An atomic model for hydrogen recombination line modelling

With application in post-processing of radiation-hydrodynamic simulations

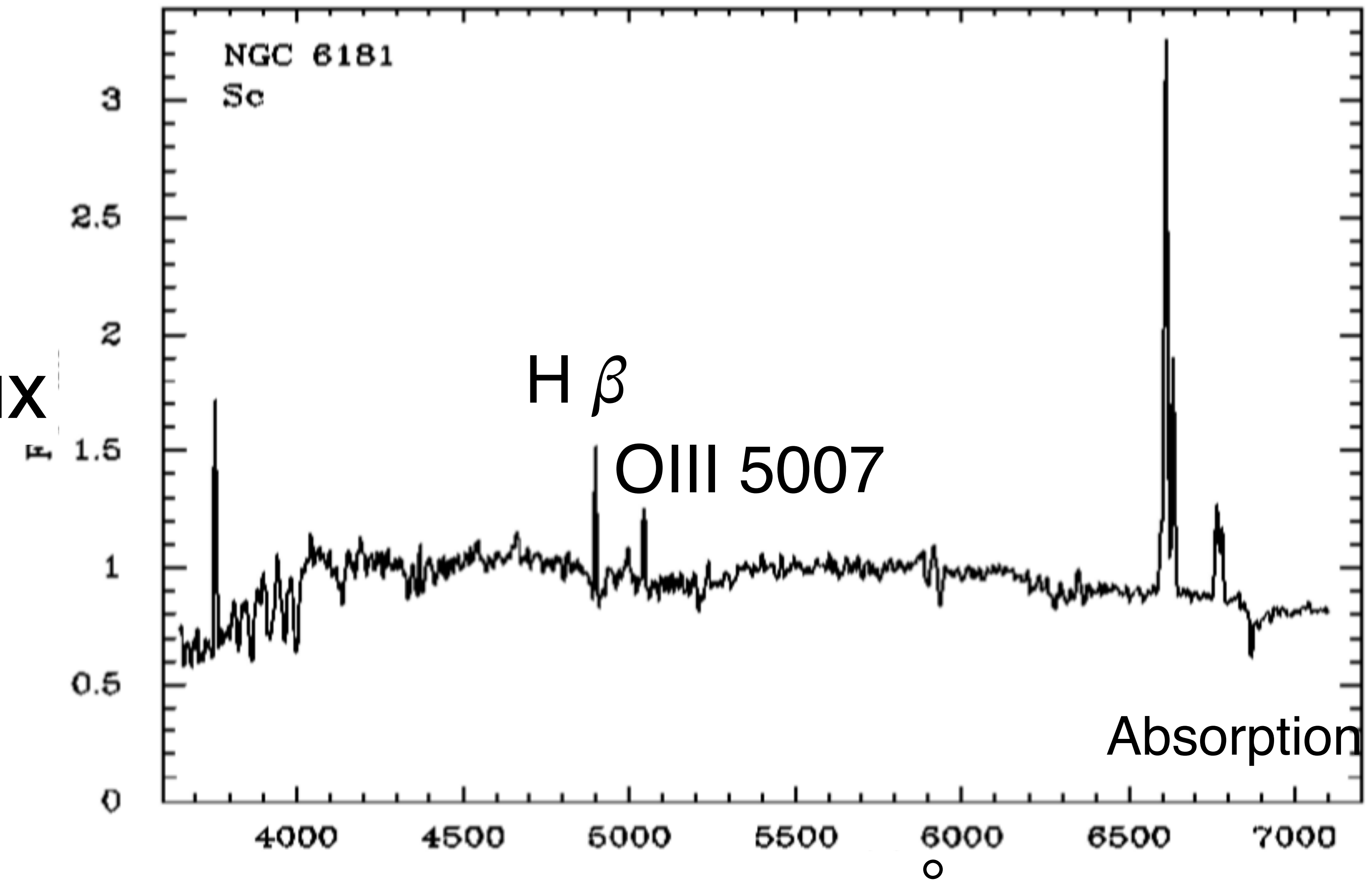
Yuankang Liu[1]

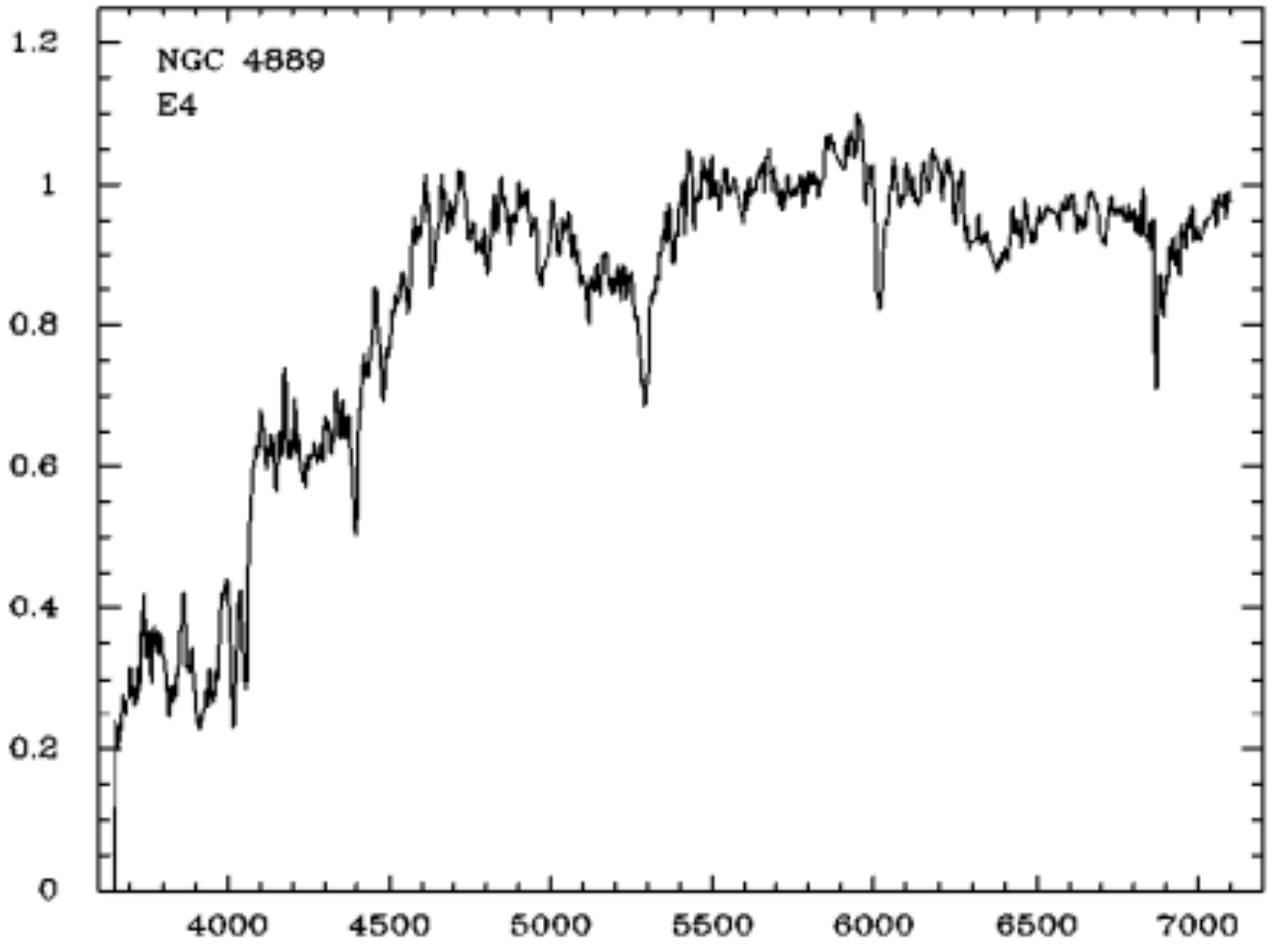
In collaboration with Tsang Keung Chan[3], Alex Richings[4]
Supervised by Tom Theuns[1] and Anna McLeod[2,1]

