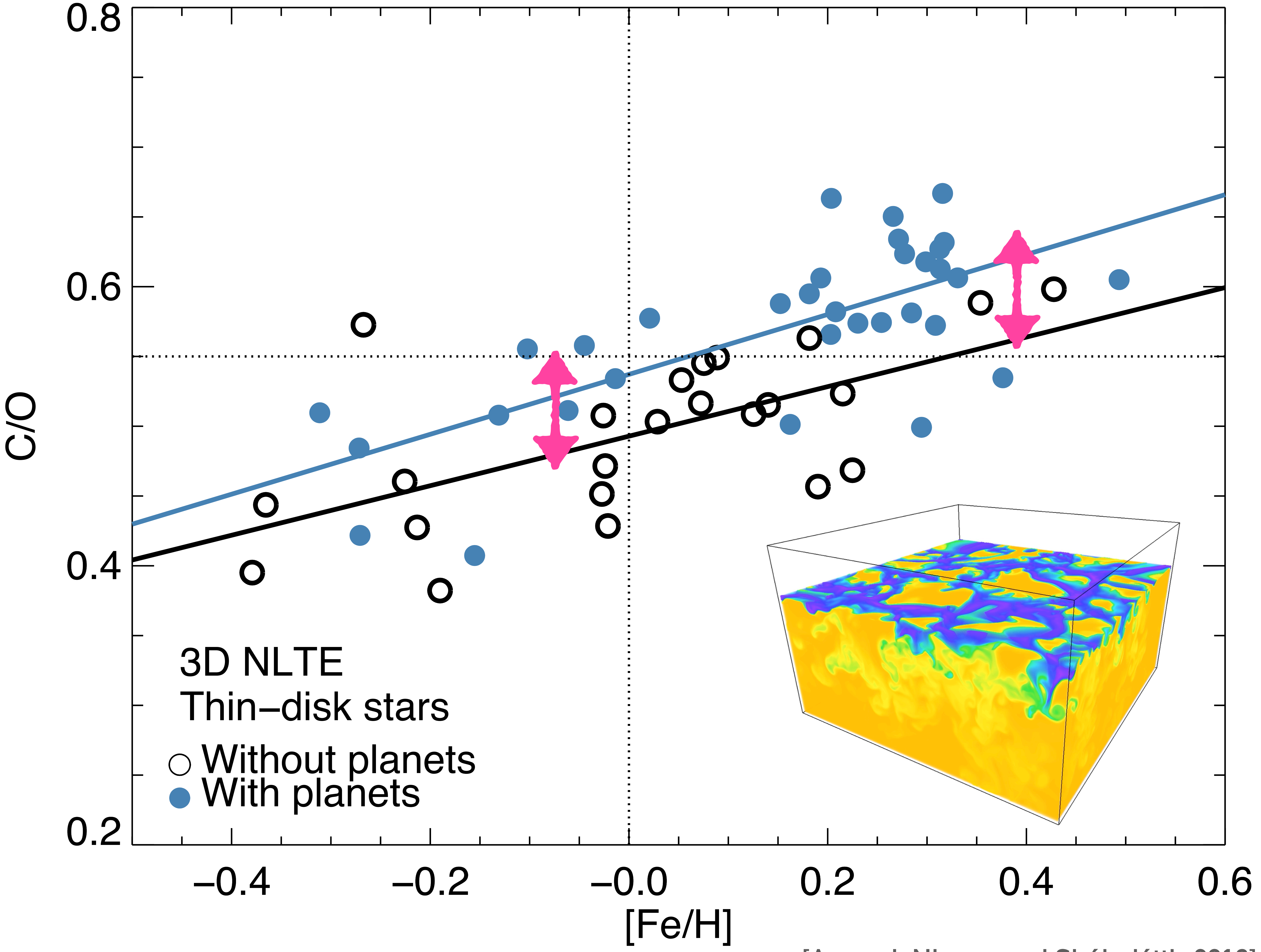

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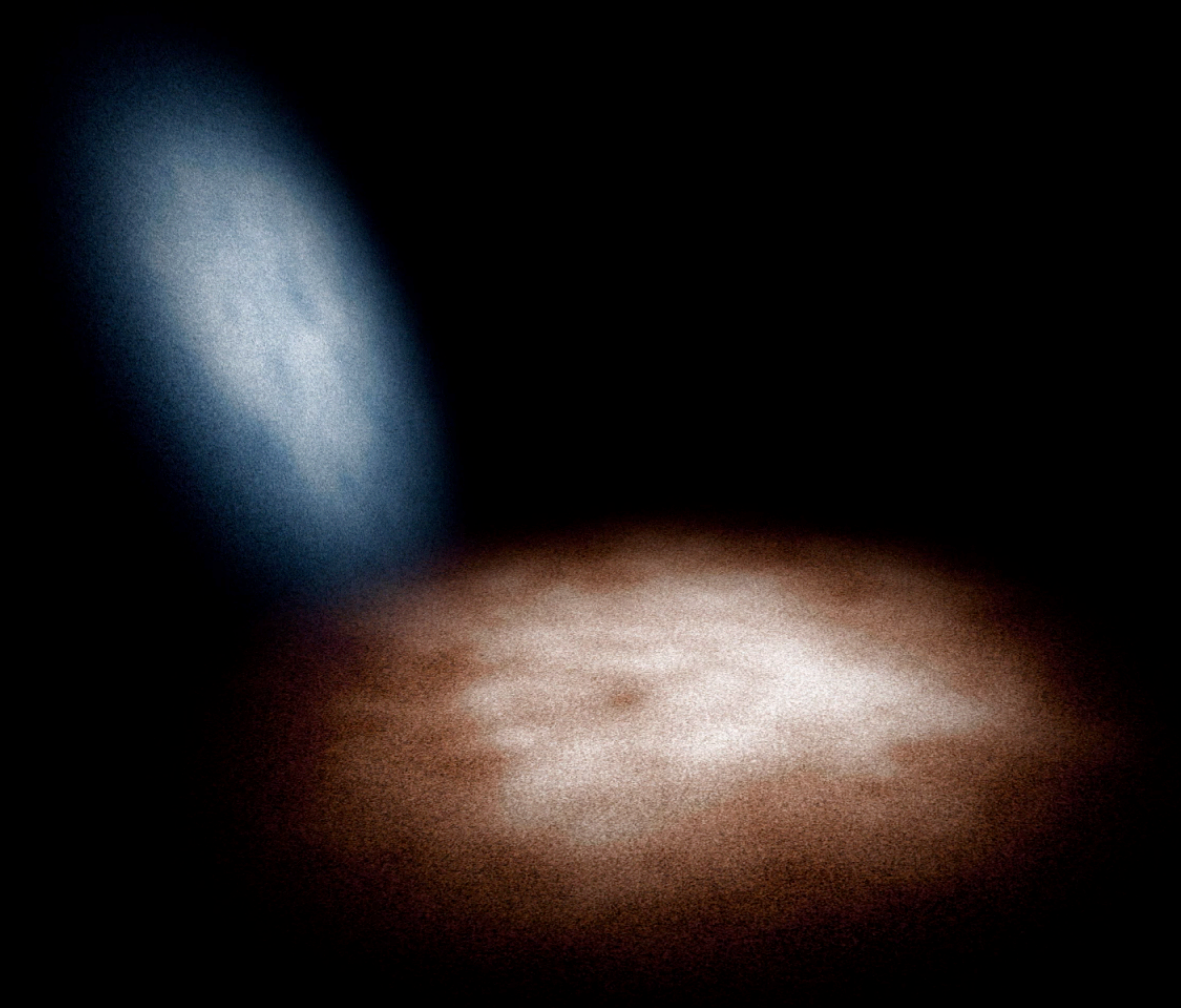
3. [Mg/Fe] accretion signature



Early days of the Milky Way, artist impression [Gabriel Pérez Díaz, SMM, IAC]

3. [Mg/Fe] accretion signature

- Mg abundances for stars in the Galaxy
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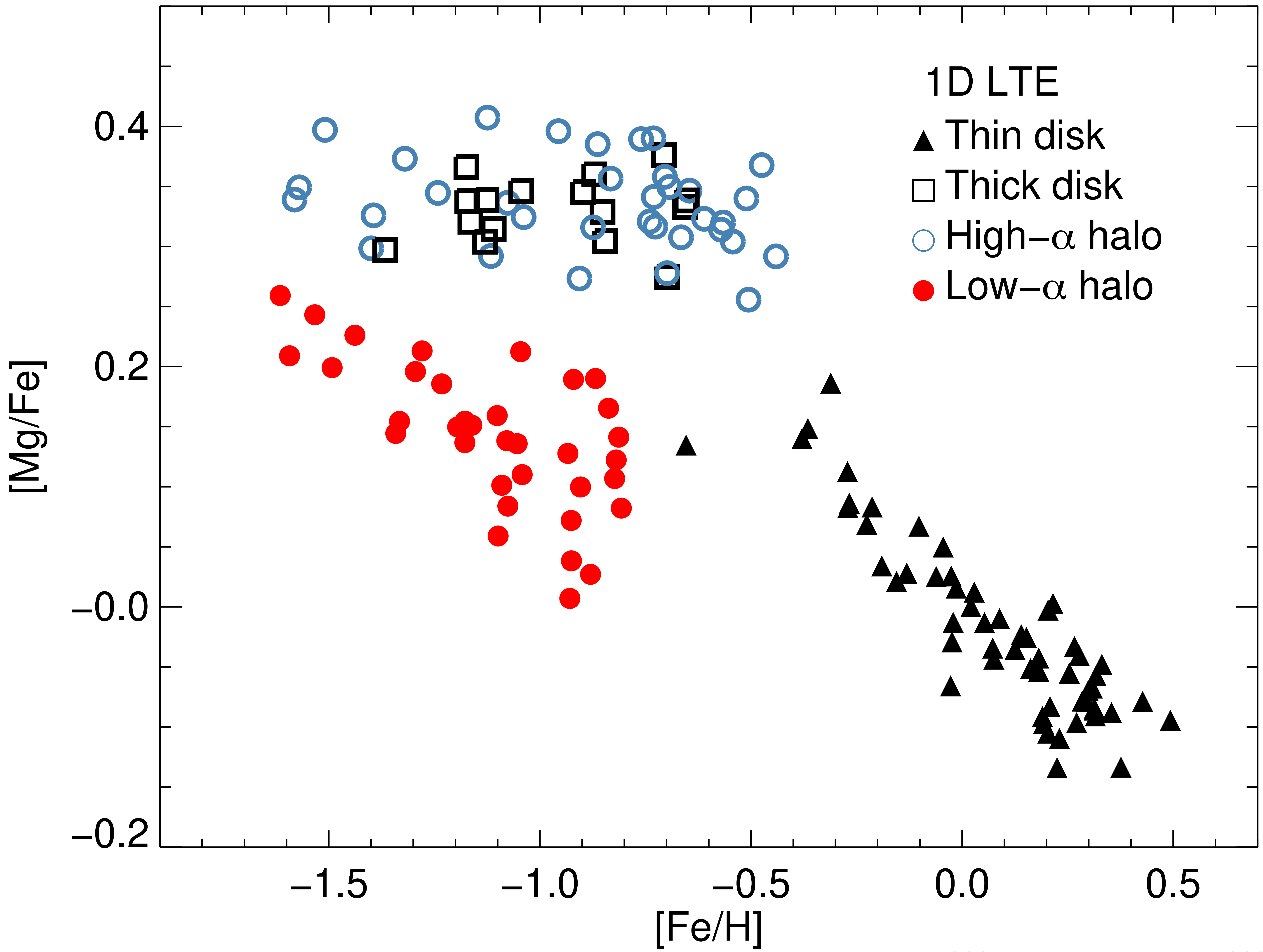

[Nissen, Amarsi, et al. 2024; Lind and Amarsi 2024]

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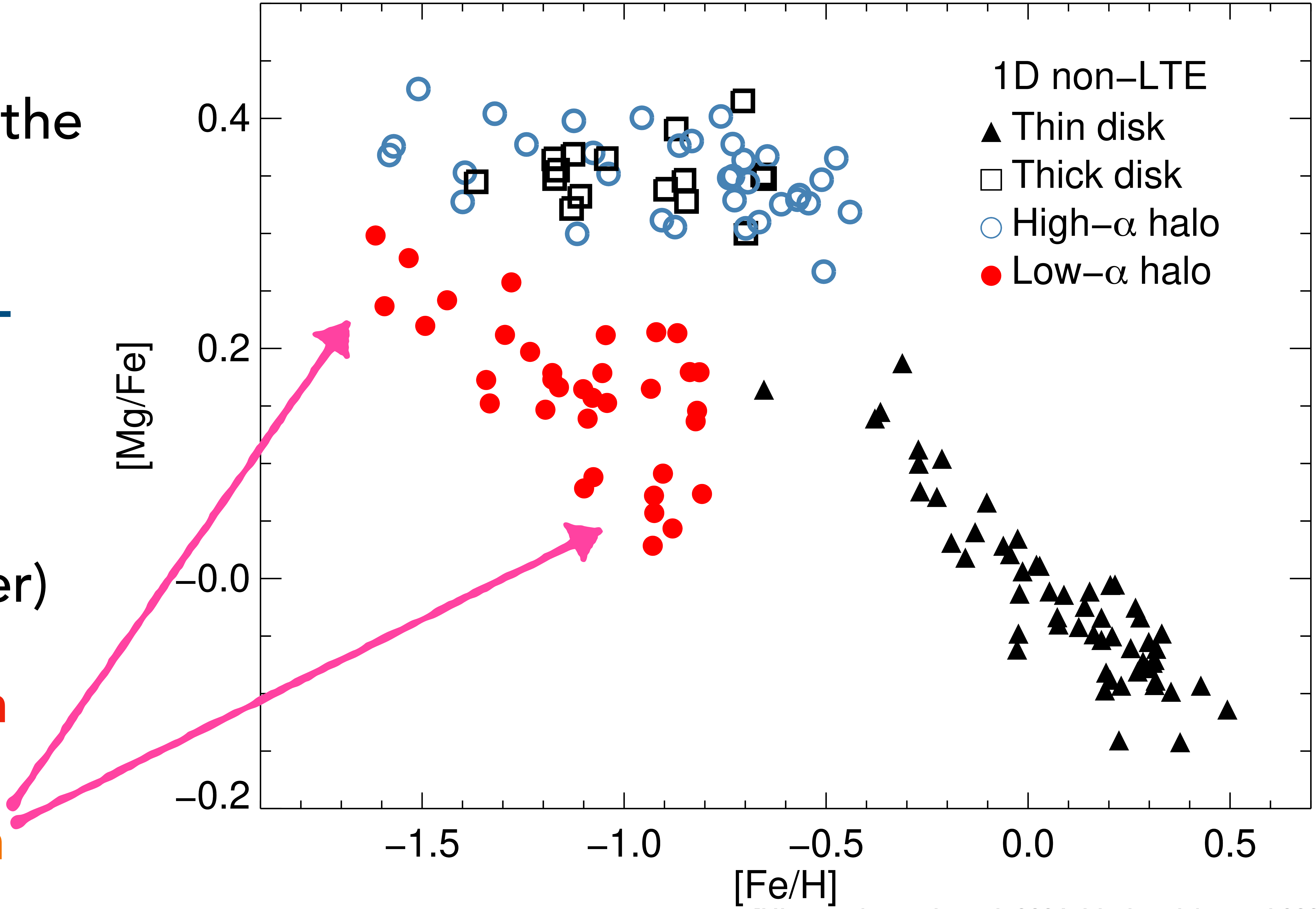

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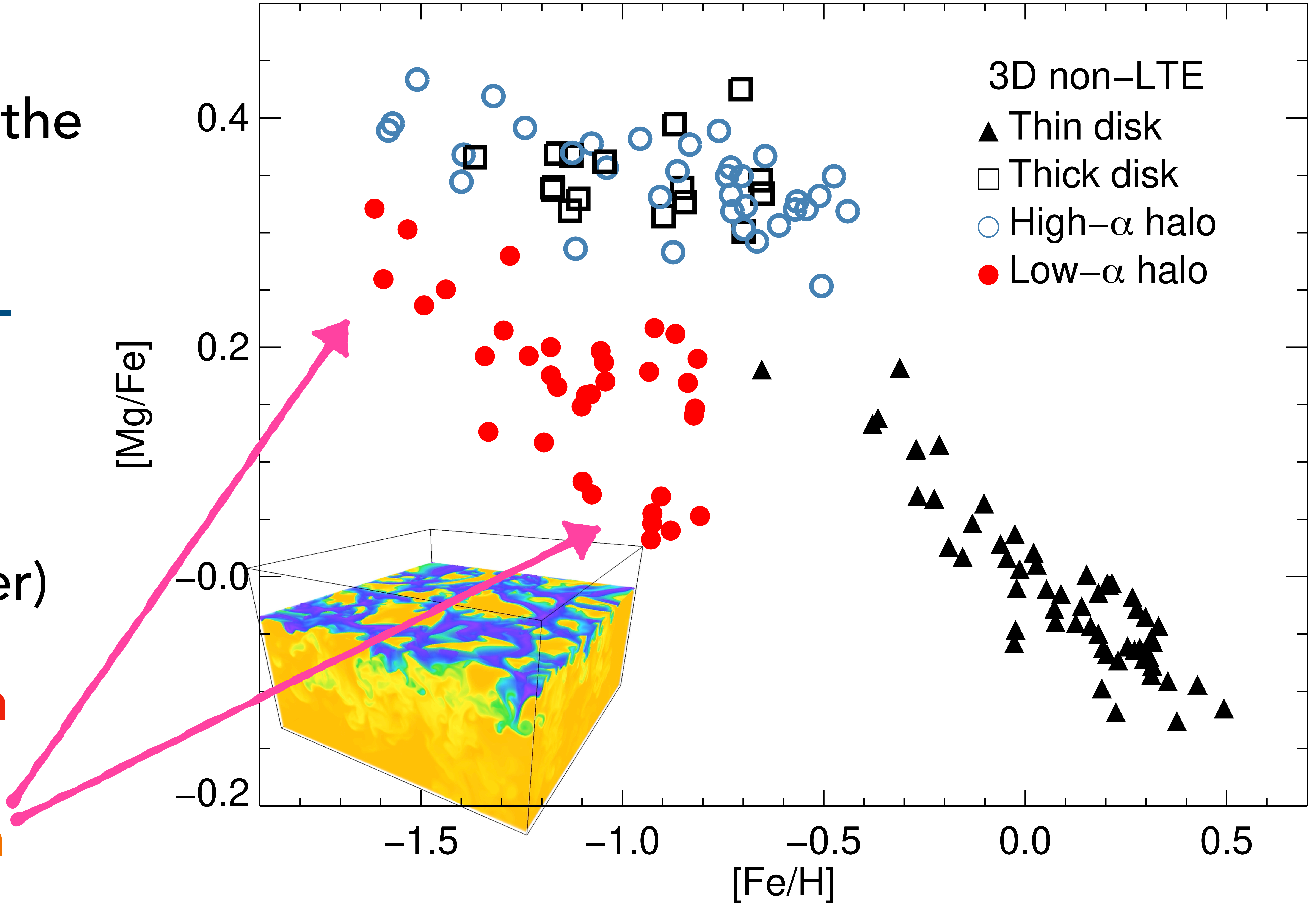