1. Institute for Computational Cosmology, Durham University
2. Centre for Extragalactic Astronomy, Durham University
3. Department of Physics, Chinese University of Hong Kong
4. E.A. Milne Centre for Astrophysics, University of Hull

Motivation

Line emission in galaxies





Kennicutt (1992)

Motivation

McLeod19

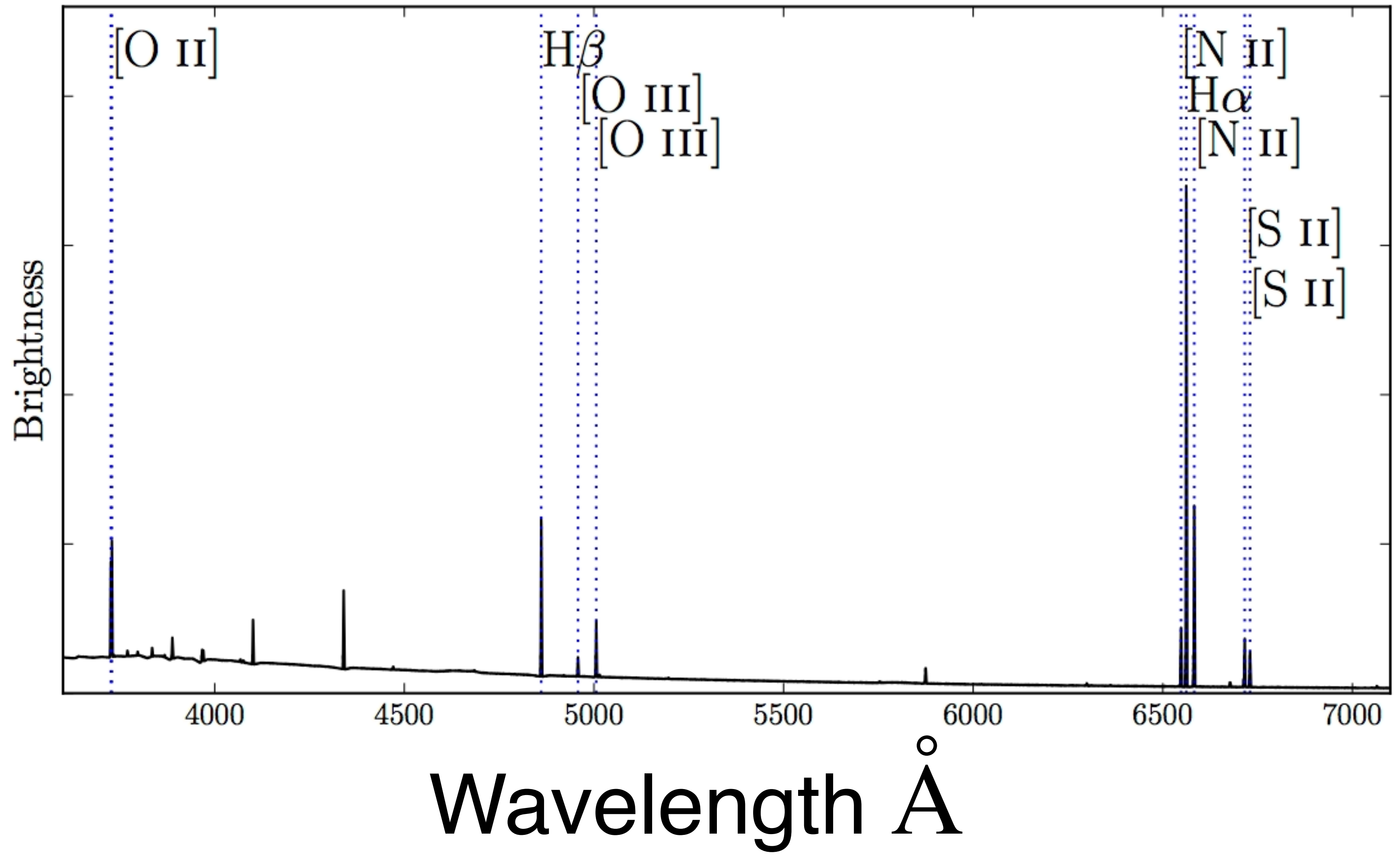
- Density
- Temperature
- Metallicity

etc.

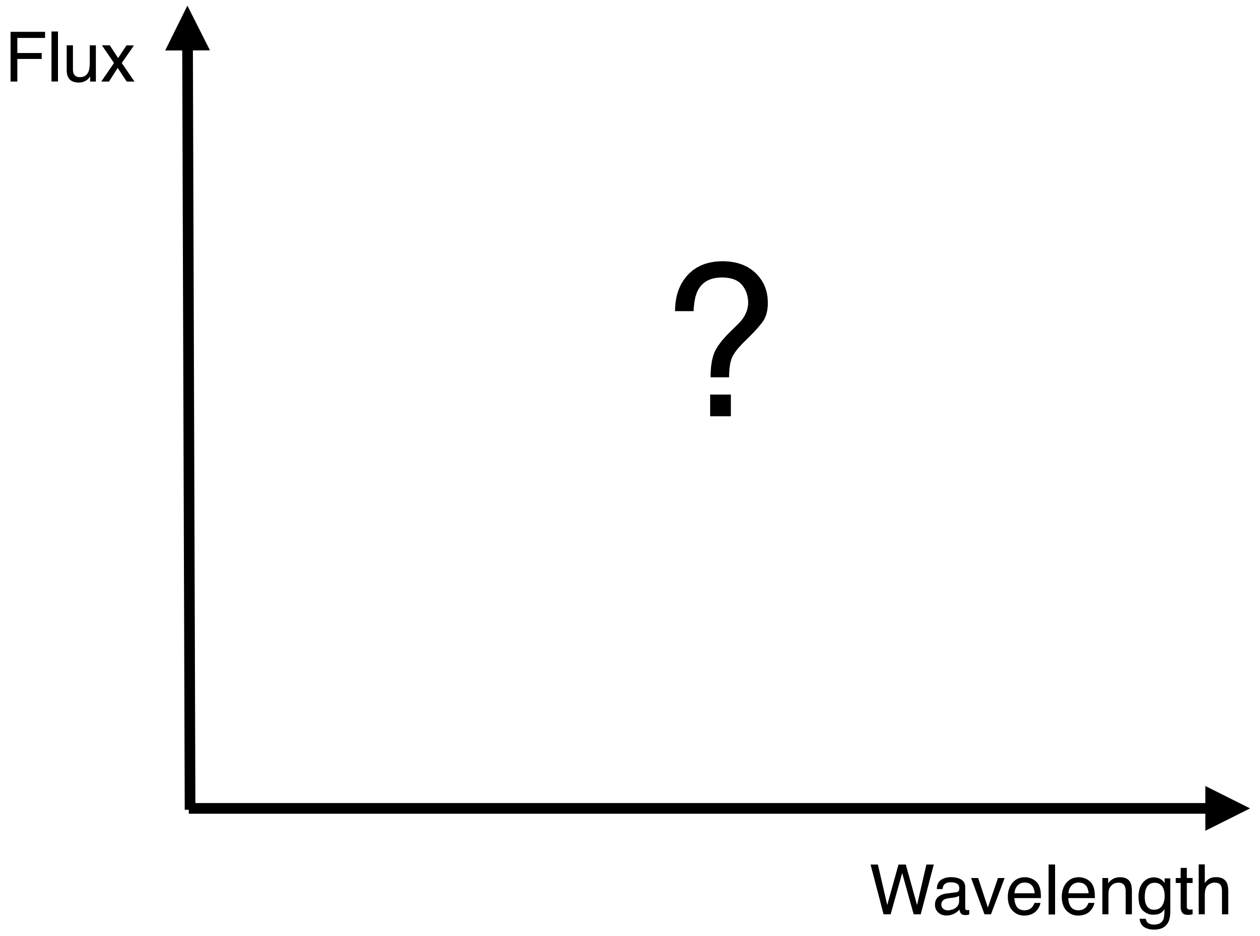
Starforge

Observation

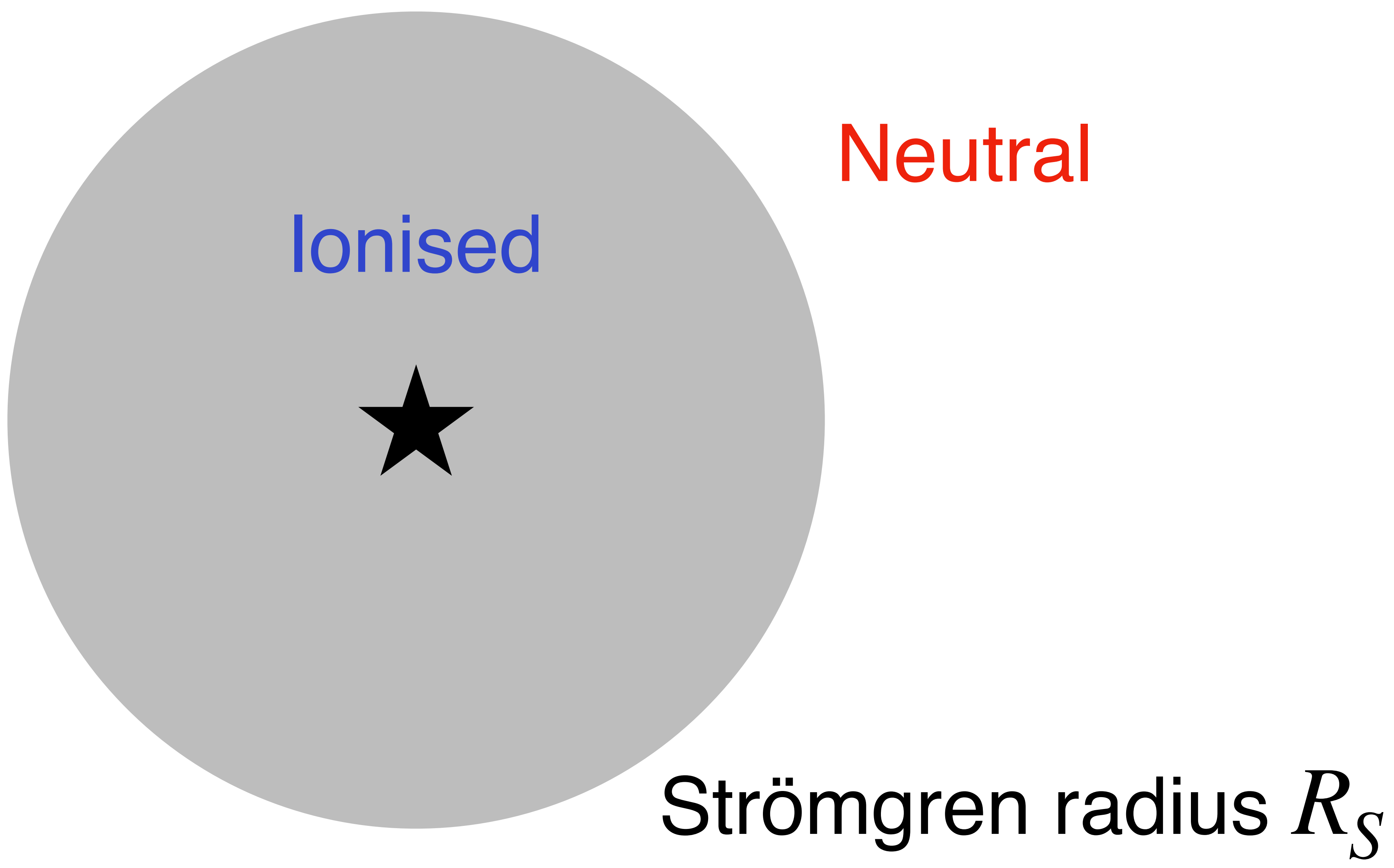
Simulation



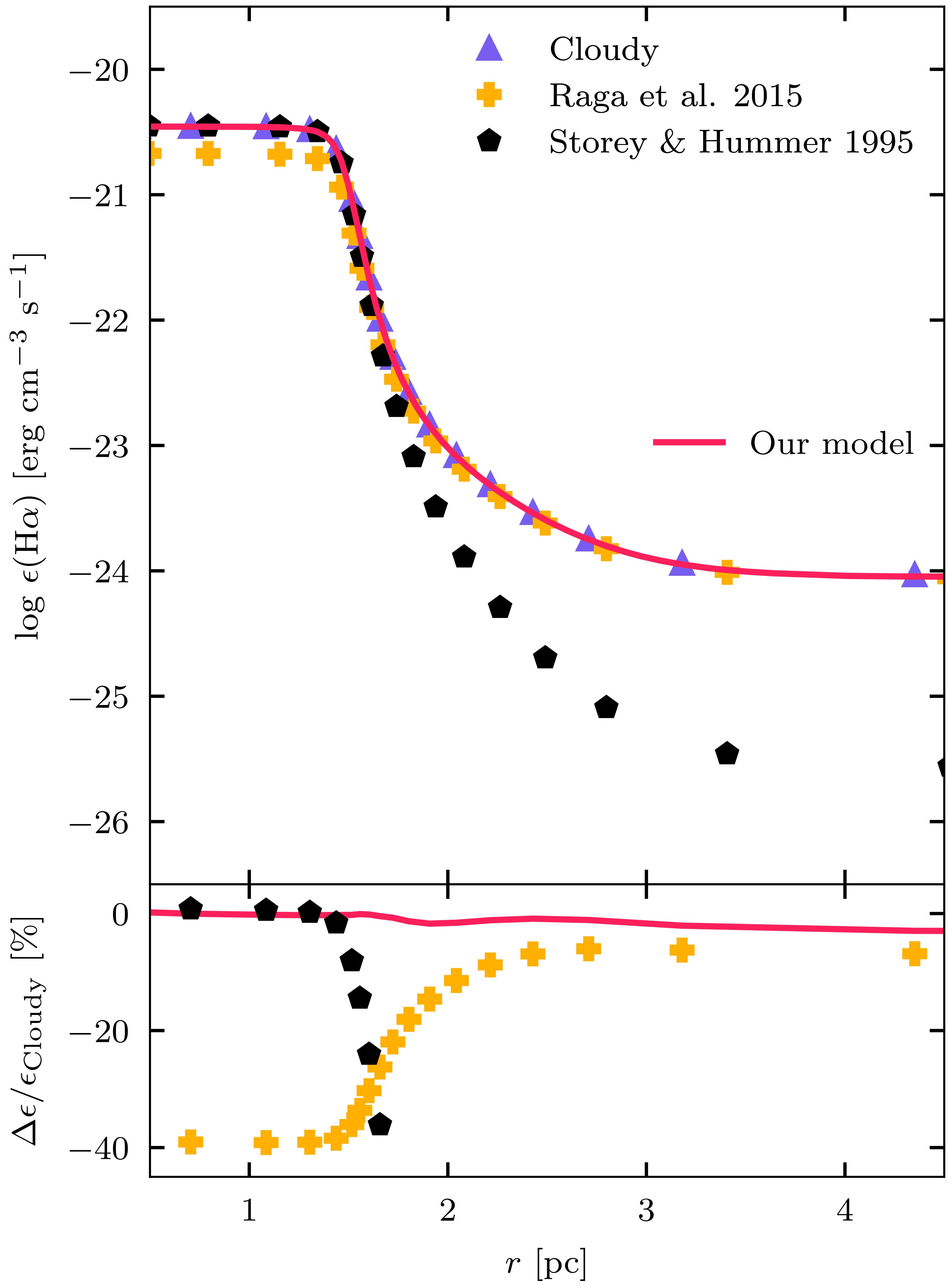
Credit: MOSFIRE Team



How do we model H II regions?