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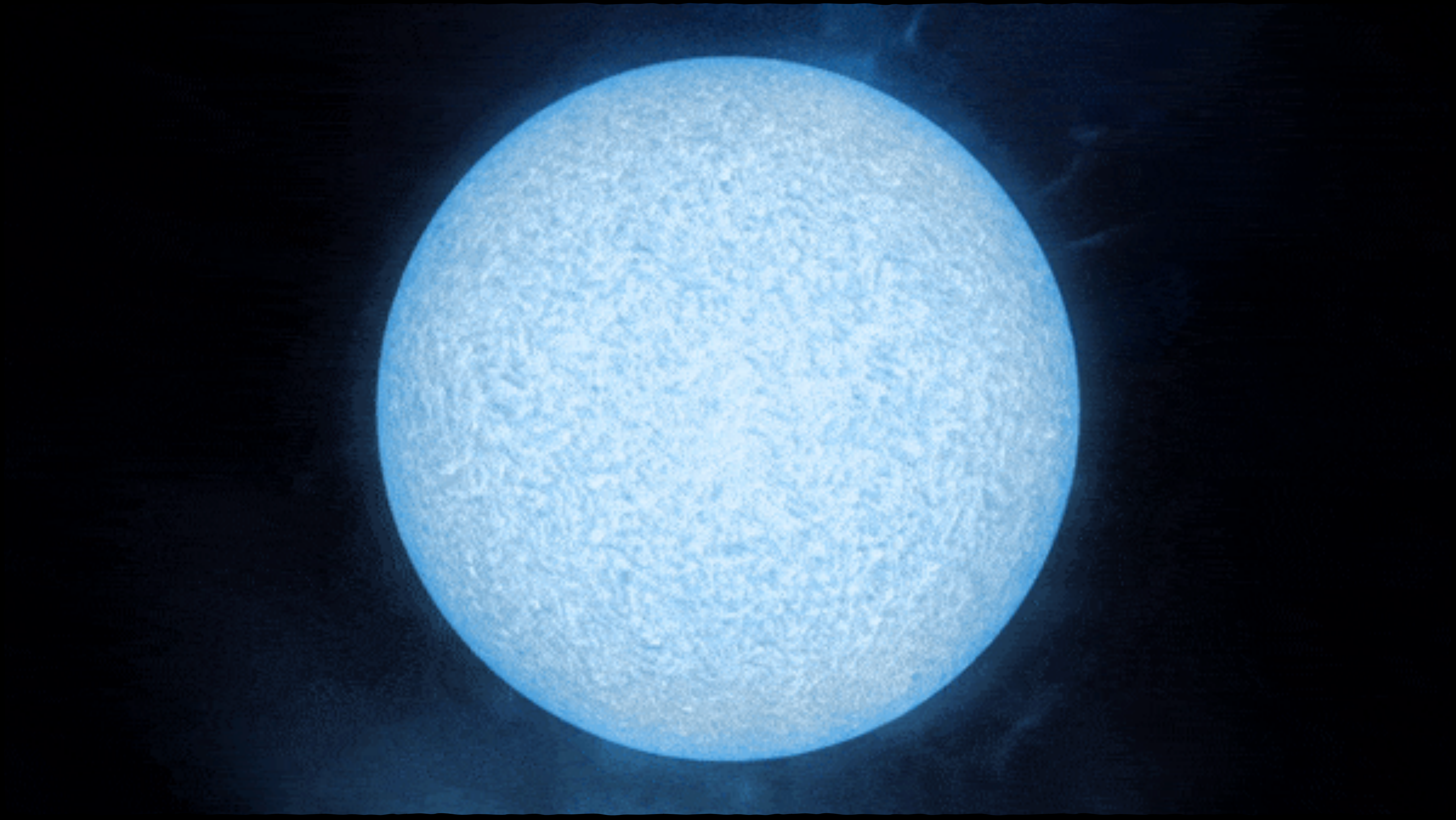
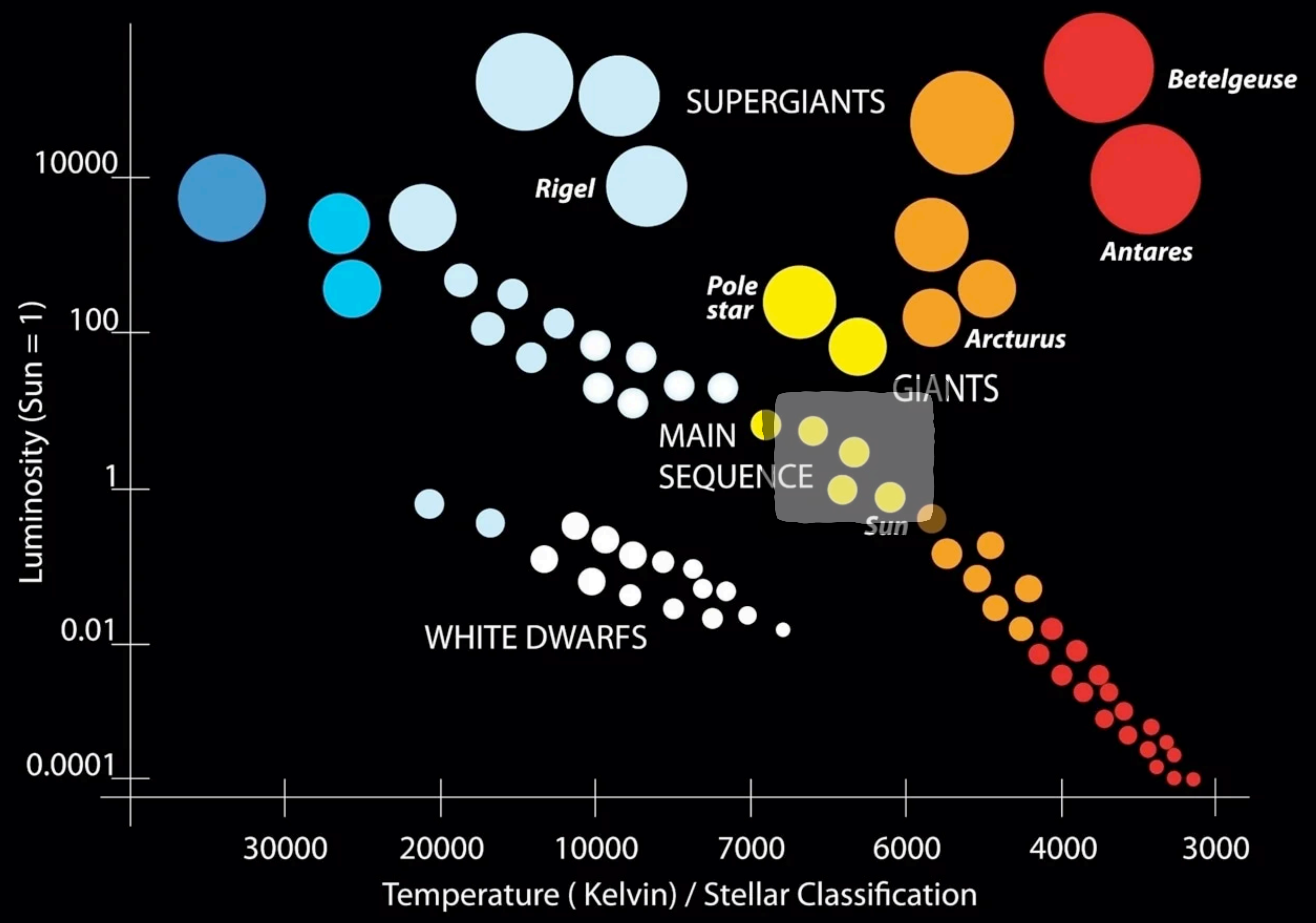
4. [C/O] Pop III signature





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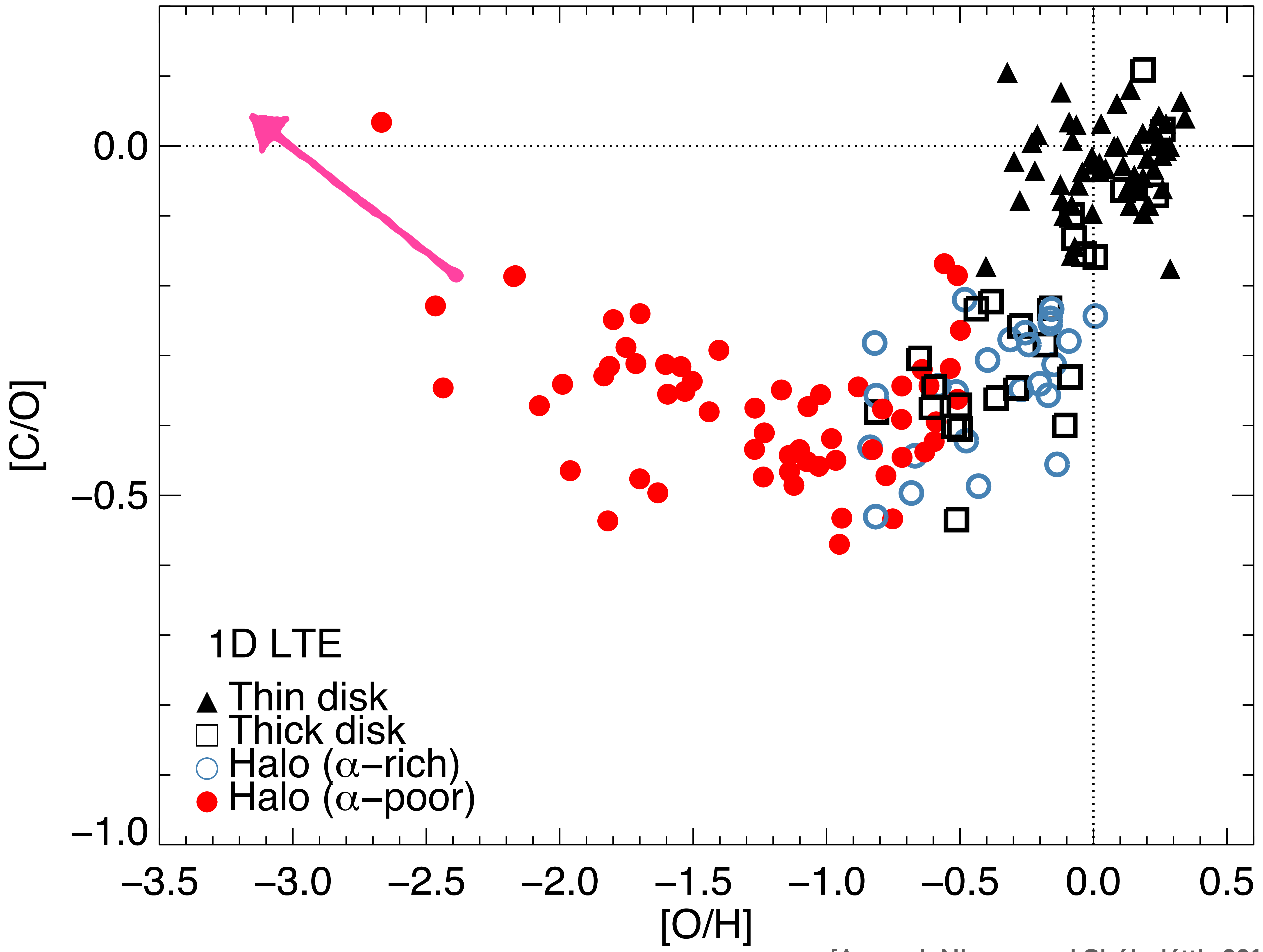

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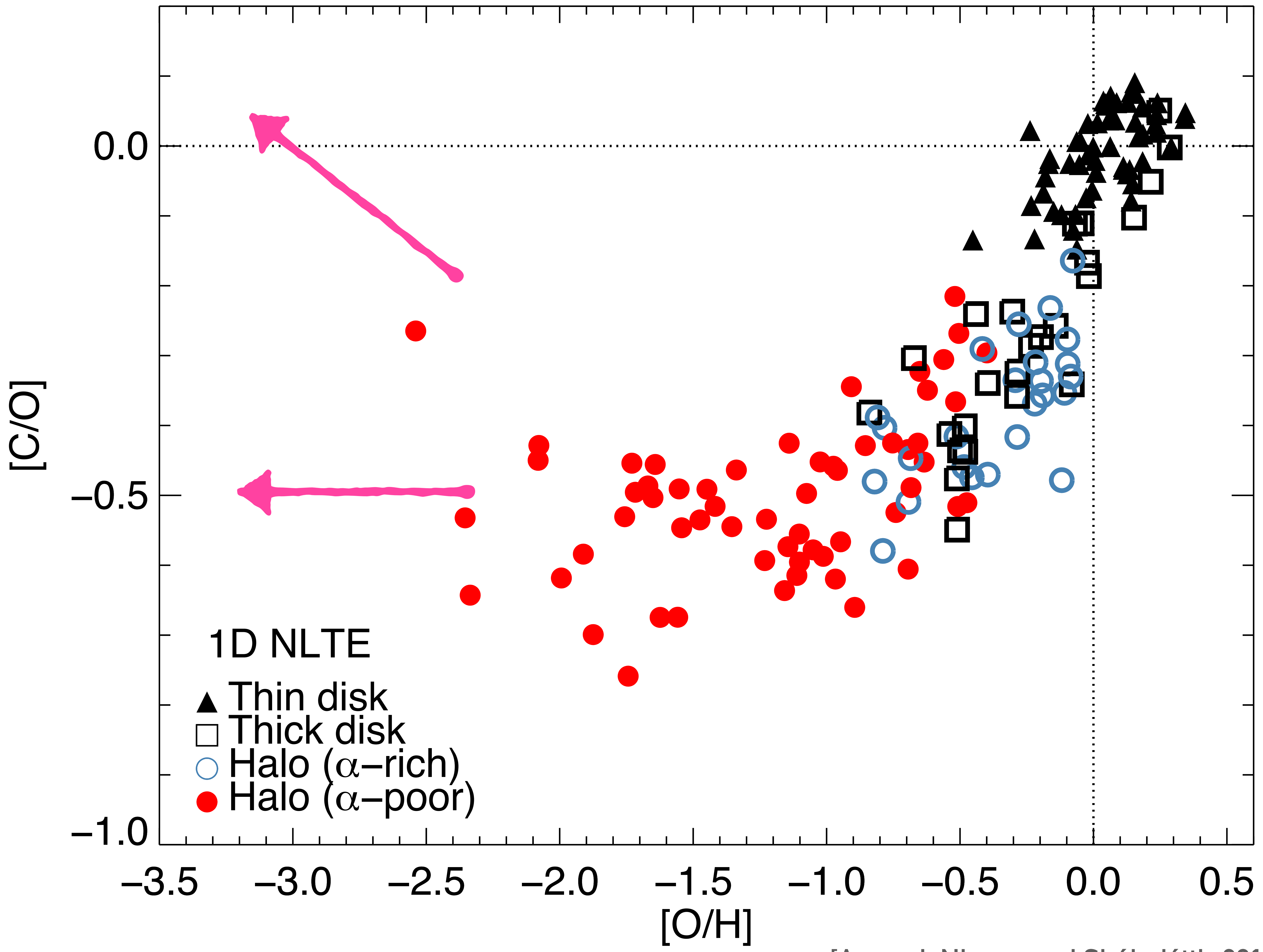

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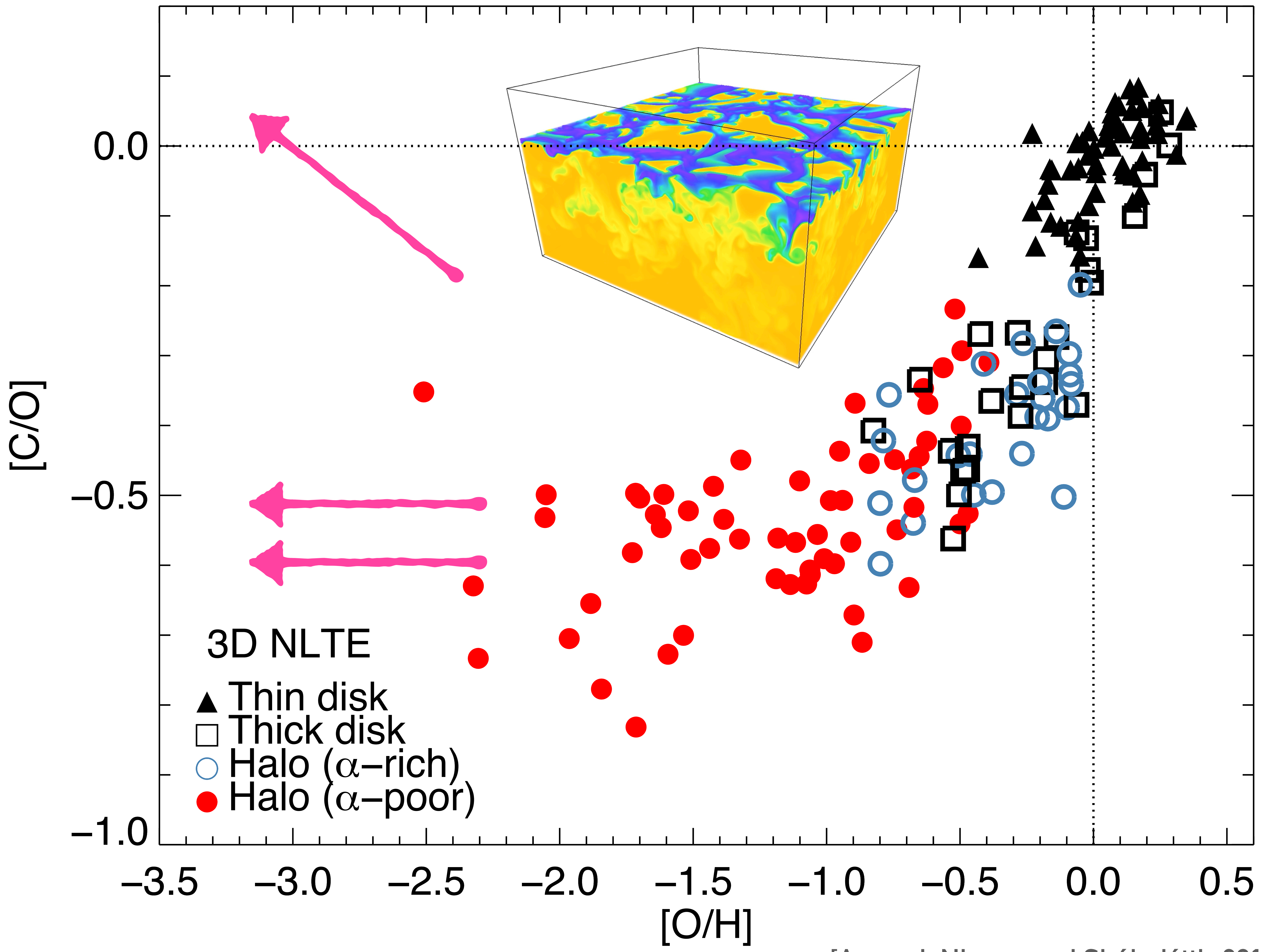