Hα emissivity profile



Cloudy:

Cloudy & Associates

Photoionization simulations for the discriminating astrophysicist since 1978

A photo-ionisation code

Storey & Hummer 1995:

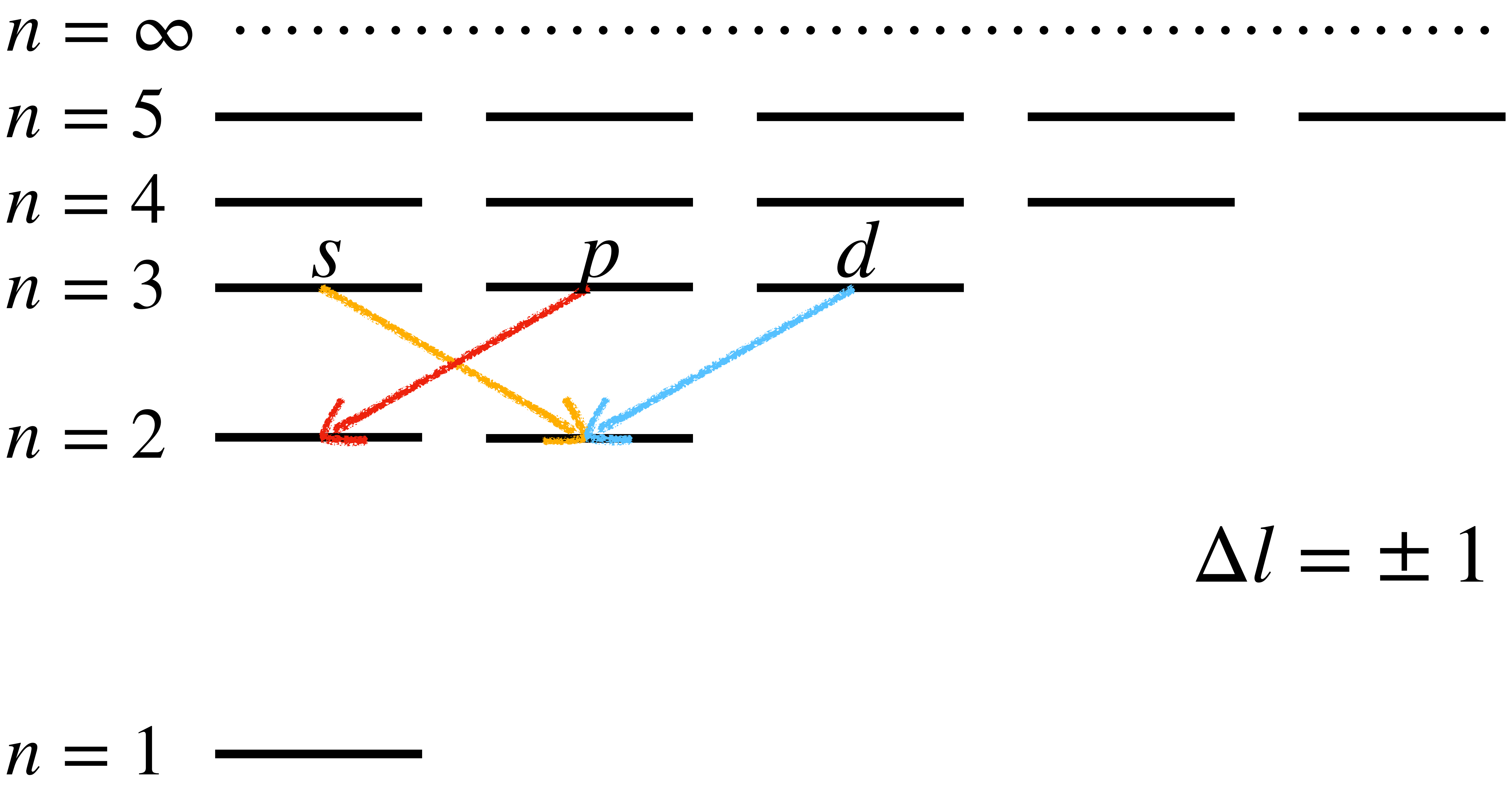
A tabulated table

Raga et al. 2015:

An analytical method

Atomic model for hydrogen

Hα as an example

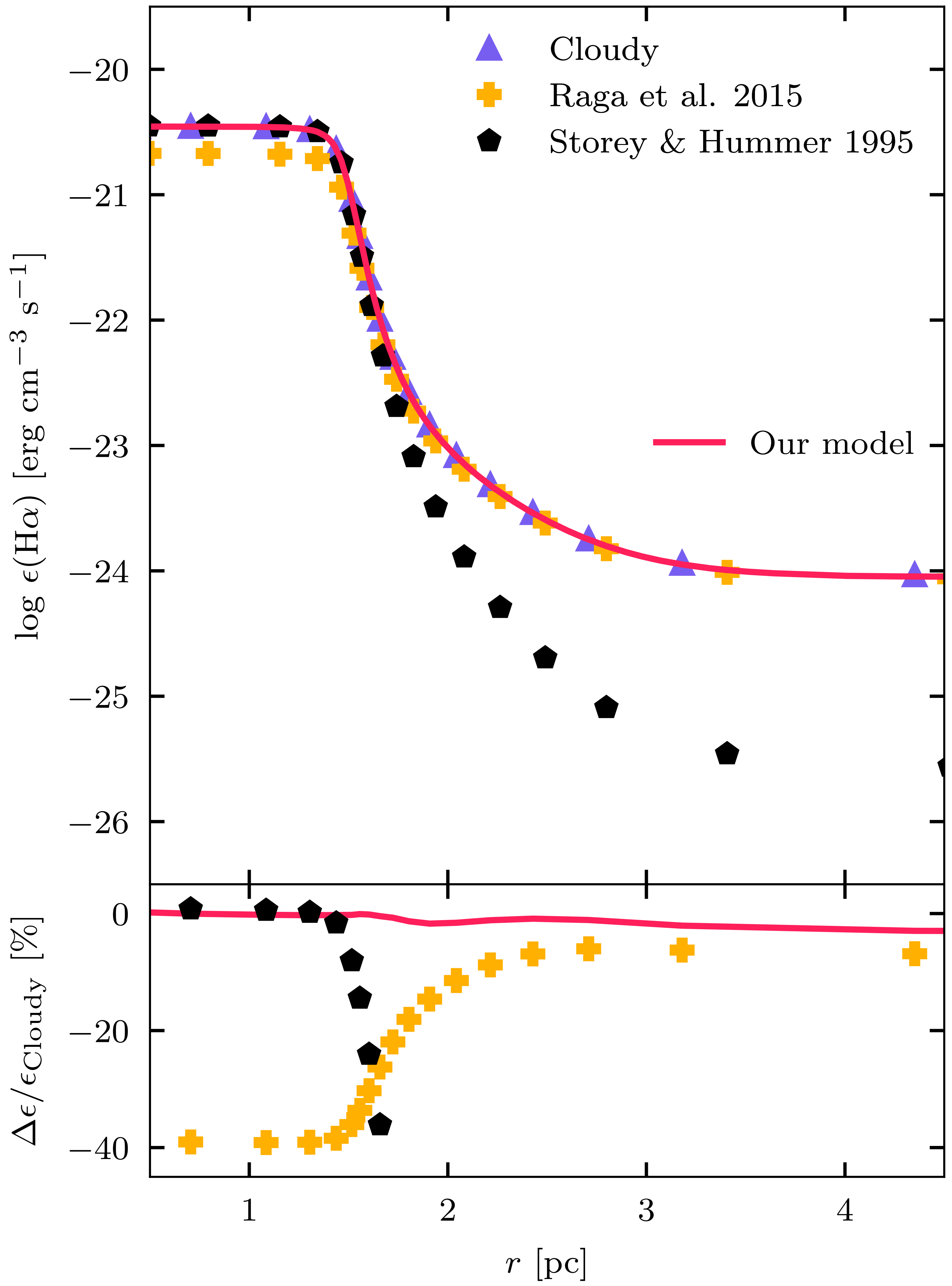


$\Delta l = \pm 1$

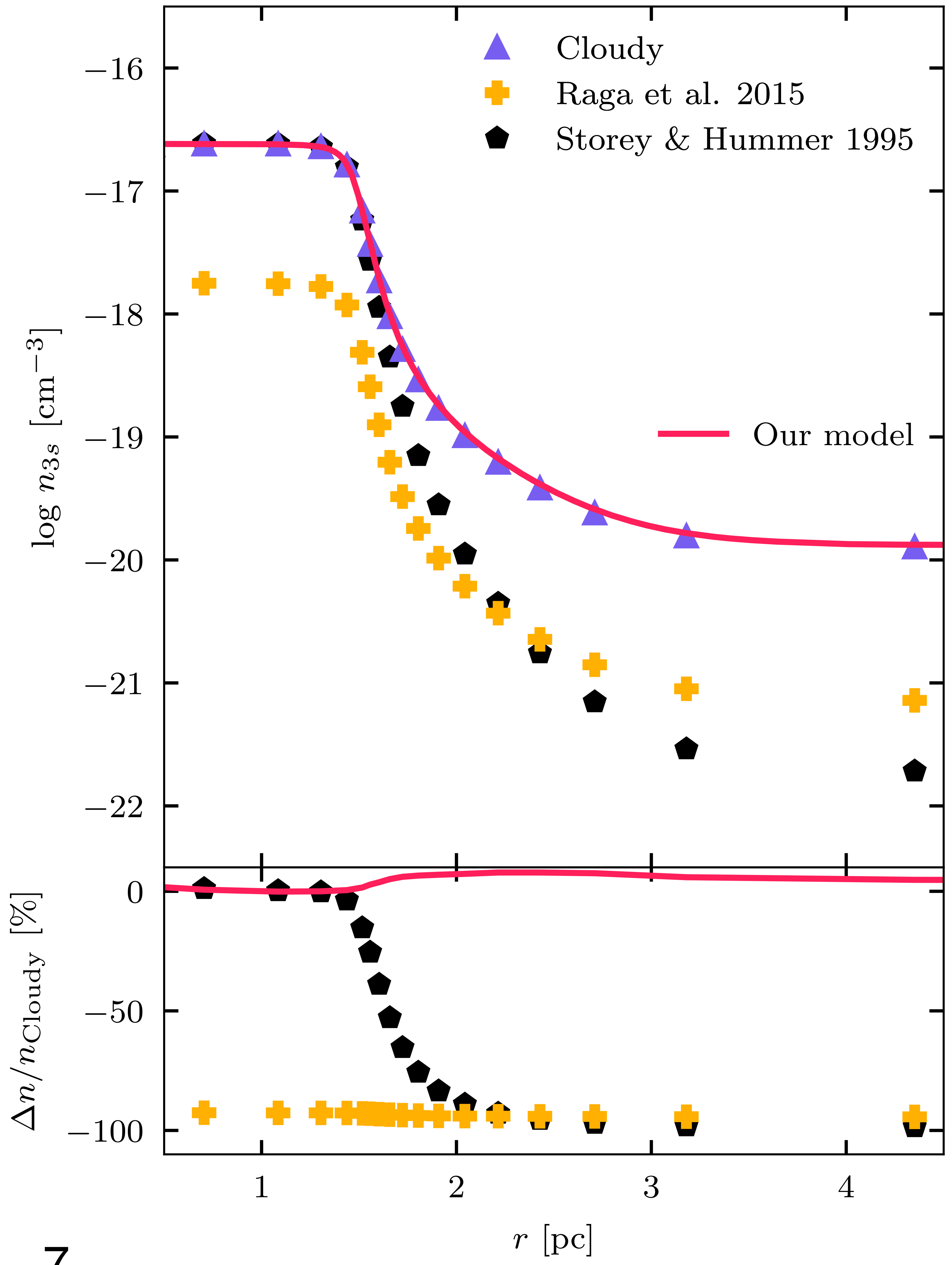
Line emissivity of Hα

$$\epsilon_{32} = (n_{3s} A_{3s,2p} + n_{3p} A_{3p,2s} + n_{3d} A_{3d,2p}) h\nu_{3\rightarrow 2}$$