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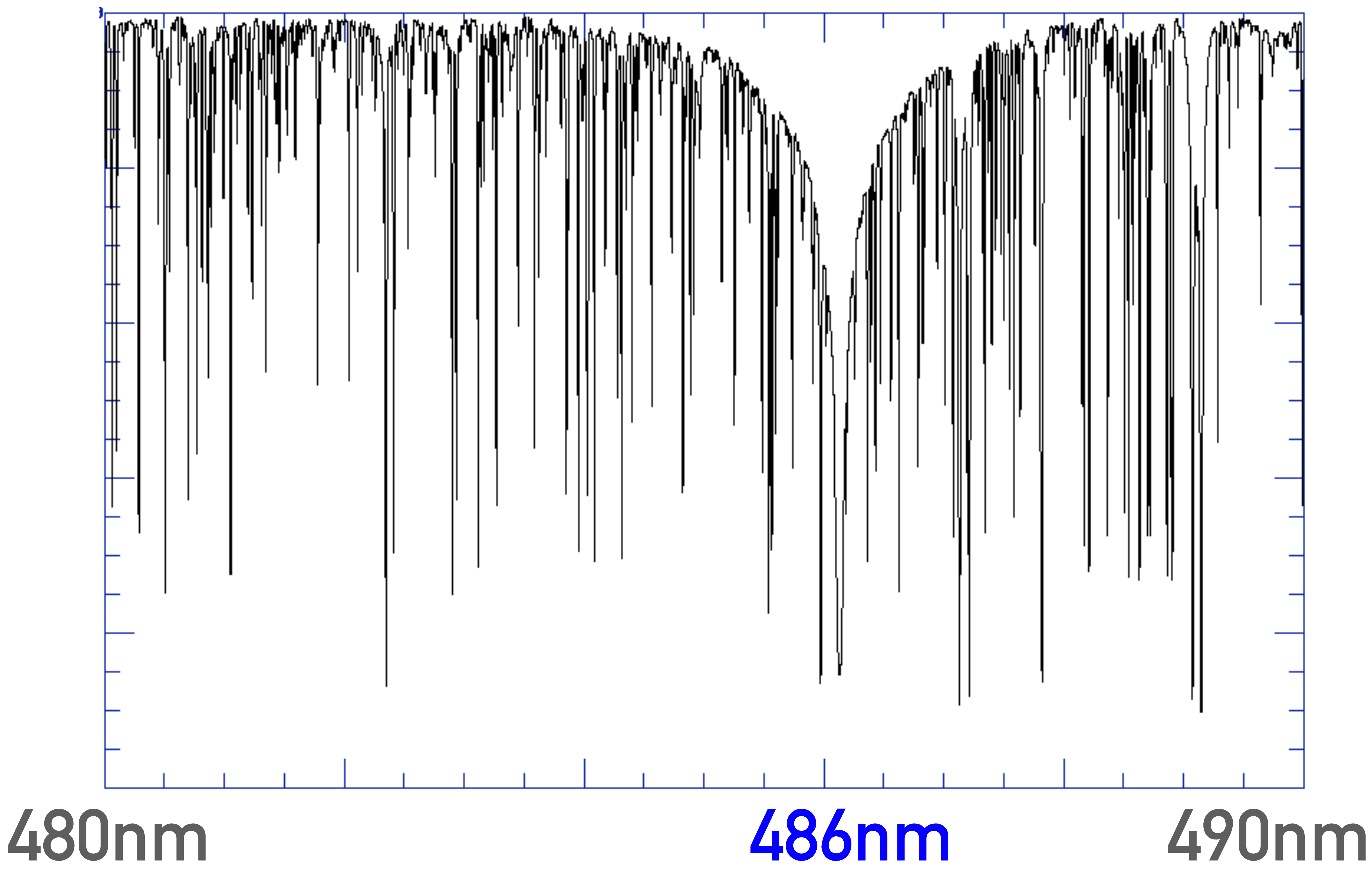
Theory and methods

When is LTE valid? How do we calculate non-LTE spectra in practice?
[See Rutten (2003) lecture notes, Hubeny & Mihalas (2015) textbook, Lind & Amarsi (2024) review]

Populations in LTE

- Absorption line strengths depend on **number of absorbers and emitters** in the correct energy states

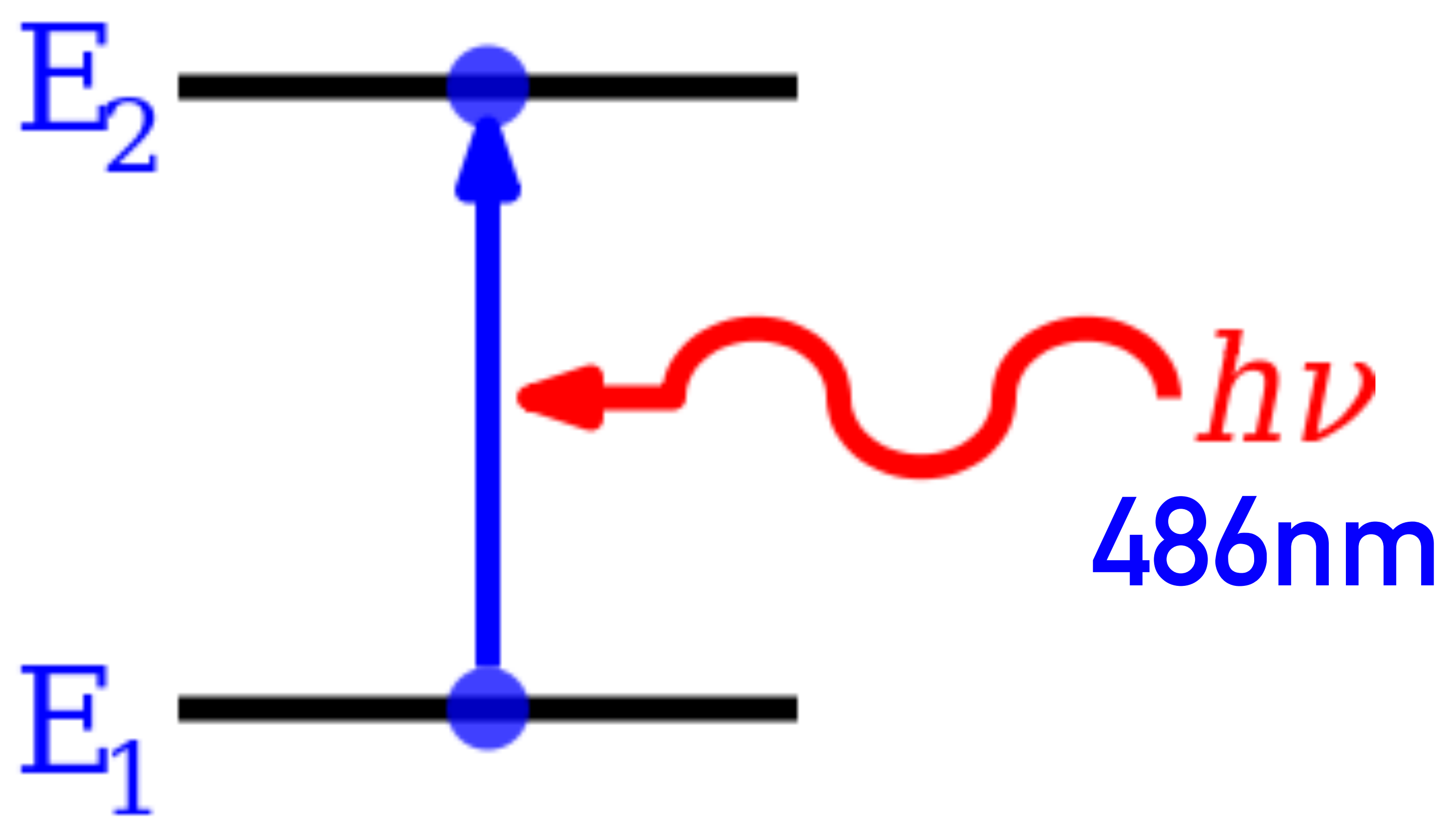


Populations in LTE

- Absorption line strengths depend on **number of absorbers and emitters** in the correct energy states

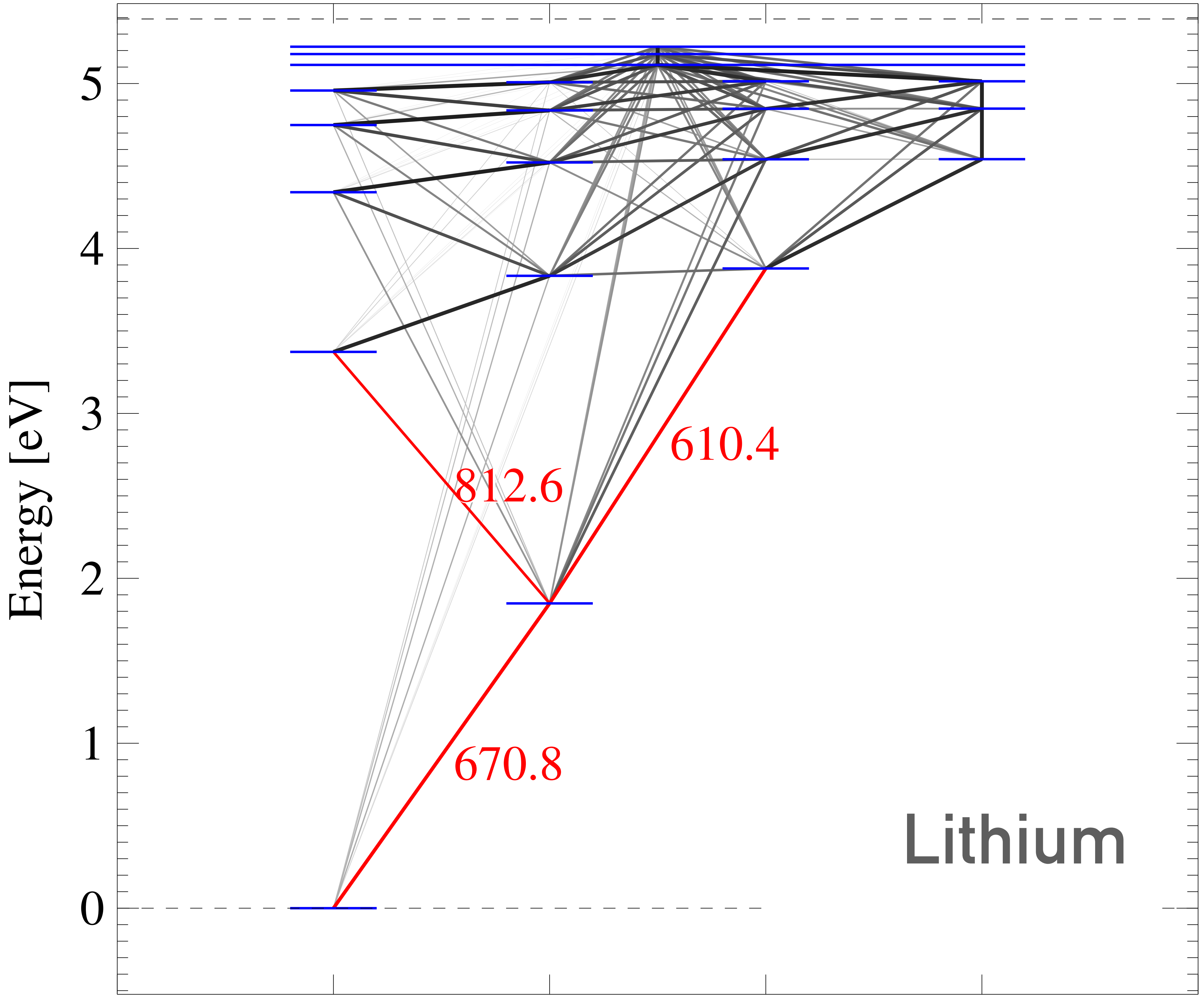
- Local thermodynamic equilibrium (LTE): trivially known via **Saha and Boltzmann distributions**

  - $$\frac{n_2}{n_1} = \frac{g_2}{g_1} \exp\left(-\frac{E_2 - E_1}{k_B T}\right)$$
  - $$n_e \frac{N_{II}}{N_I} = \frac{2}{\Lambda^3} \frac{Z_2}{Z_1} \exp\left(-\frac{E_{II} - E_I}{k_B T}\right)$$



Populations in non-LTE

- More general solution: solve the rate equations to find **statistical equilibrium**
  - $n_i \Sigma_j [R_{ij} + C_{ij}] = \Sigma_j n_j [R_{ji} + C_{ji}]$
- ***C*** are collisional rates, depend on **local Maxwellian-averaged** cross-sections
- ***R*** takes into account **non-local photons**
  - e.g. for bound-bound absorption, $R_{lu} = \int_0^\infty B_{lu} J_\nu \varphi\left(\nu - \nu_0\right) \mathrm{d}\nu$, mean radiation field J_ν determined via **radiative transfer**



[Wang, Nordlander, et al. 2021]

Interpretation

- Radiation in atmosphere is non-Planckian
  - At a particular layer in the atmosphere, locally-generated photons are scattering out and escaping (TE assumes all emitted photons are immediately reabsorbed) — photon losses
  - Photons escaping from other (mostly deeper) layers scatter into the layer you are trying to model — photon pumping, overexcitation/overionisation

Stagger simulations + Balder non-LTE post-processing [Thomas Nordlander, Australian National University]

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Interpretation

For which stars do we typically expect stronger non-LTE effects?
High or low $\log g$?
High or low $T_{\rm eff}$?

- Radiation in atmosphere is non-Planckian
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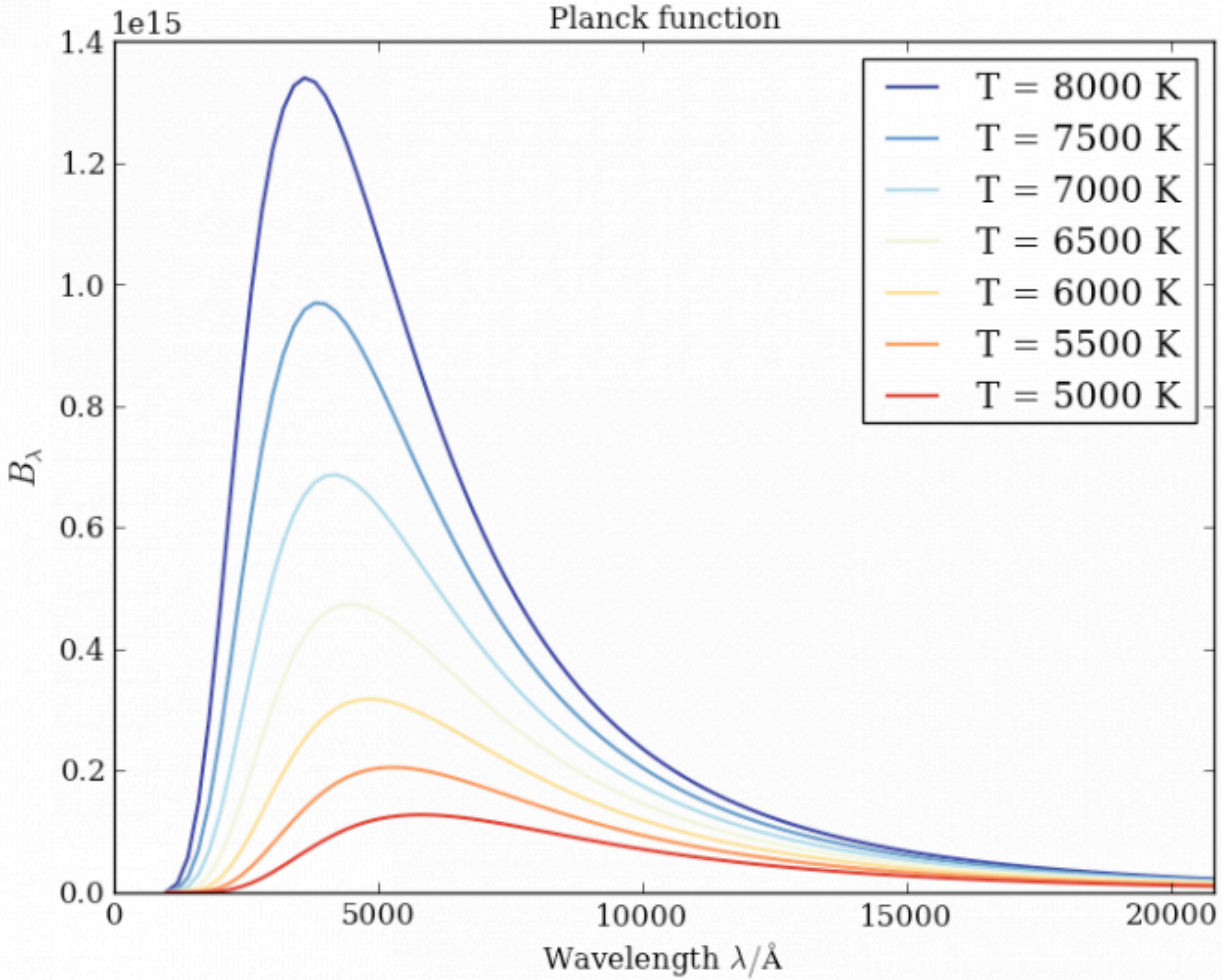
  - Photons **escaping** from other (mostly deeper) layers scatter into the layer you are trying to model — photon pumping, overexcitation/**overionisation**
- Particles have LTE (Maxwellian) velocities (Hubeny and Mihalas chapter 4)
- Competition between **collisions** (LTE) and (escaping) **radiation** (non-LTE)

Interpretation

- **Lower $\log g$**
  - Lower gas pressure
  - Fewer collisions to bring system to LTE
- **Higher T_{eff}**
  - Larger (escaping) UV flux (dB/dT is large in the UV), more photon pumping
  - Usually have high density of atomic/ ionic lines and important photoionisation thresholds in the UV

Beware there are exceptions, and cancellation effects, depending on the species and spectral line