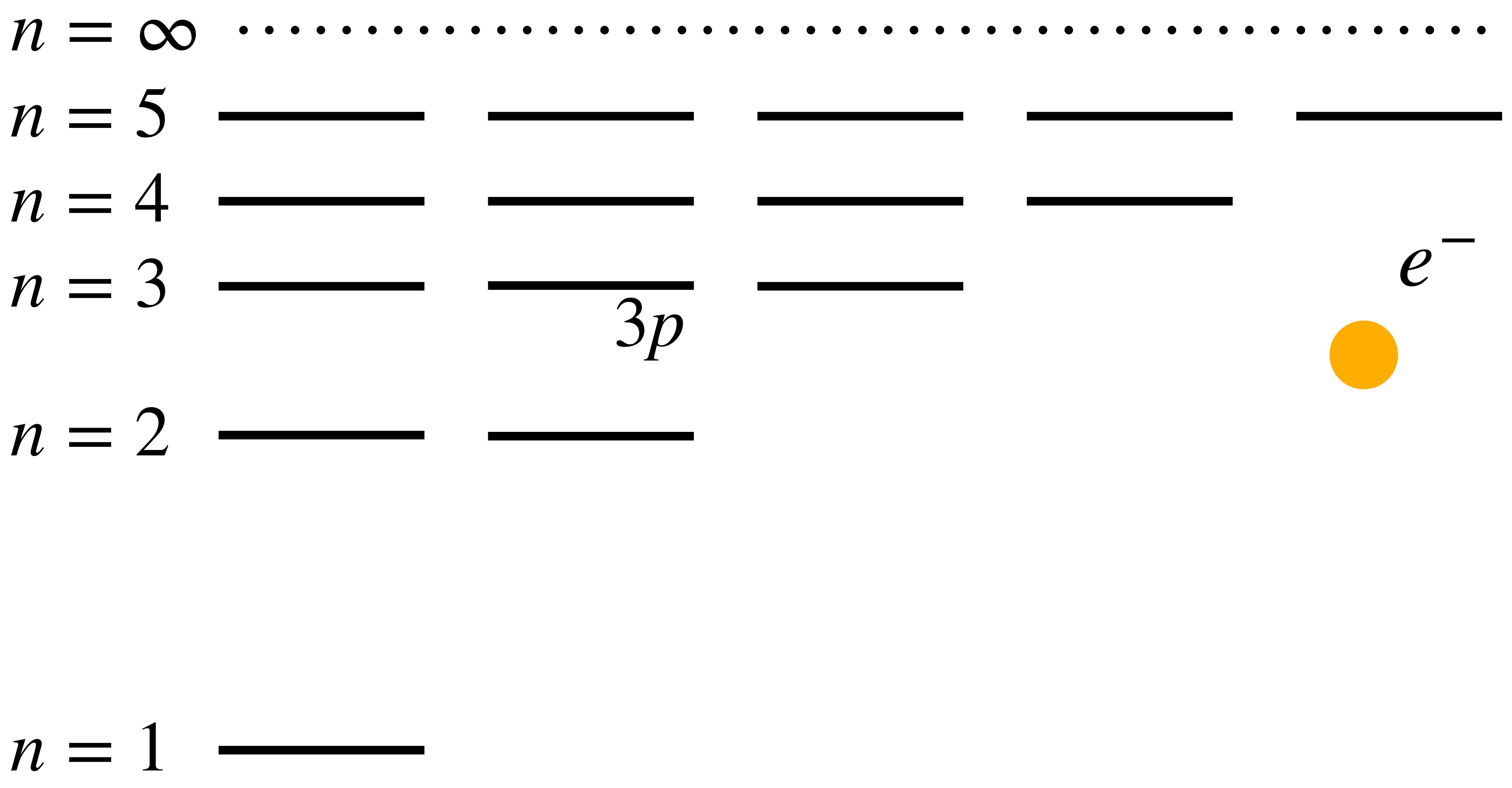
Hα emissivity profile



n_{3s} level population profile

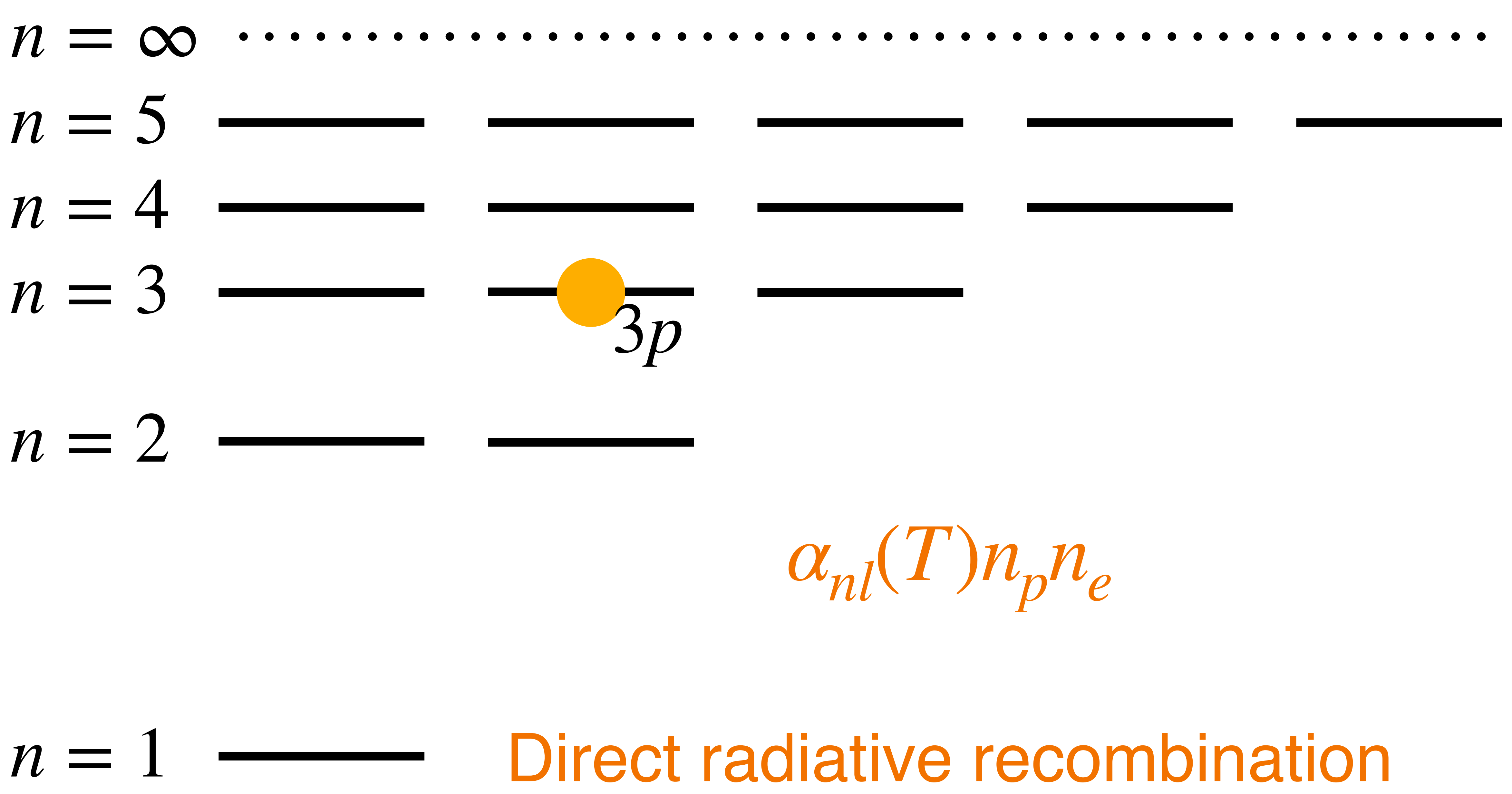


Atomic model for hydrogen
Rate equation



Atomic model for hydrogen

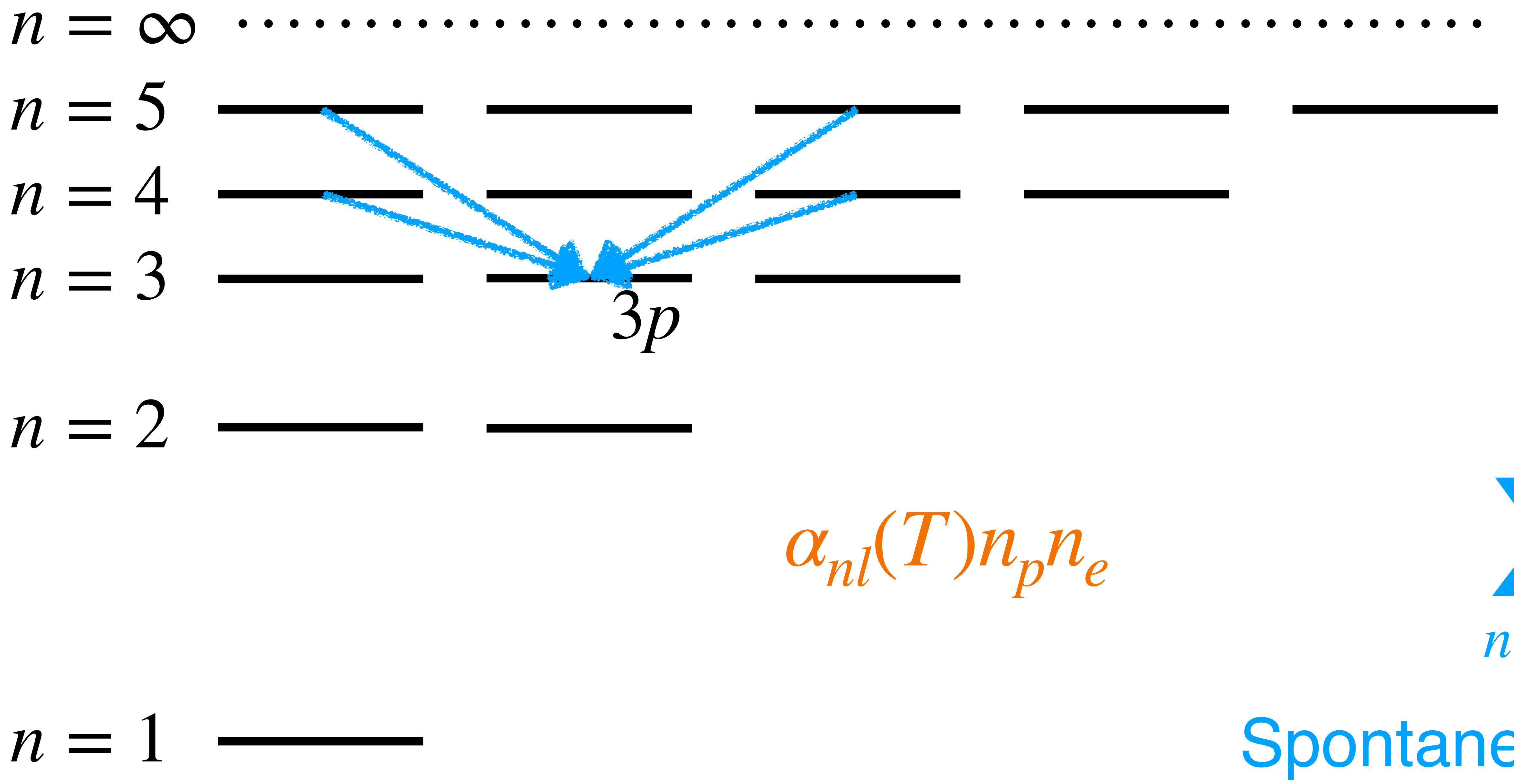
Rate equation



$$\Delta l = \pm 1$$

Atomic model for hydrogen

Rate equation



$\alpha_{nl}(T) n_p n_e$

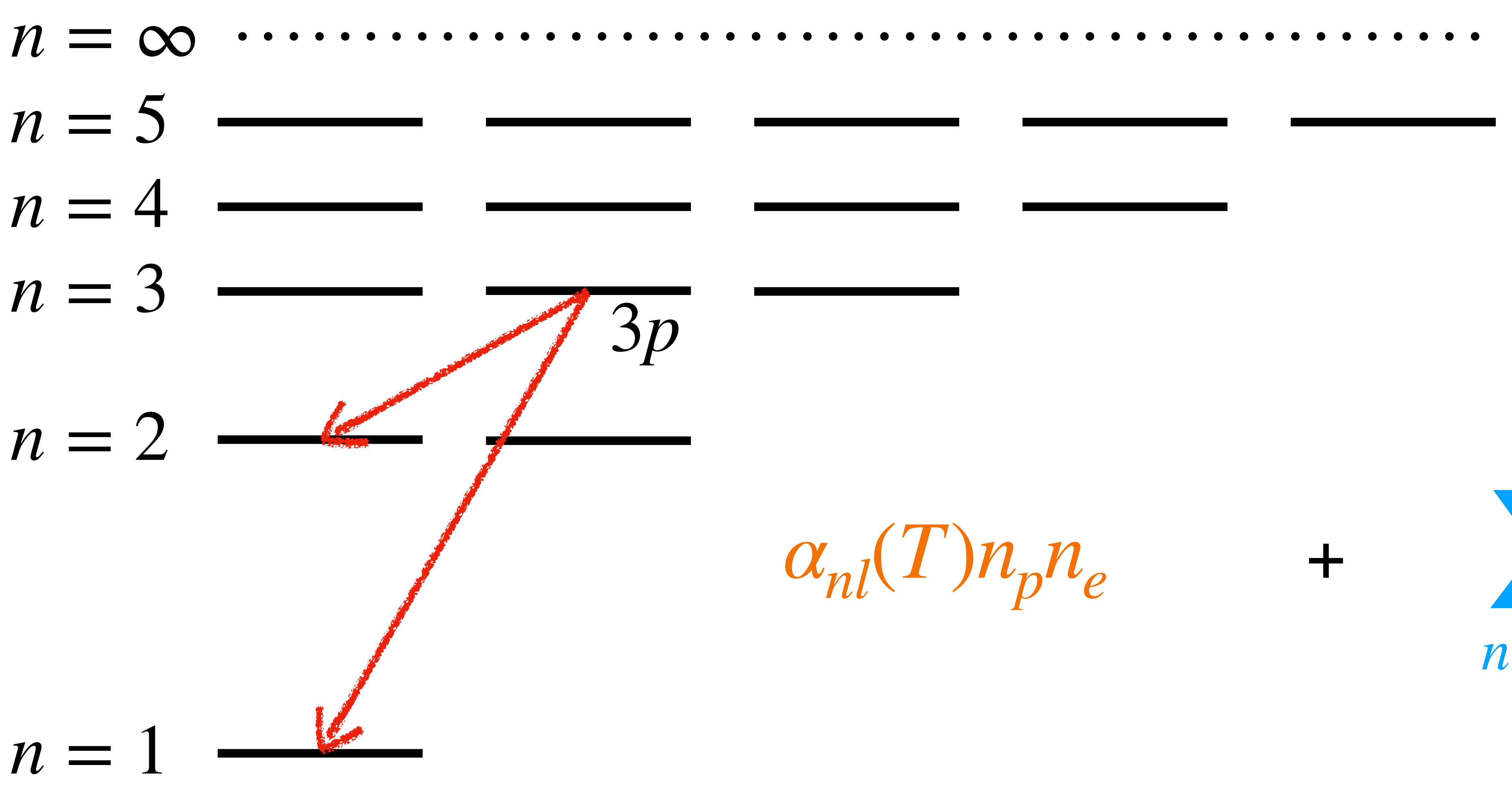