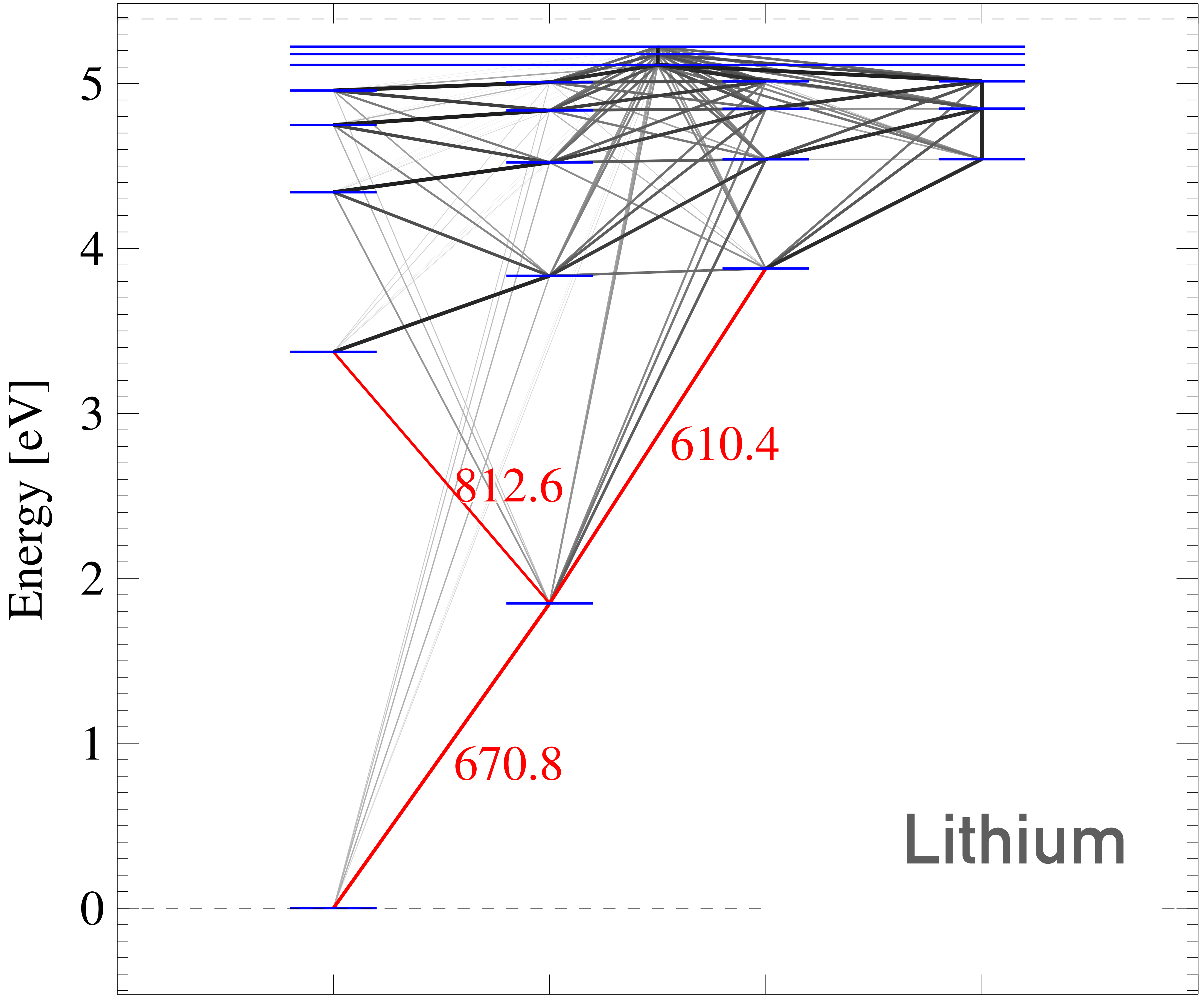
Non-LTE codes

- Commonly used codes include MULTI, DETAIL, TLUSTY, CLOUDY,…
- (Examples in this presentation use **BALDER**, an offshoot of Multi3D, with links to MULTI)
- One **uncertainty** is the equation of state and **background opacities** of the non-LTE code
  - Background opacities block the radiation from the species of interest, generally (but not always) reducing departures from LTE
  - Good to check when was the last time this was updated

The model atom

- Energies, statistical weights, partition functions
- Radiation: transition rates (Einstein A's), photoionisation cross-sections
- Collisions: (low-energy) collision cross-sections (free electrons; hydrogen in cool stars)

- Non-LTE solution is only as good as the input atomic (and ionic) data
- This compilation of data is called the "model atom"
- Significant effort to construct and test model atoms
- Relevant atomic/molecular data are often missing/inaccurate



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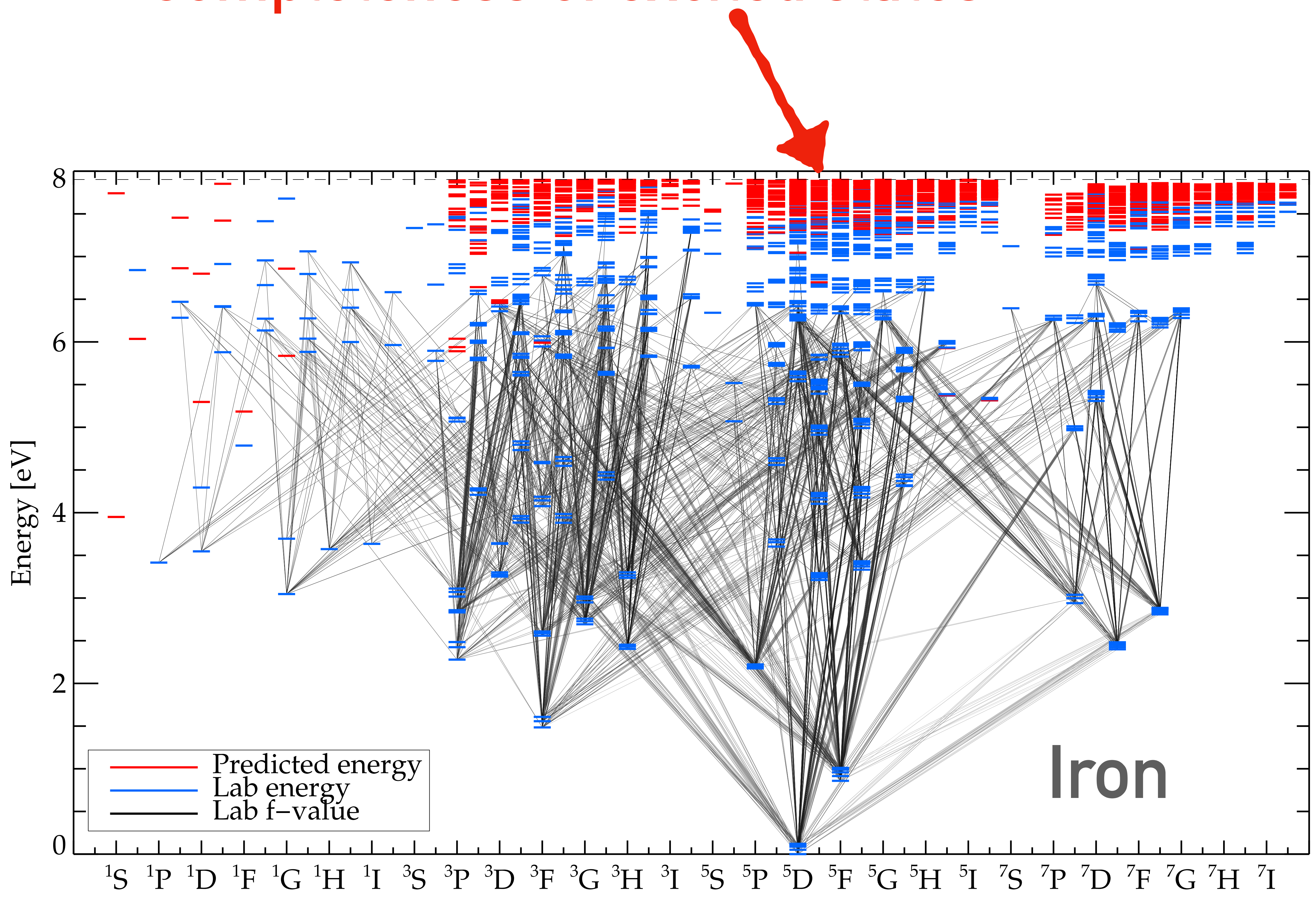
Some **uncertainties** for hot stars:

- Photoionisation cross-sections (e.g. hydrogenic vs R-matrix)
- Electron collisions (e.g. van Regemorter or Seaton recipes vs R-matrix)
- **Completeness of excited states**



[Lind and Amarsi 2024]

Typical non-LTE effects

Are non-LTE spectral lines stronger or weaker than LTE spectral lines?

S I infrared triplet in detail

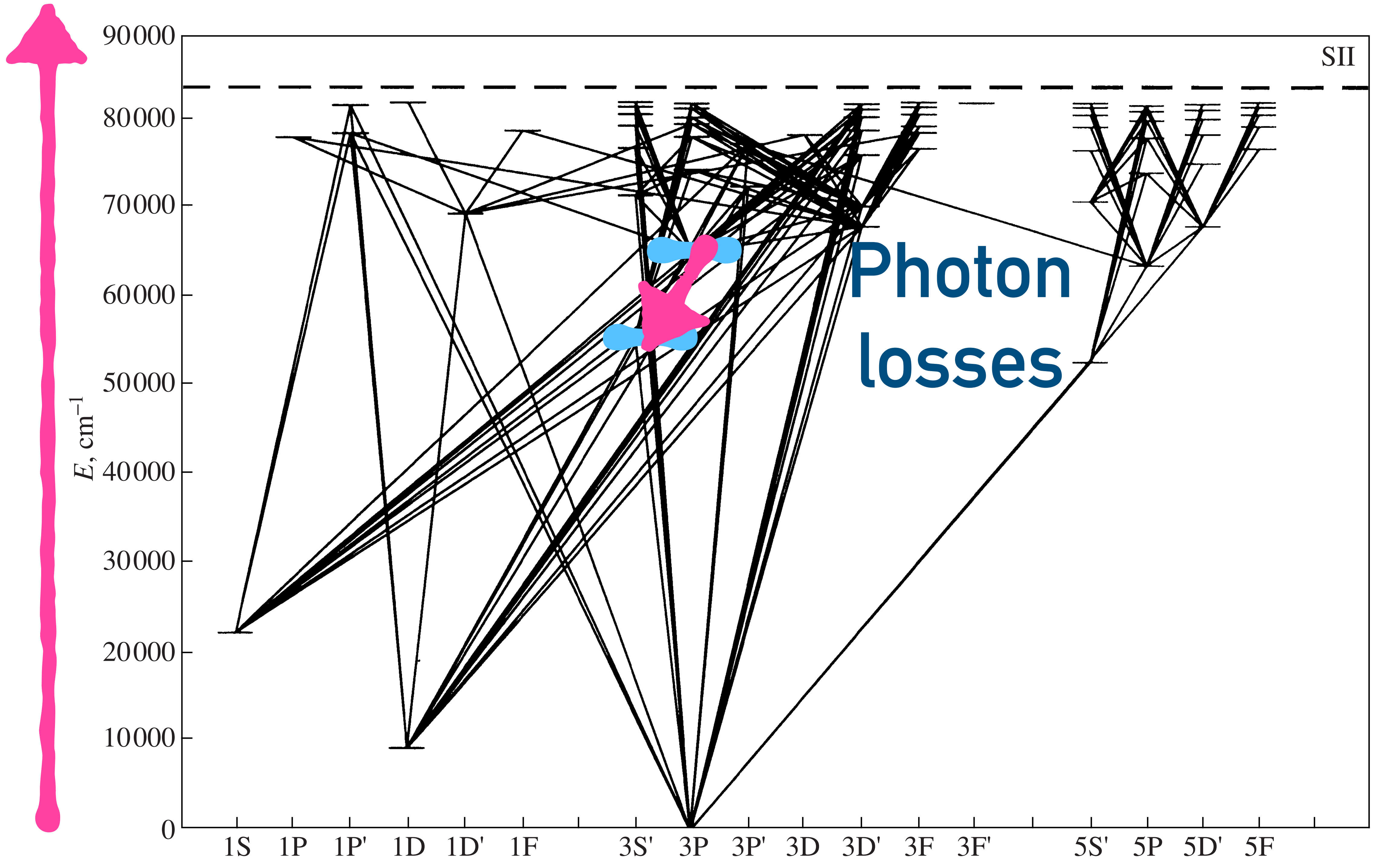
In non-LTE, the blue component gets stronger, the middle component gets weaker — why?

[Kochukhov et al. 2024]

S I infrared triplet in detail

- Transition from $4s\,^3S_1^*$ to $4p\,^3P_{2,0,1}$
- In the model, the $4p\,^3P_{2,0,1}$ level populations have identical departures from LTE
- But middle line component ($4p\,^3P_0$) gets weaker while other line components ($4p\,^3P_{2,1}$) get stronger
- Understand this by looking at **departure coefficients**

Overionisation



Various competing effects

[Korotin 2009]

Departure coefficients $b = \frac{n_{\rm NLTE}}{n_{\rm LTE}}$

- Line **source function** goes as ratio of upper and lower level b's, b_u / b_l
  - Lower source function = stronger line
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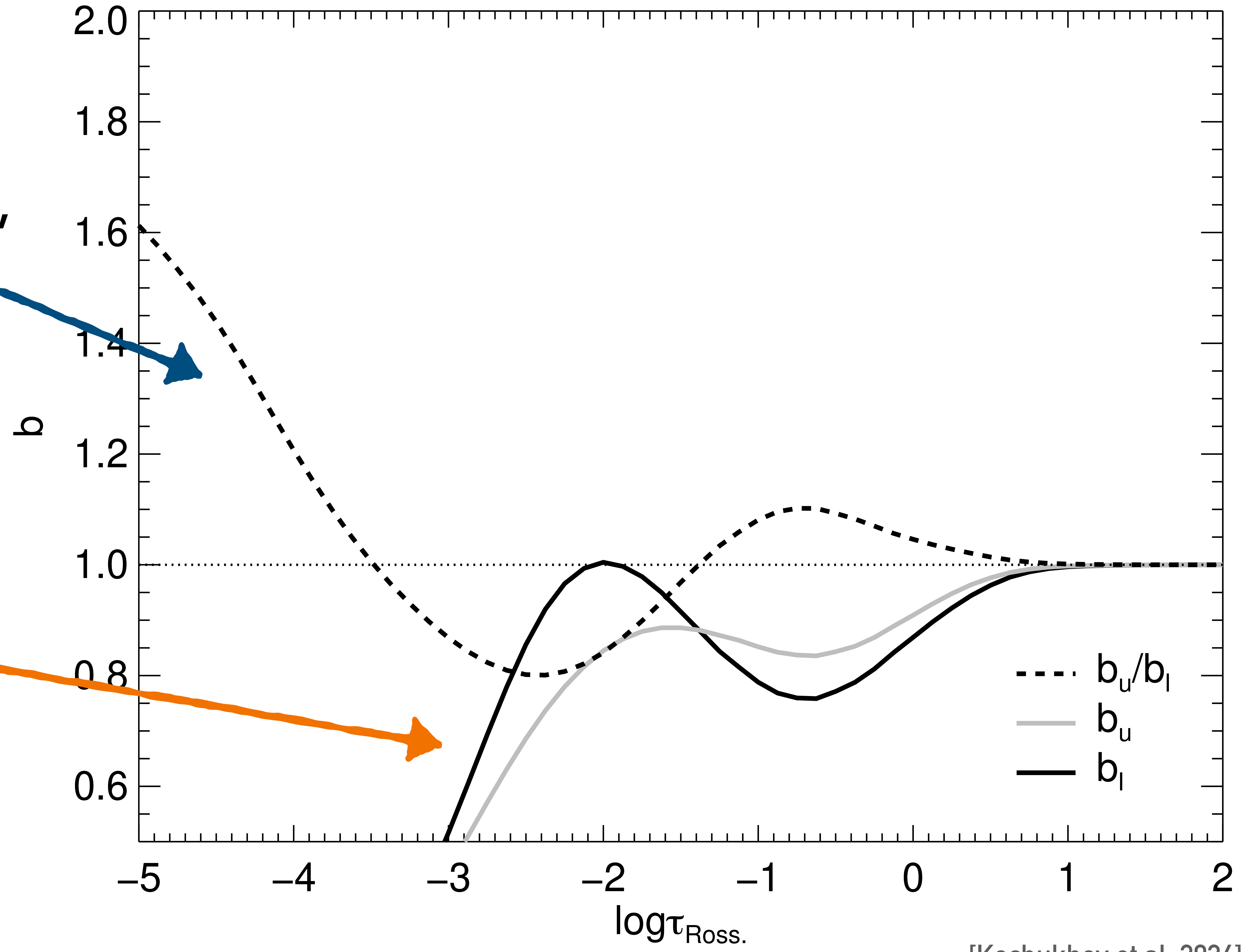

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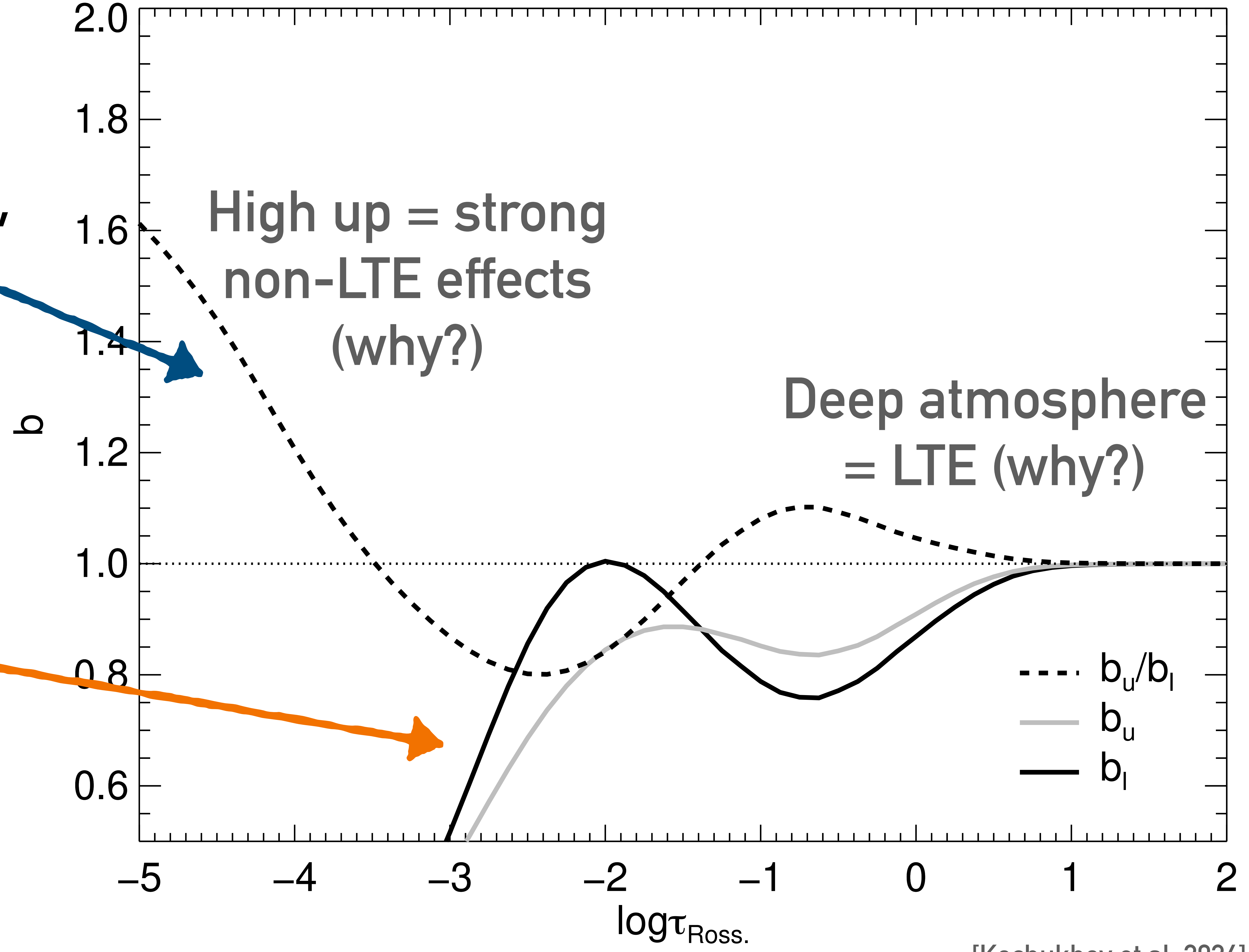

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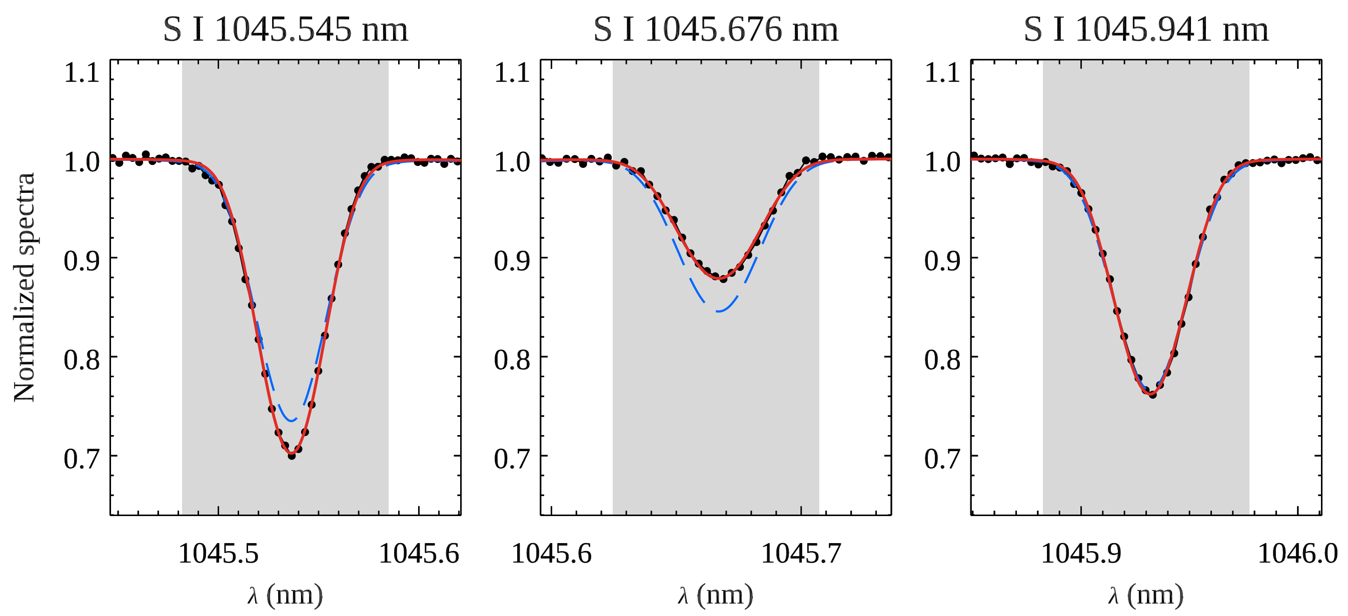

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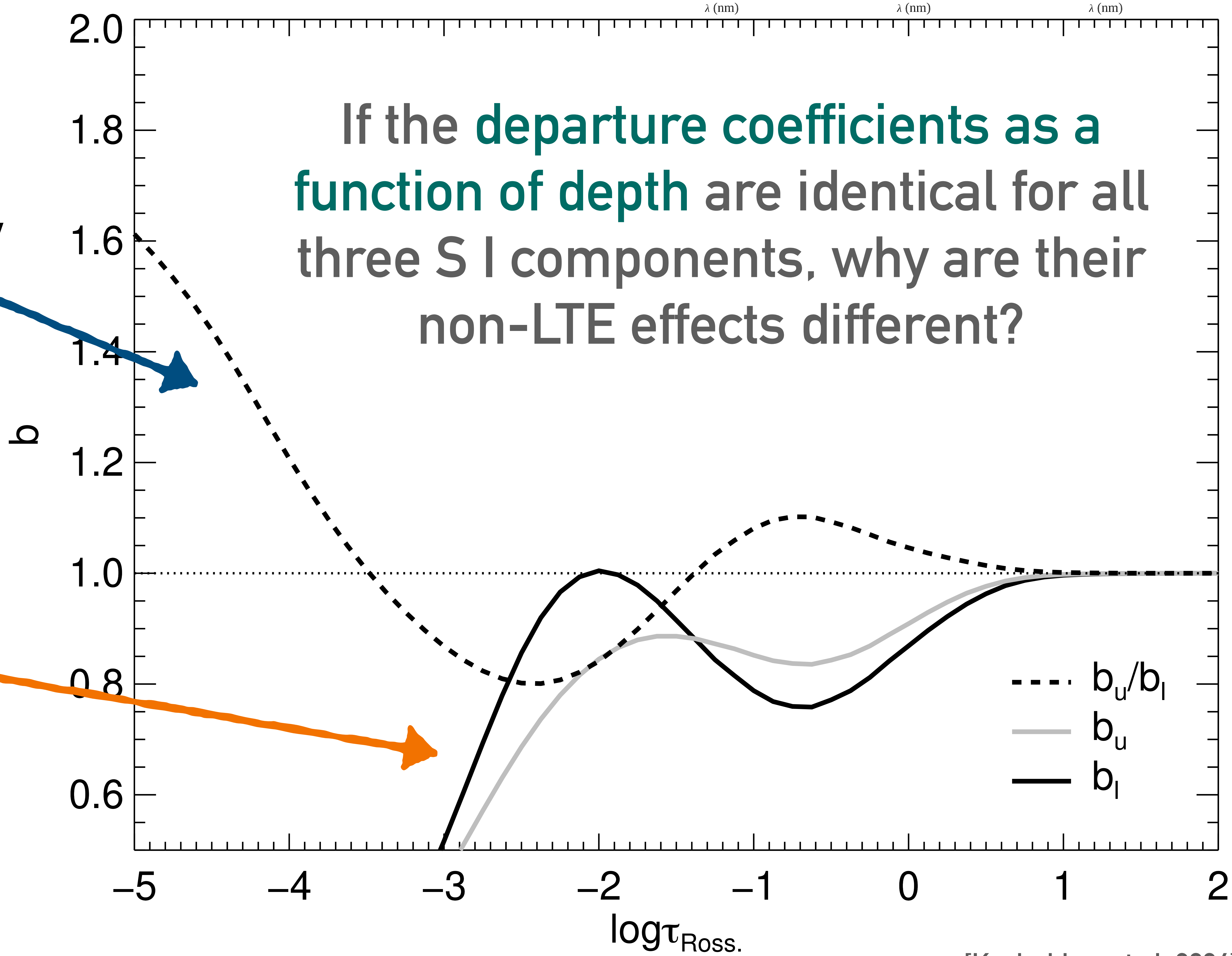

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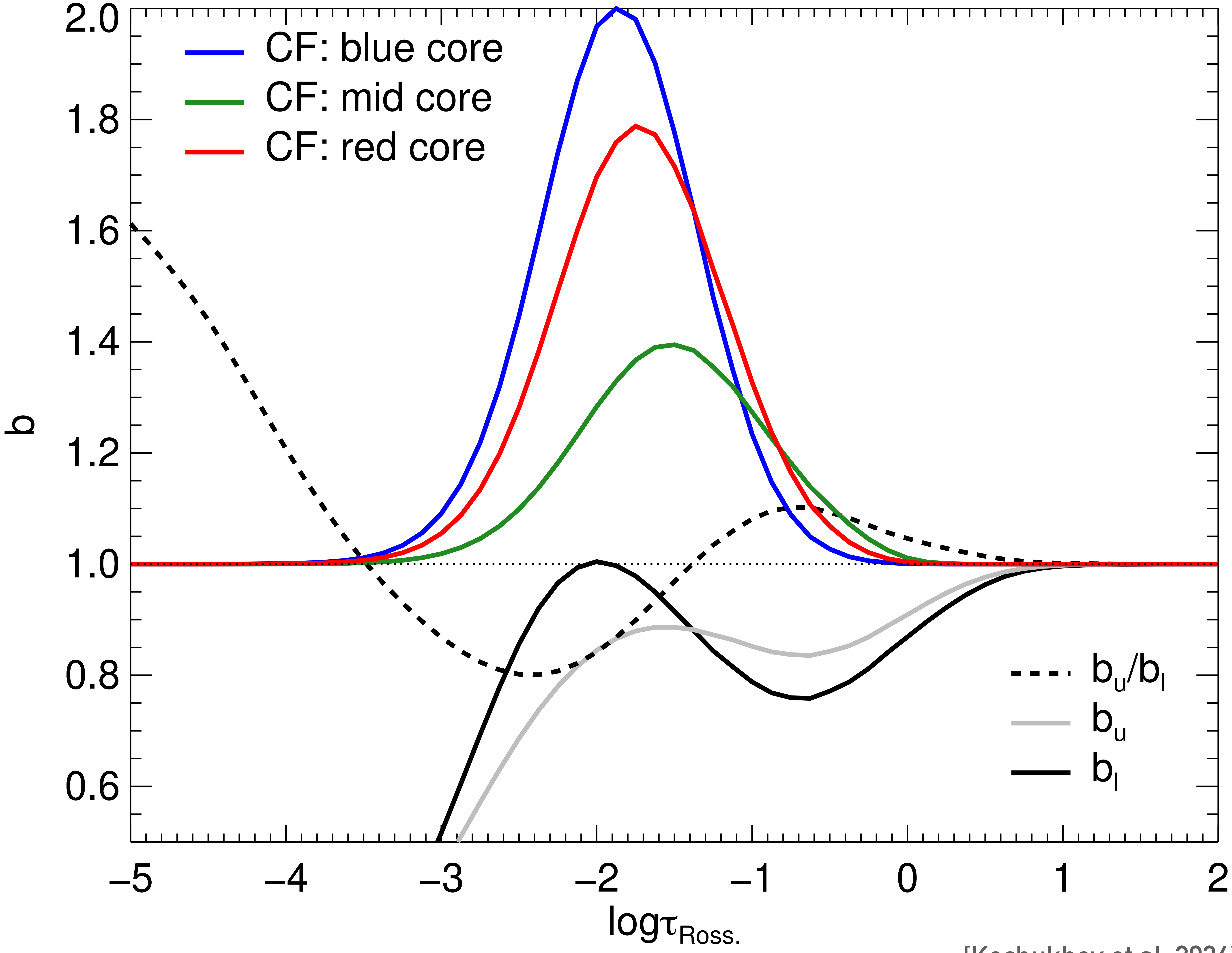

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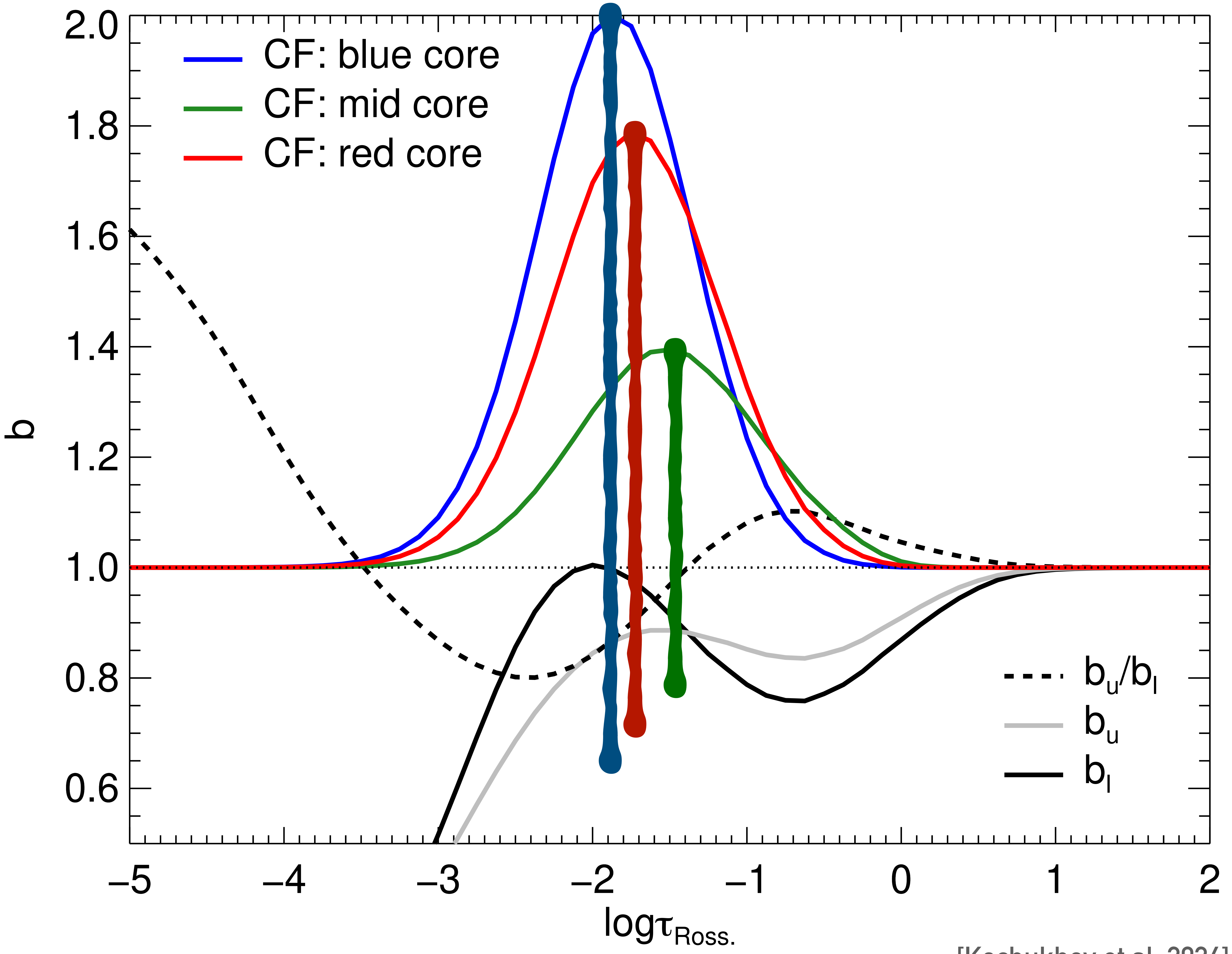

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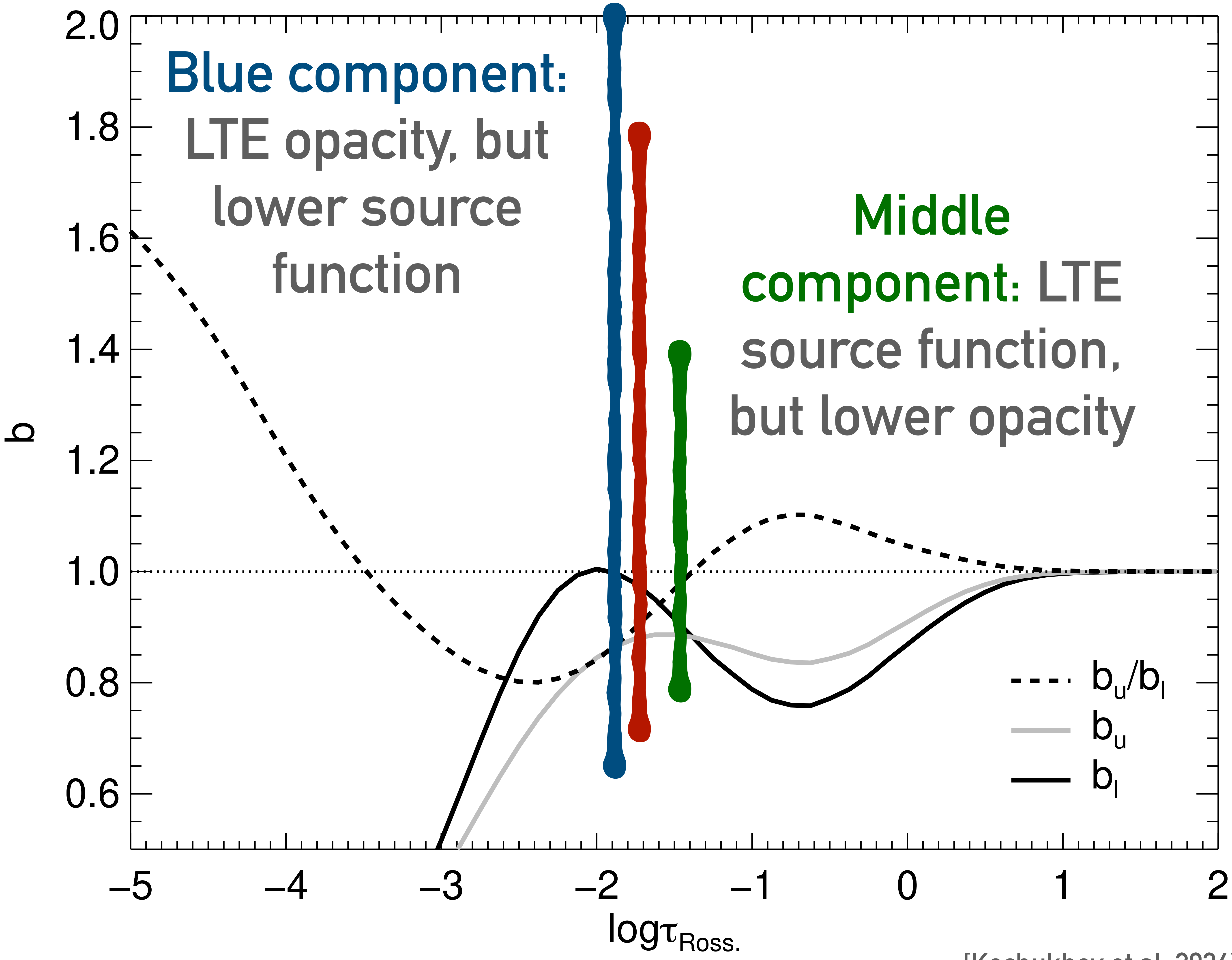