$$\sum_{n'>n}^{\infty} \sum_{L'=L\pm1} n_{n'L'} A_{n'L',nL}$$

Spontaneous decay from higher levels

$\Delta l = \pm 1$

Atomic model for hydrogen

Rate equation



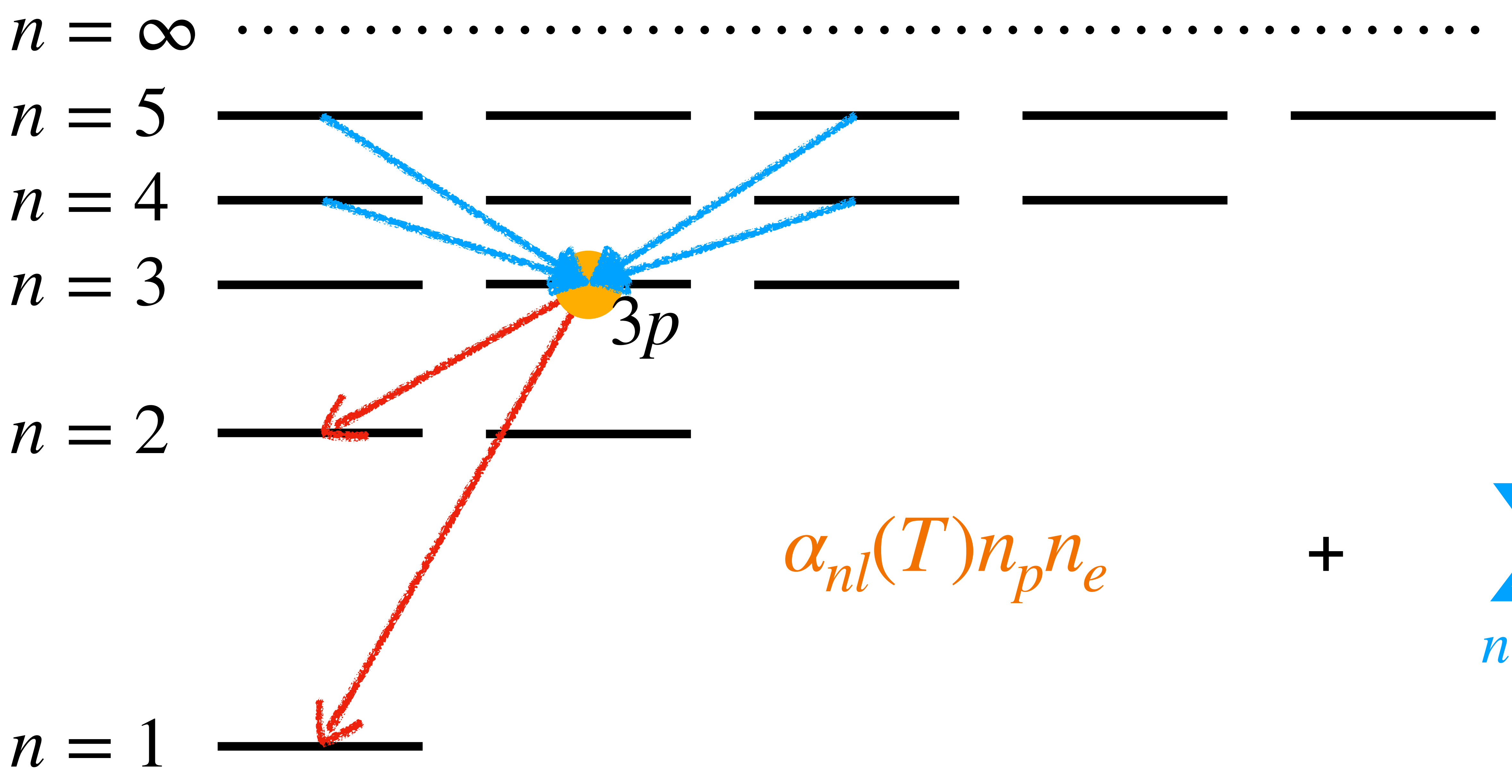
$$\alpha_{nl}(T) n_p n_e \quad + \quad \sum_{n'>n}^{\infty} \sum_{L'=L\pm 1} n_{n'L'} A_{n'L',nL} \quad = \quad n_{nl} \sum_{n''=n_0}^{n-1} A_{nL,n''L''}$$