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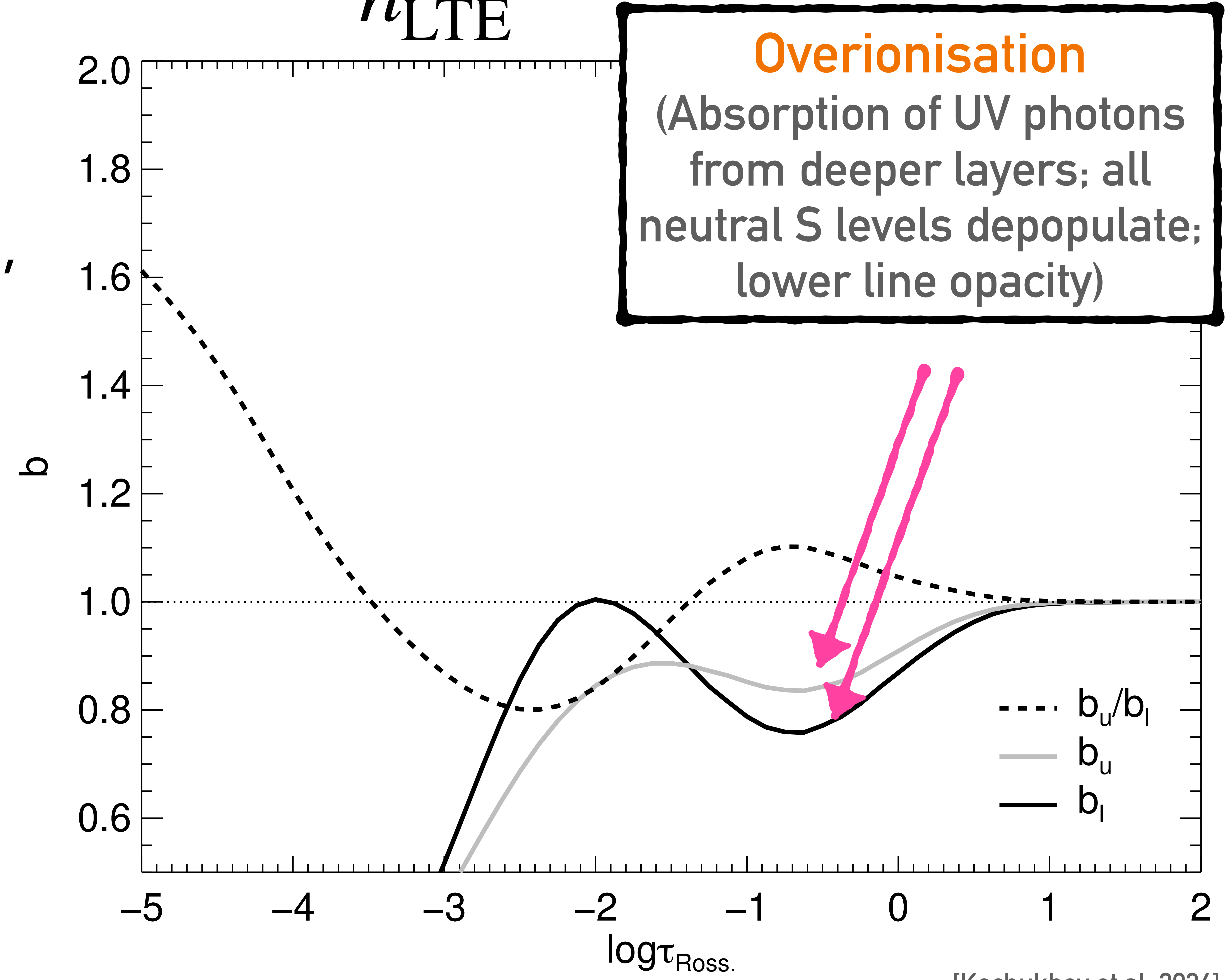

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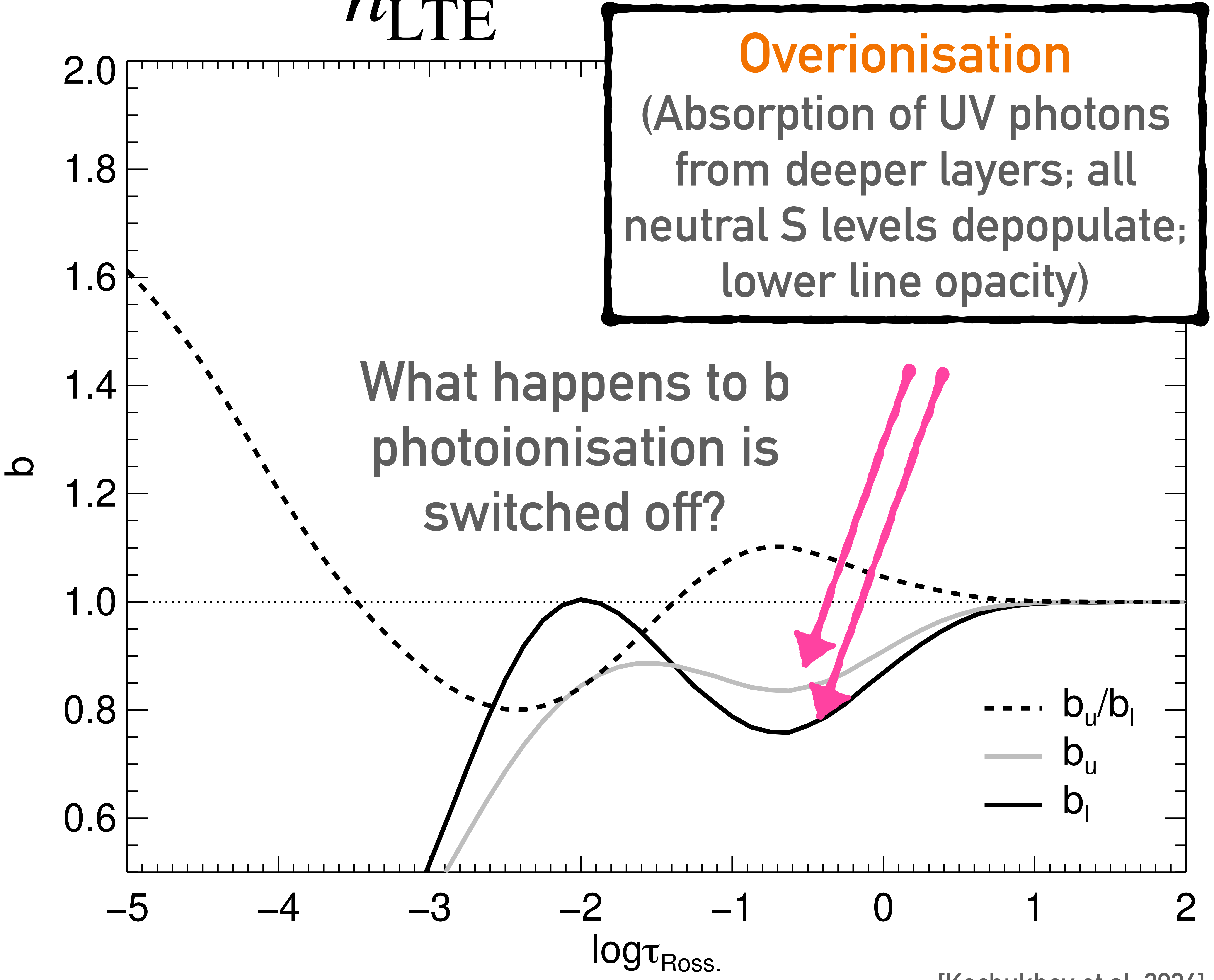

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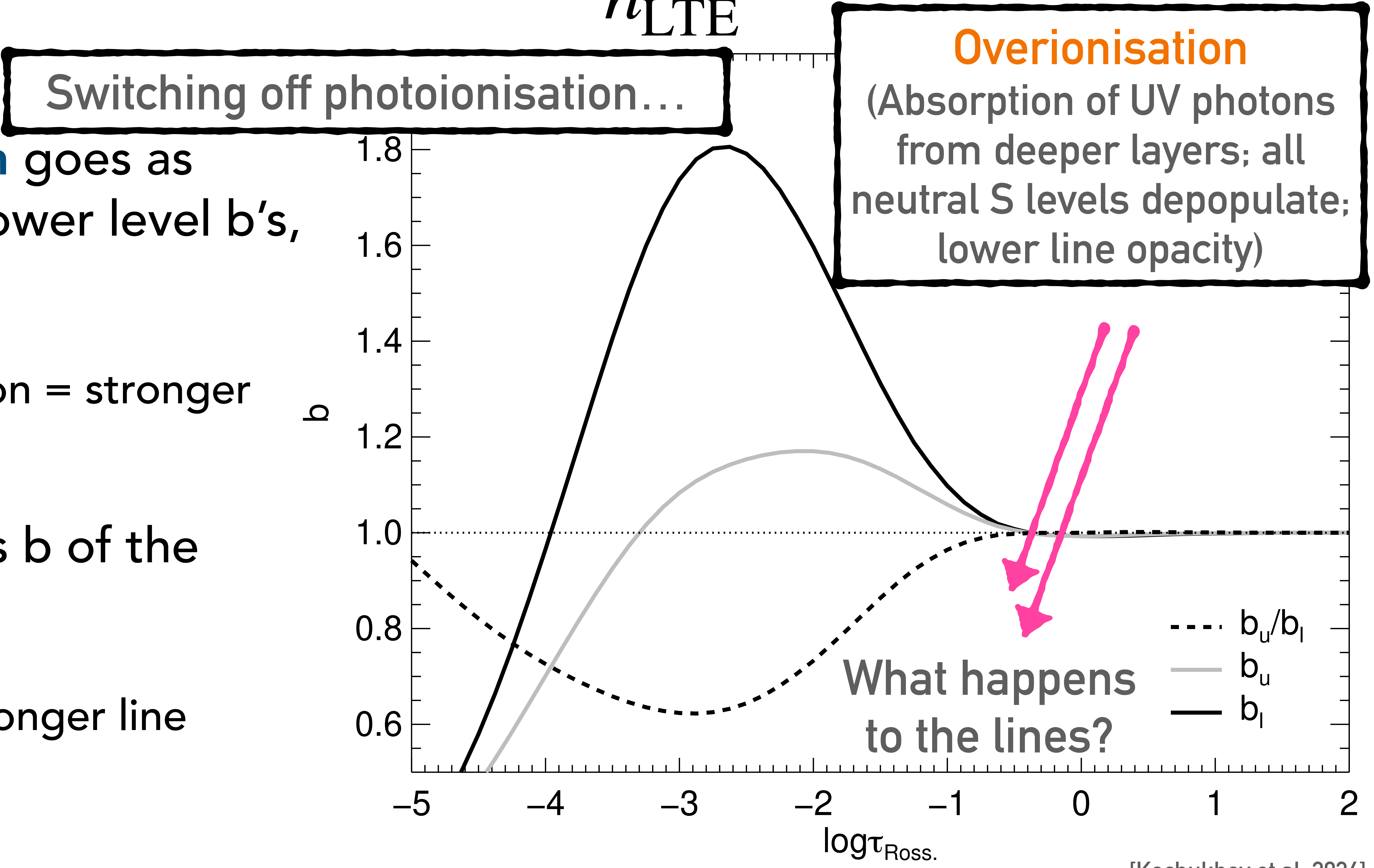

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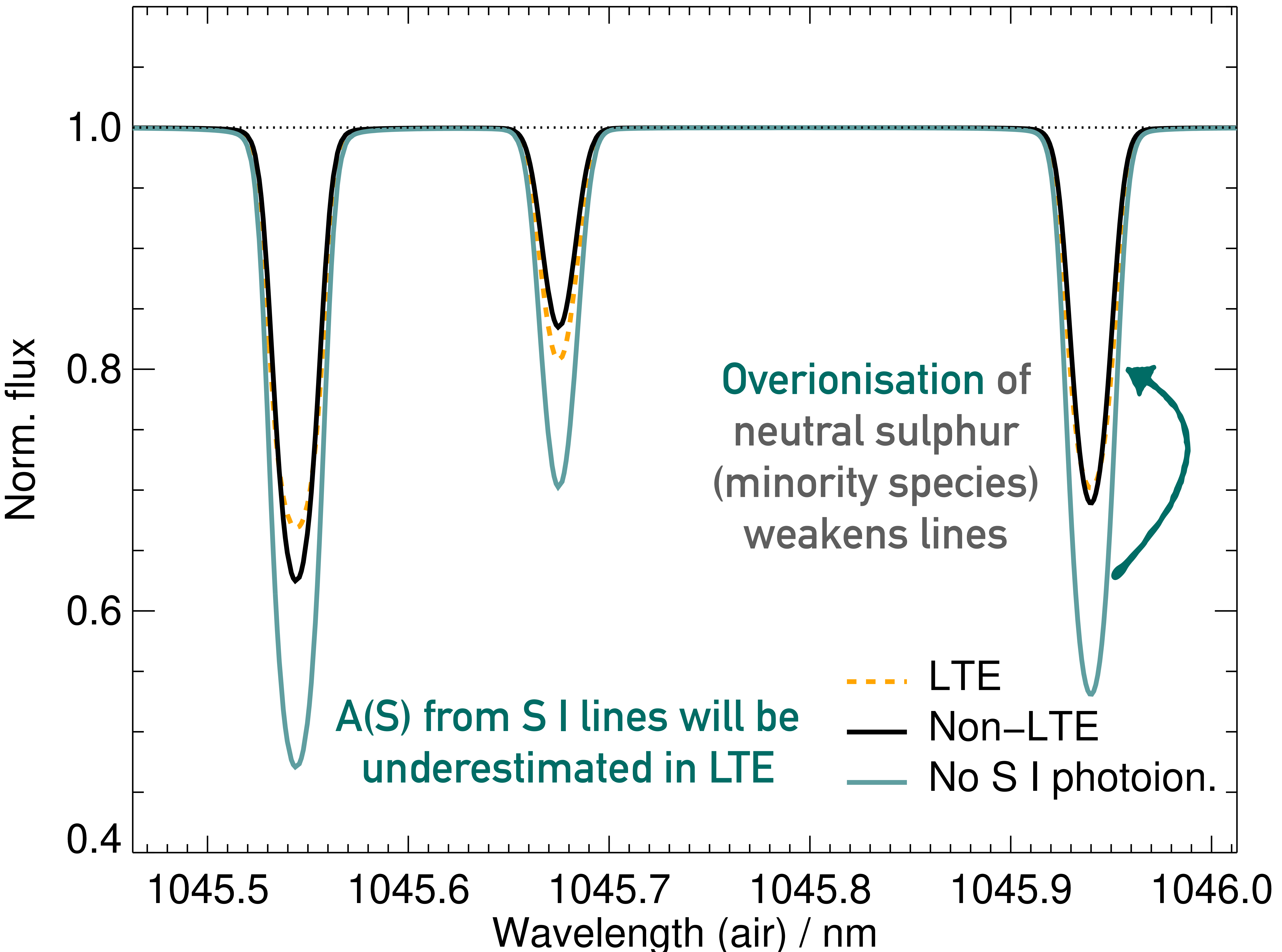

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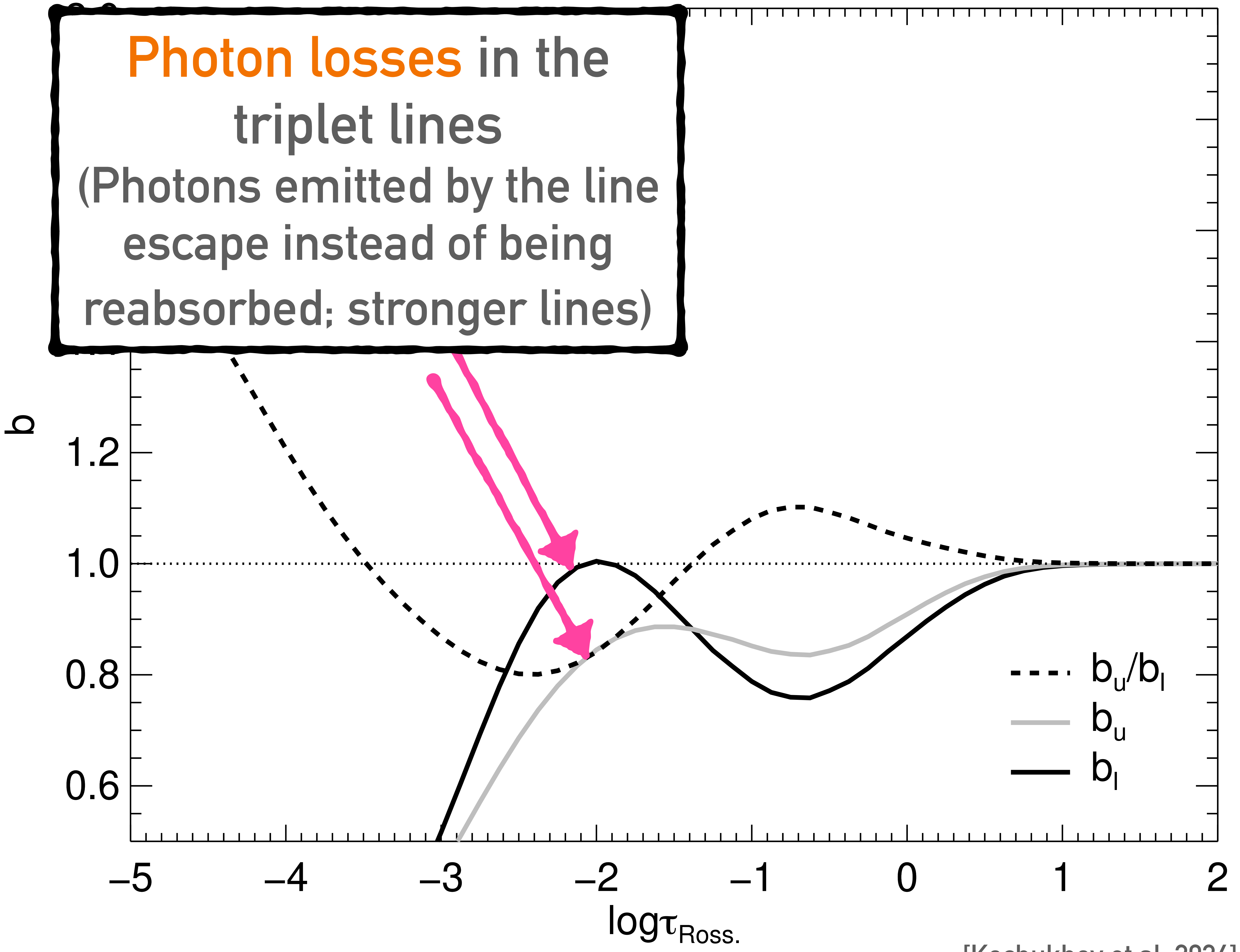

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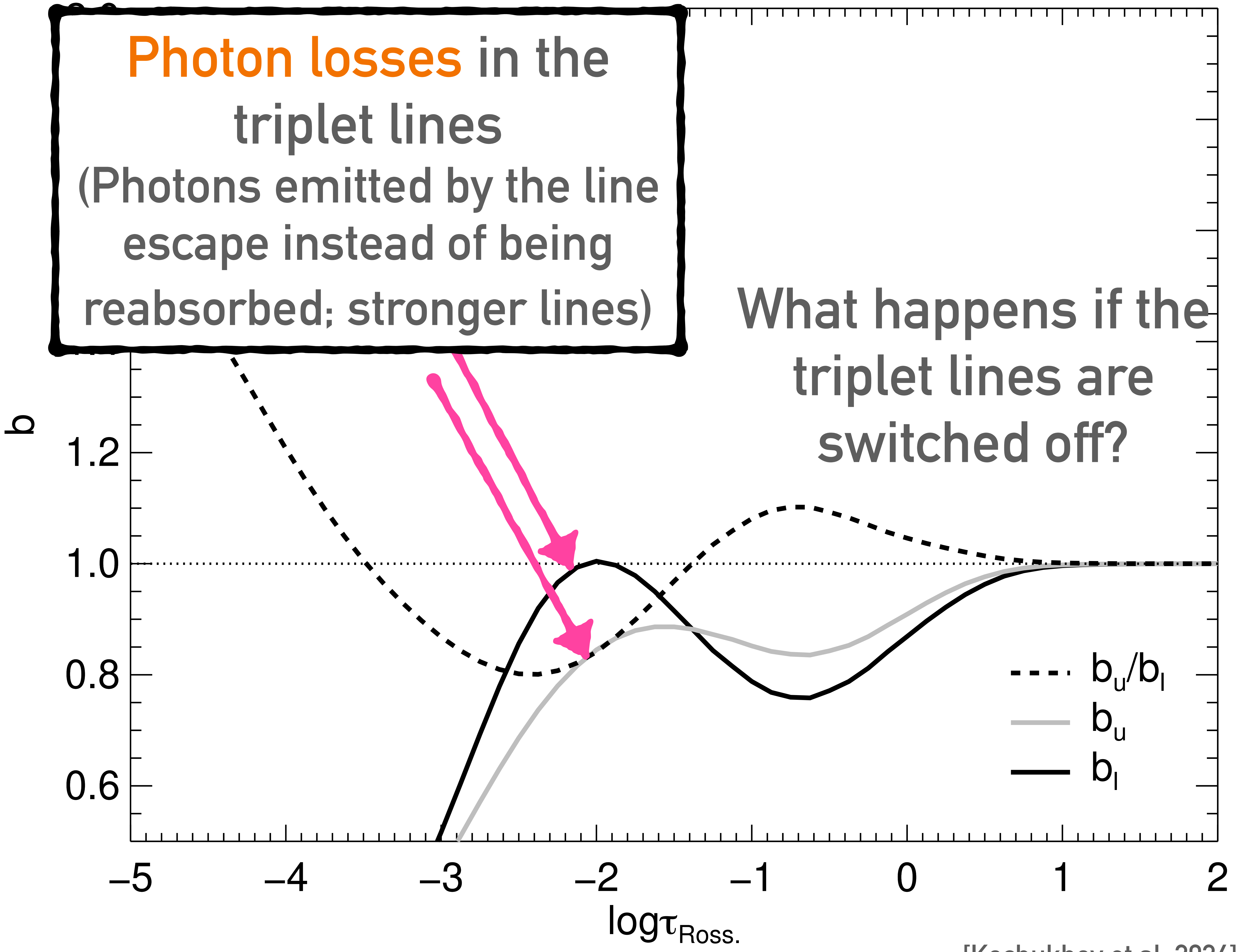

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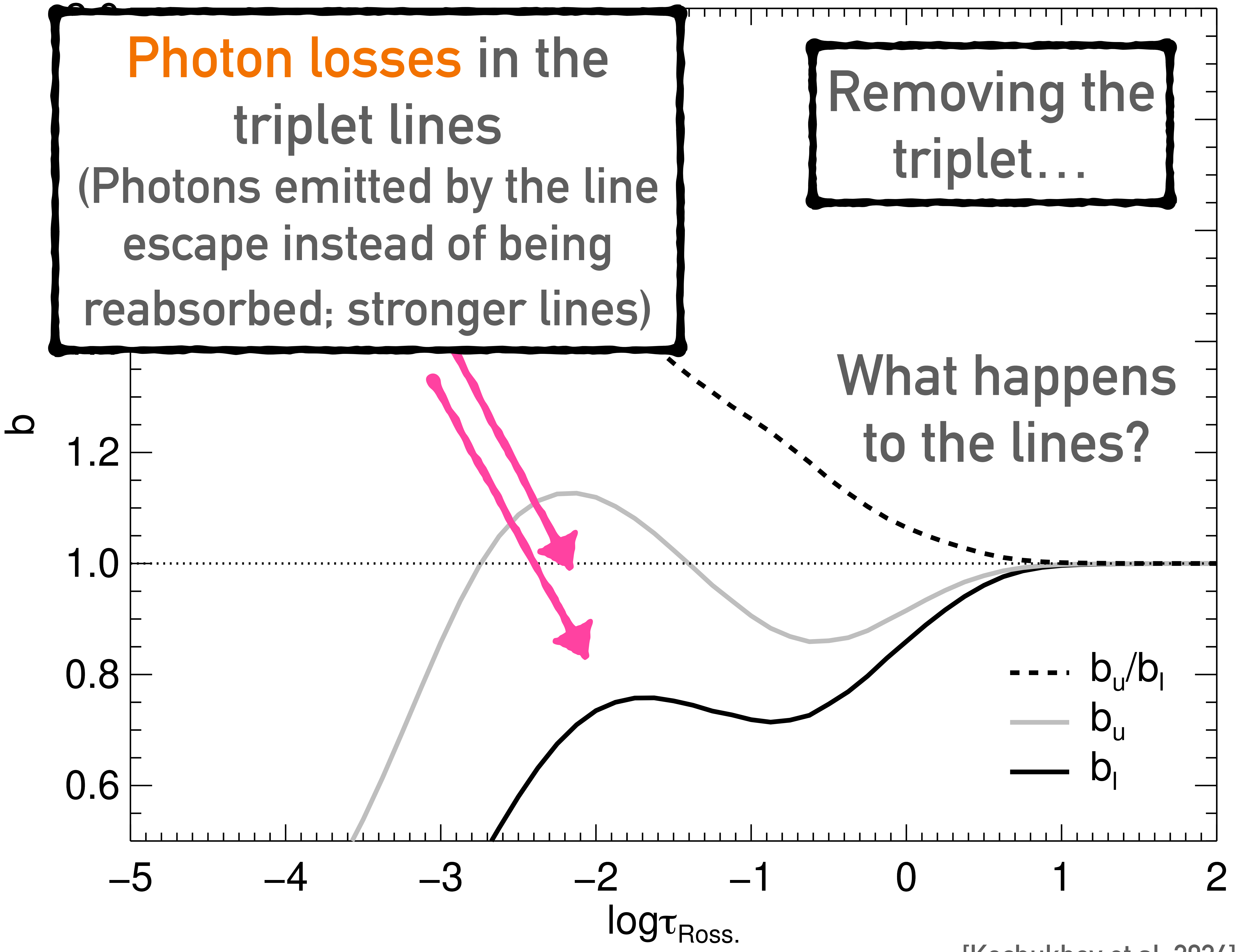
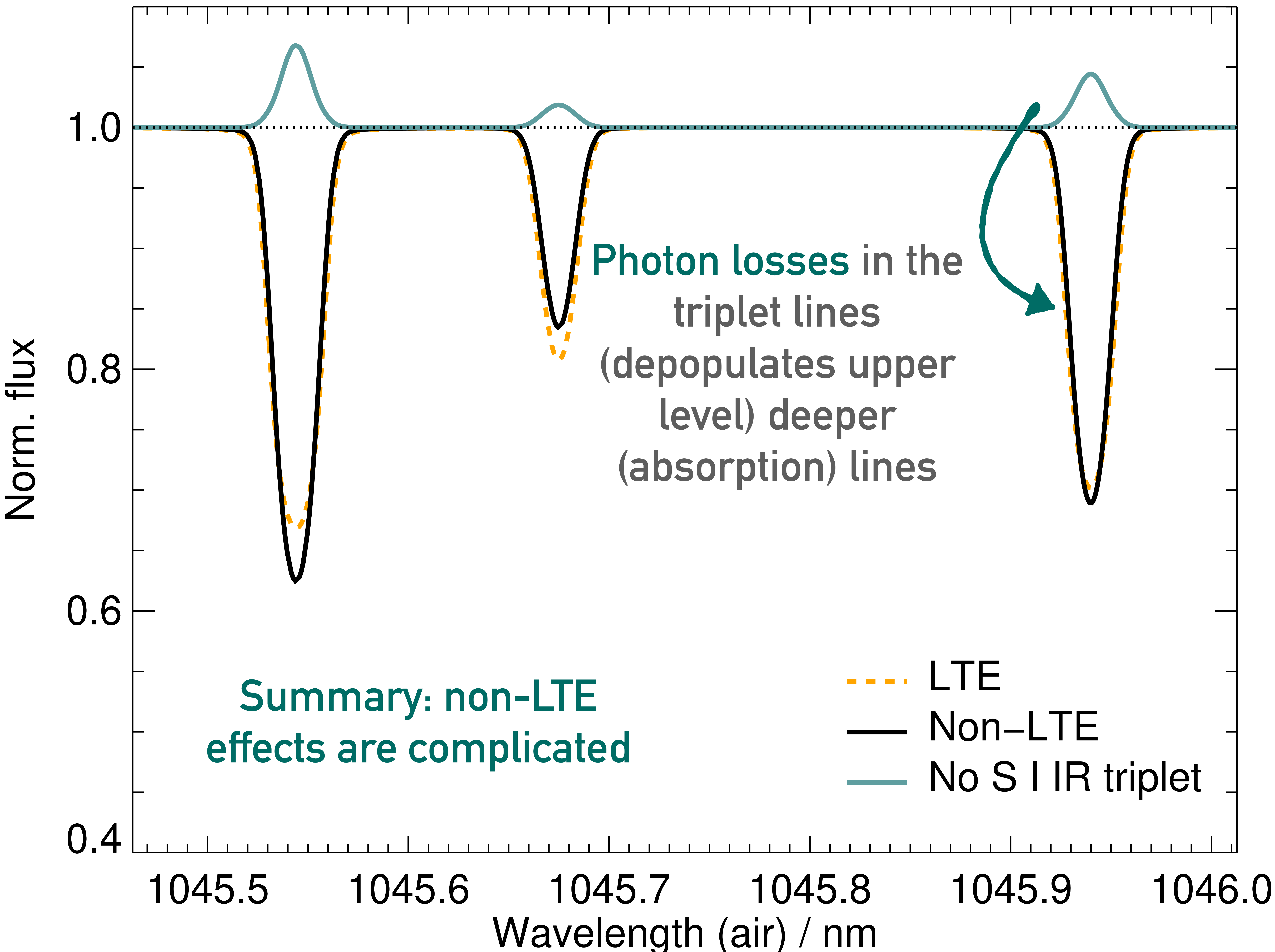


[Kochukhov et al. 2024]



[Kochukhov et al. 2024]

Applying non-LTE corrections

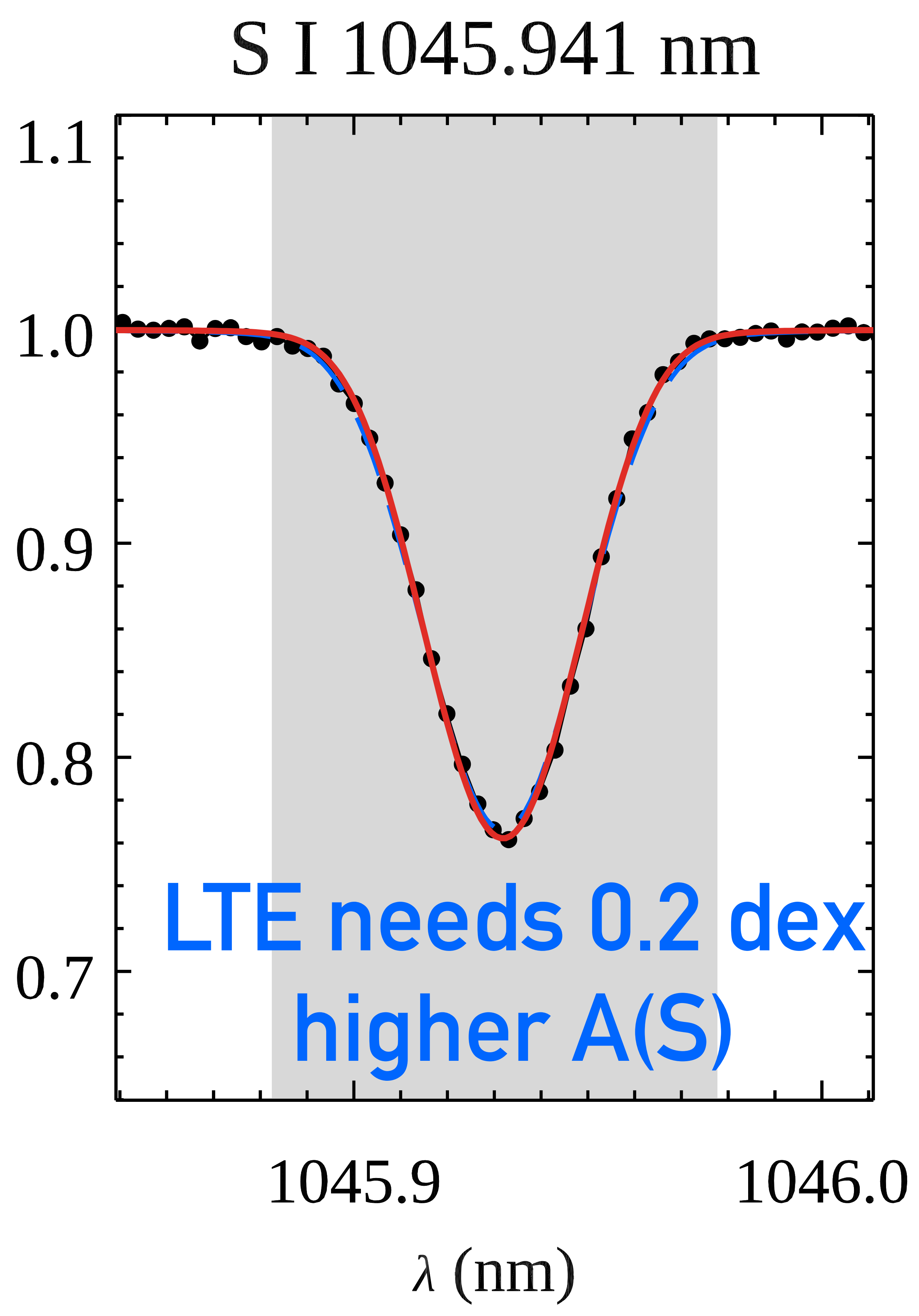
How can we carry out non-LTE spectral analyses in practice?

Correcting LTE results

- Non-LTE calculations are more expensive than LTE ones
  - For a whole spectrum: 10-50 times more computationally expensive
  - For a single line: 1000-5000 times more computationally expensive
  - Excludes code overheads + the **human cost** of constructing the model atom(s)
- Instead, **users** can correct LTE results with non-LTE data pre-computed by **modellers**
  1. Using abundance corrections
  2. Using departure coefficients

1. Abundance corrections

- Given spectral line, model atmosphere, **modeller** calculates spectral lines in non-LTE and in LTE for different abundances
- For a given LTE abundance A_{LTE}, **modeller** finds non-LTE abundance A_{NLTE} such that non-LTE and LTE equivalent widths agree
- **Modeller** creates a grid of abundance corrections $\Delta = A_{\mathrm{NLTE}} - A_{\mathrm{LTE}}$
- **User** interpolates $\Delta = \Delta(T_{\mathrm{eff}}, \log g, [\mathrm{Fe/H}], A_{\mathrm{LTE}}, \xi_{\mathrm{mic.}})$



$\Delta = -0.2$

[Kochukhov et al. 2024]

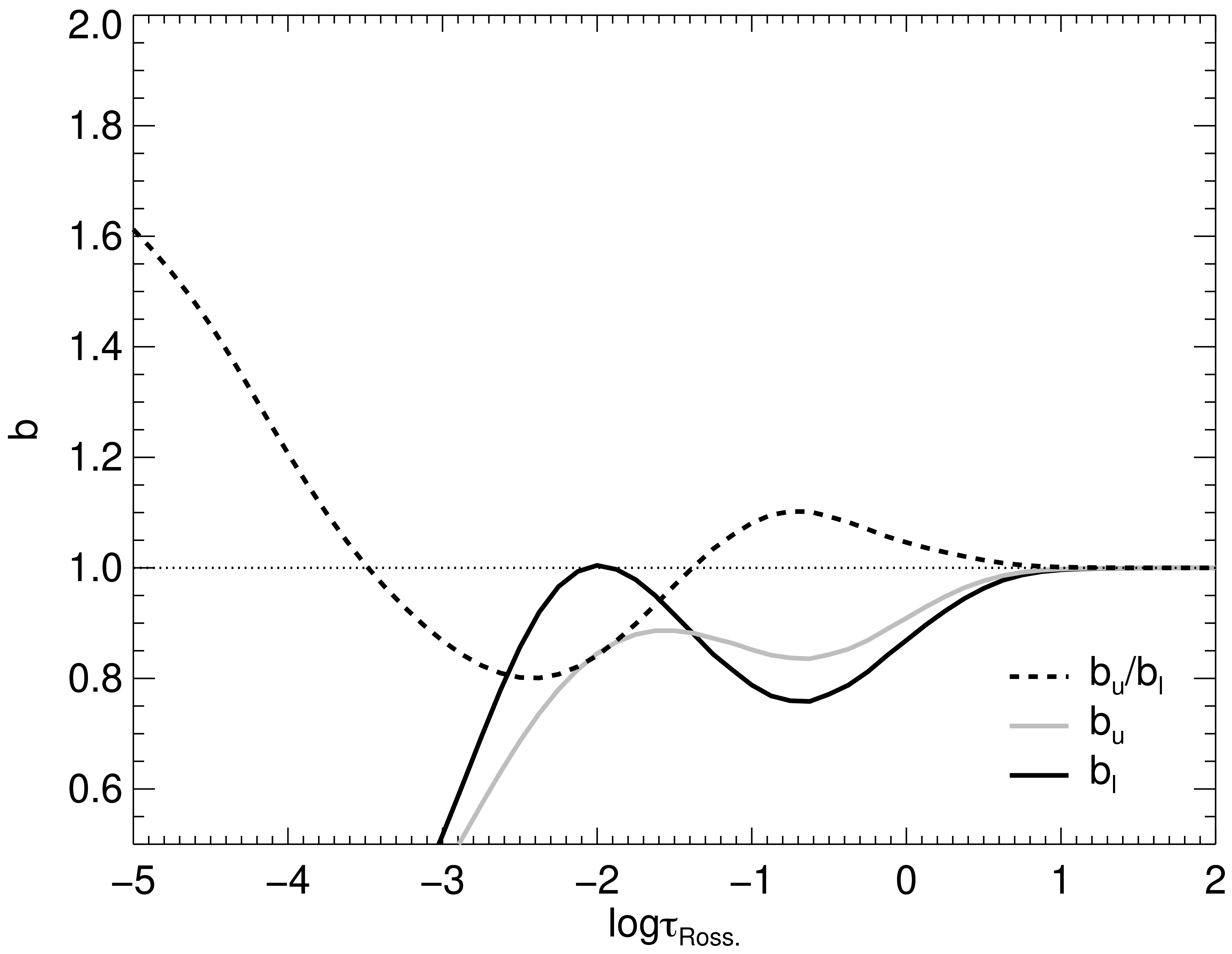
2. Departure coefficients

- Given model atmosphere, abundance, **modeller** calculates departure coefficients

- **User** takes departure coefficients $b = b(T_{\rm eff}, \log g, [{\rm Fe/H}], A_{\rm NLTE}, \xi_{\rm mic.})$ and reads them into an LTE code

- LTE code corrects line opacity using b_l and line source function using b_u/b_l, interpolating if necessary

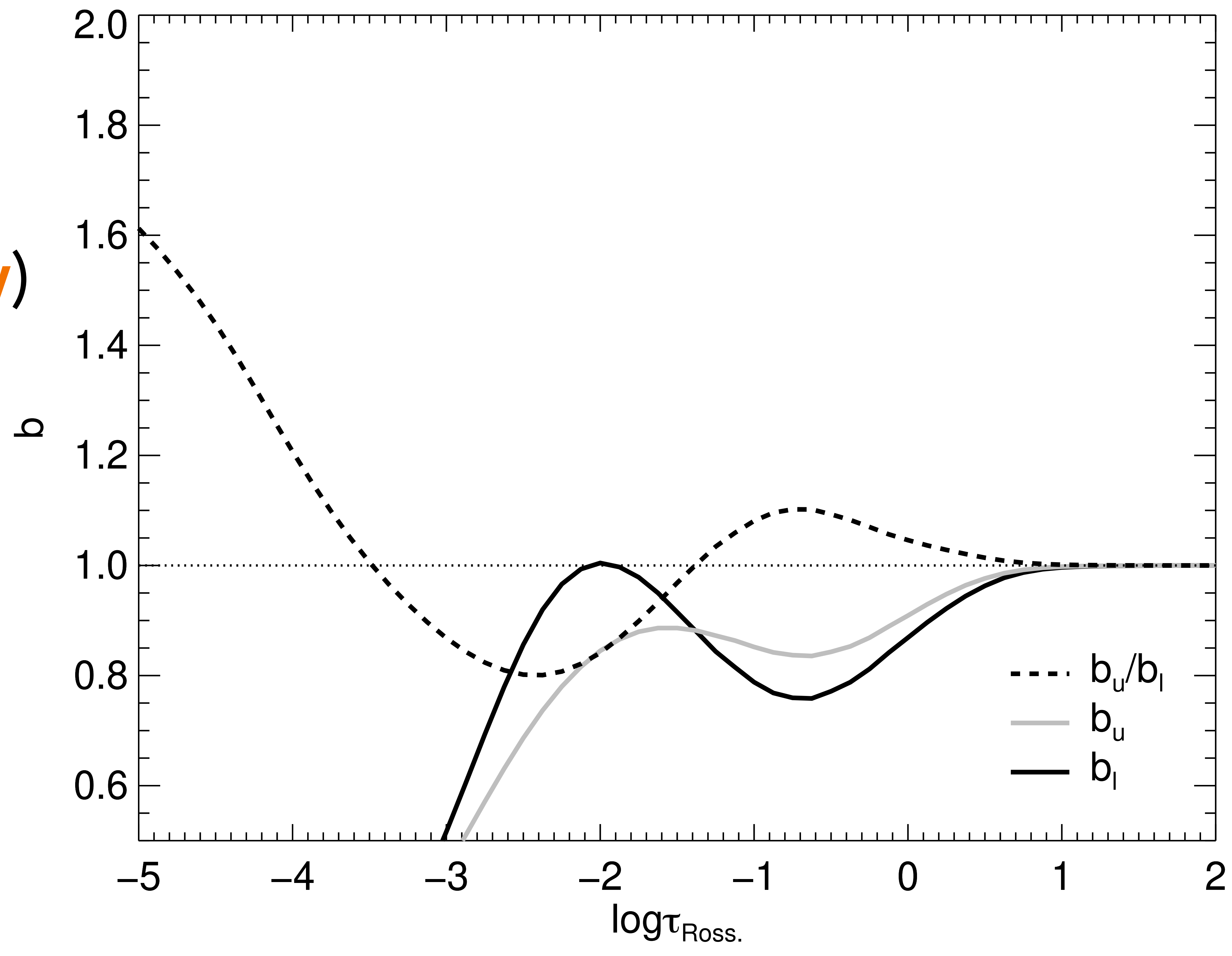
- **User** gets **non-LTE spectra** with LTE cost



[Kochukhov et al. 2024]

2. Departure coefficients

- Many LTE codes support reading and interpolating departure coefficients e.g.
  - PySME (Wehrhahn+ 2023; Nik's tutorial tomorrow)
  - Turbospectrum (Gerberg+ 2023)
  - Synmast (Kochukhov+ 2010)
  - (Various others)
- Straightforward to implement into your favourite LTE code

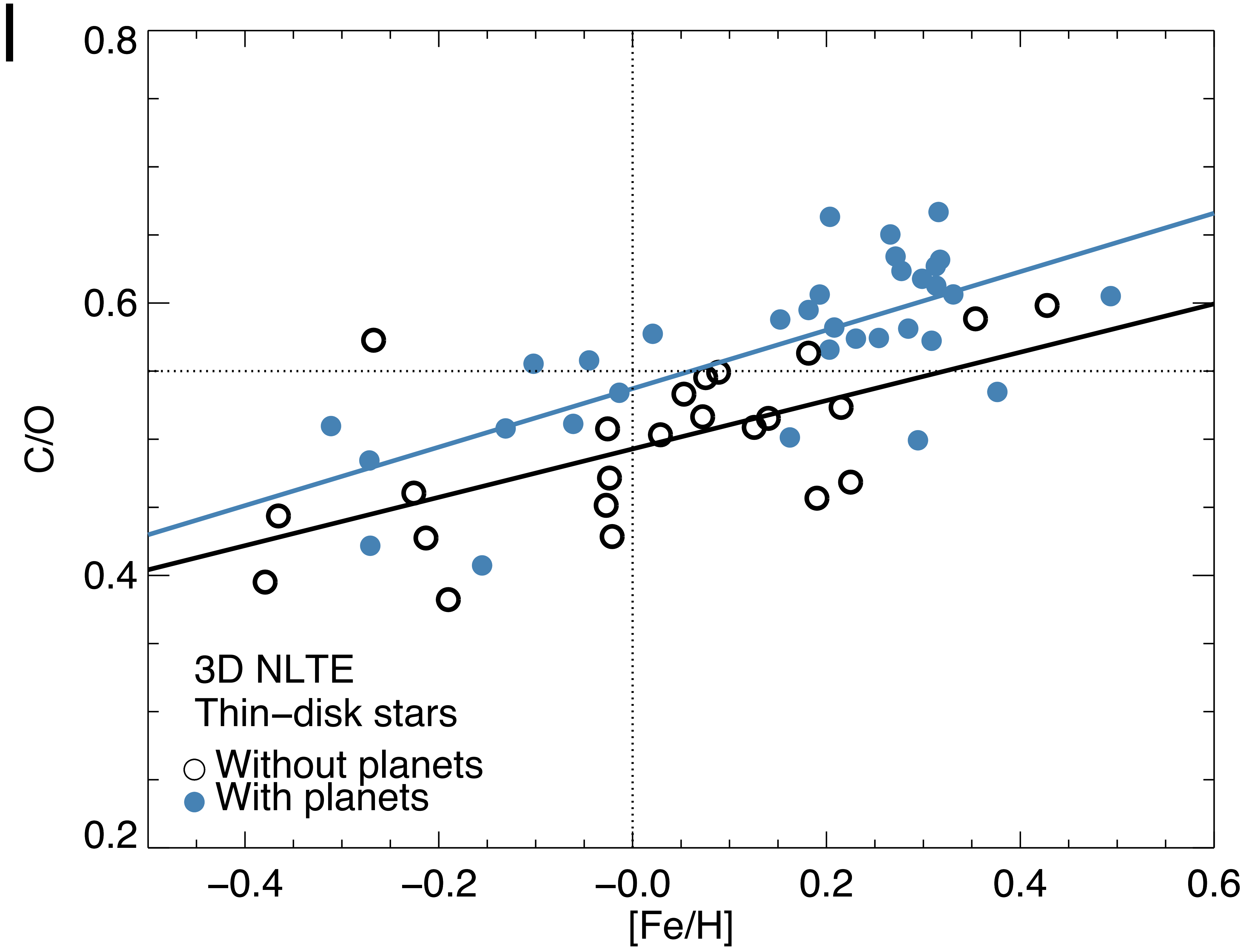


[Kochukhov et al. 2024]

Conclusion

Conclusion

- Taking non-LTE effects into account can reveal interesting **new astrophysics**

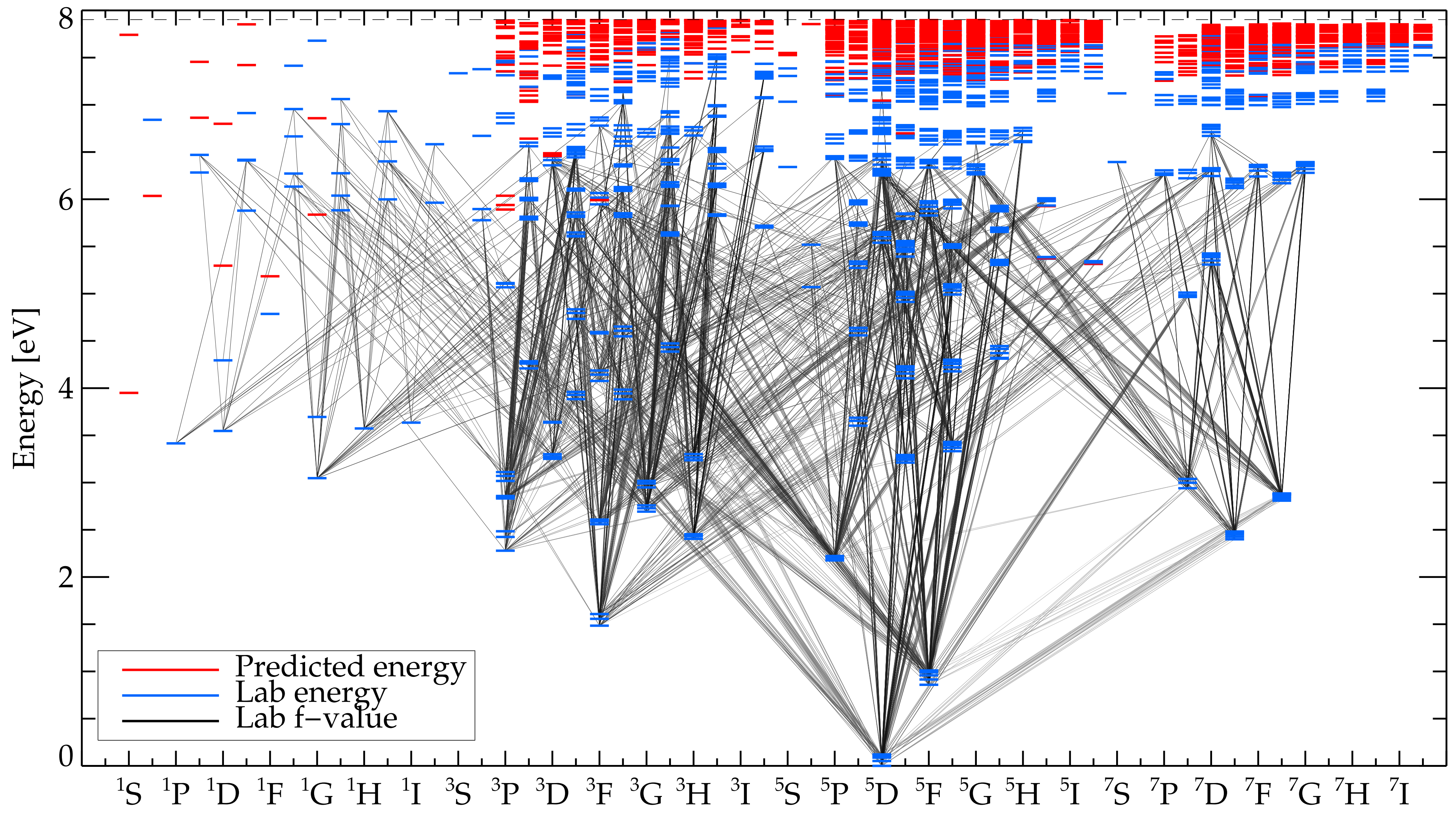


[Amarsi, Nissen and Skúladóttir 2019]

Conclusion

- Taking non-LTE effects into account can reveal interesting **new astrophysics**
- LTE is valid in the limit of **large collisions**; but anticipate large non-LTE effects in hot stars

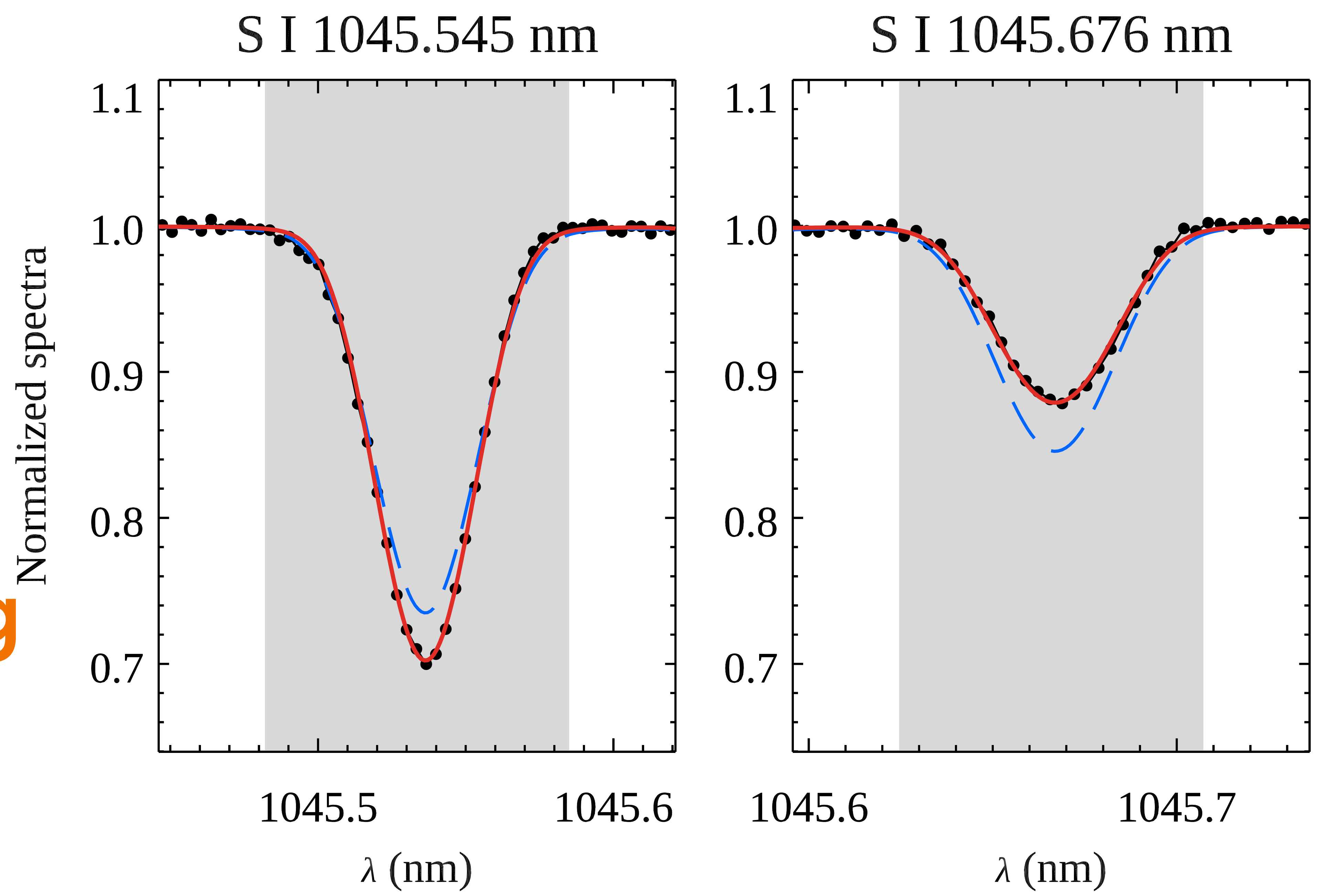
$$n_i \Sigma_j [R_{ij} + C_{ij}] = \Sigma_j n_j [R_{ji} + C_{ji}]$$



[Lind and Amarsi 2024]

Conclusion

- Taking non-LTE effects into account can reveal interesting new astrophysics
- LTE is valid in the limit of large collisions; but anticipate large non-LTE effects in hot stars
- Non-LTE line strengthening and line weakening effects, depending on the stellar parameters, abundances, species, and spectral line

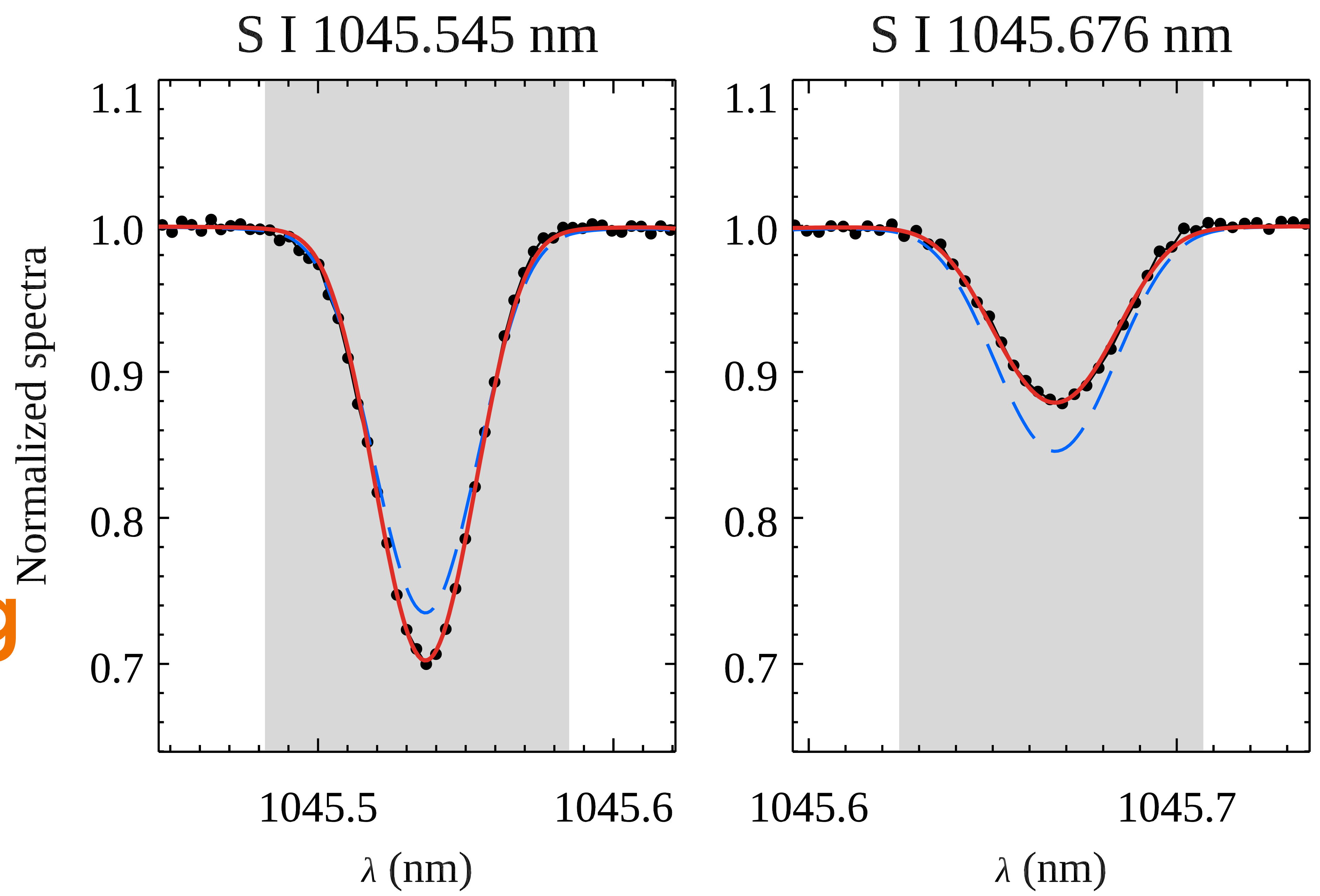


[Kochukhov et al. 2024]

Conclusion

- Taking non-LTE effects into account can reveal interesting **new astrophysics**
- LTE is valid in the limit of **large collisions**; but anticipate large non-LTE effects in hot stars
- Non-LTE **line strengthening and line weakening** effects, depending on the stellar parameters, abundances, species, and spectral line
- Interpolate **pre-computed grids of departure coefficients** to get non-LTE spectra on the fly

Non-LTE with BALDER
Synthesis with SYNMAST



[Kochukhov et al. 2024]