Spontaneous decay to lower levels

$$\Delta l = \pm 1$$

Atomic model for hydrogen

Rate equation

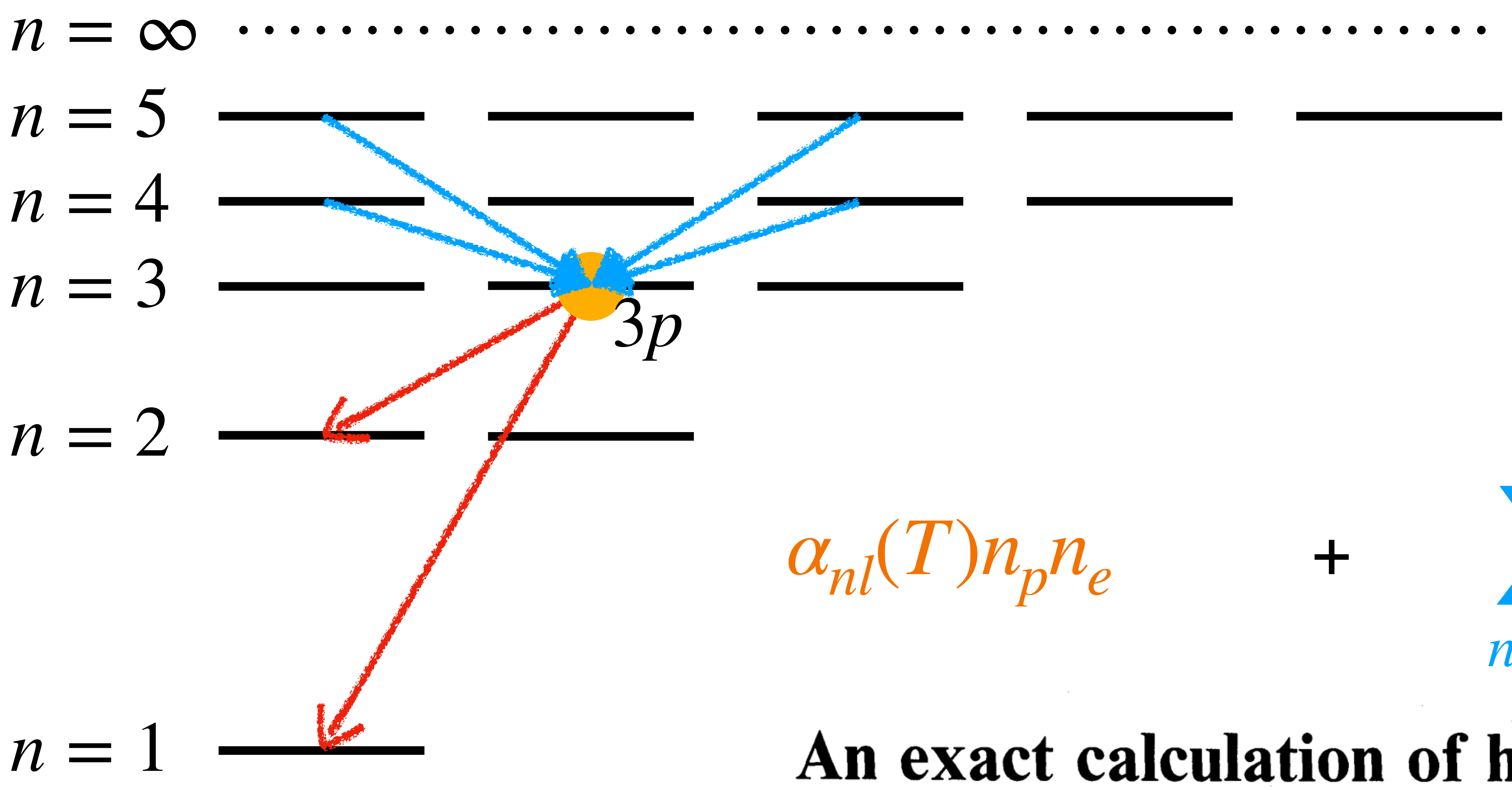


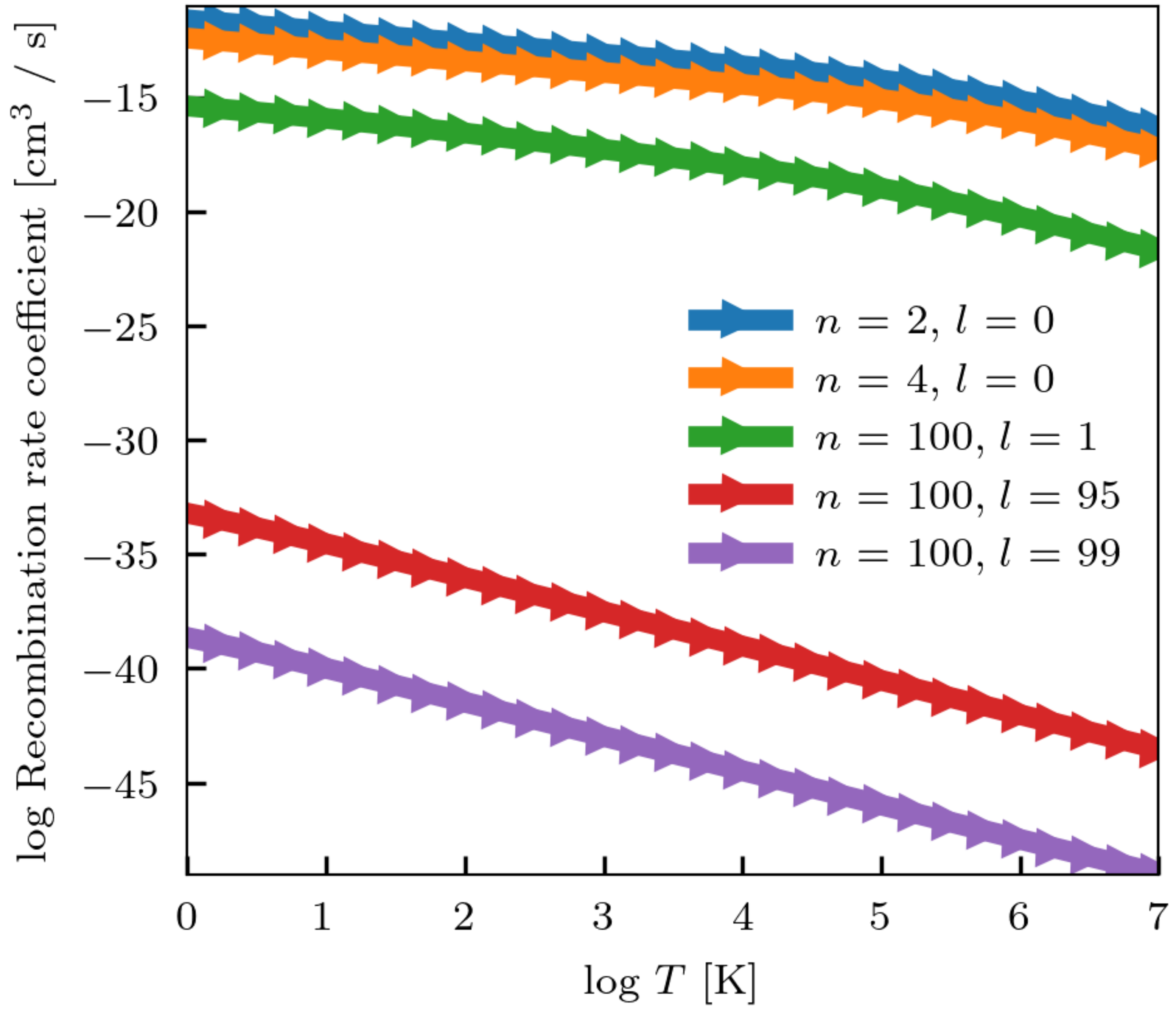
$$\alpha_{nl}(T)n_p n_e \quad + \quad \sum_{n'>n}^{\infty} \sum_{L'=L\pm1} n_{n'L'} A_{n'L',nL} \quad = \quad n_{nl} \sum_{n''=n_0}^{n-1} A_{nL,n''L''}$$

Population | De-population

Atomic model for hydrogen

Rate equation





$$\alpha_{nl}(T) n_p n_e + \sum_{n'>n}^{\infty} \sum_{L'=L\pm1} n_{n'L'} A_{n'L',nL} = n_{nl} \sum_{n''=n_0}^{n-1} A_{nL,n''L''}$$

An exact calculation of hydrogenic radial integrals and oscillator strengths, for principal quantum numbers up to $n \approx 1000$

D. Hoang-Binh

LAM, Observatoire de Paris, F-92195 Meudon Cedex, France

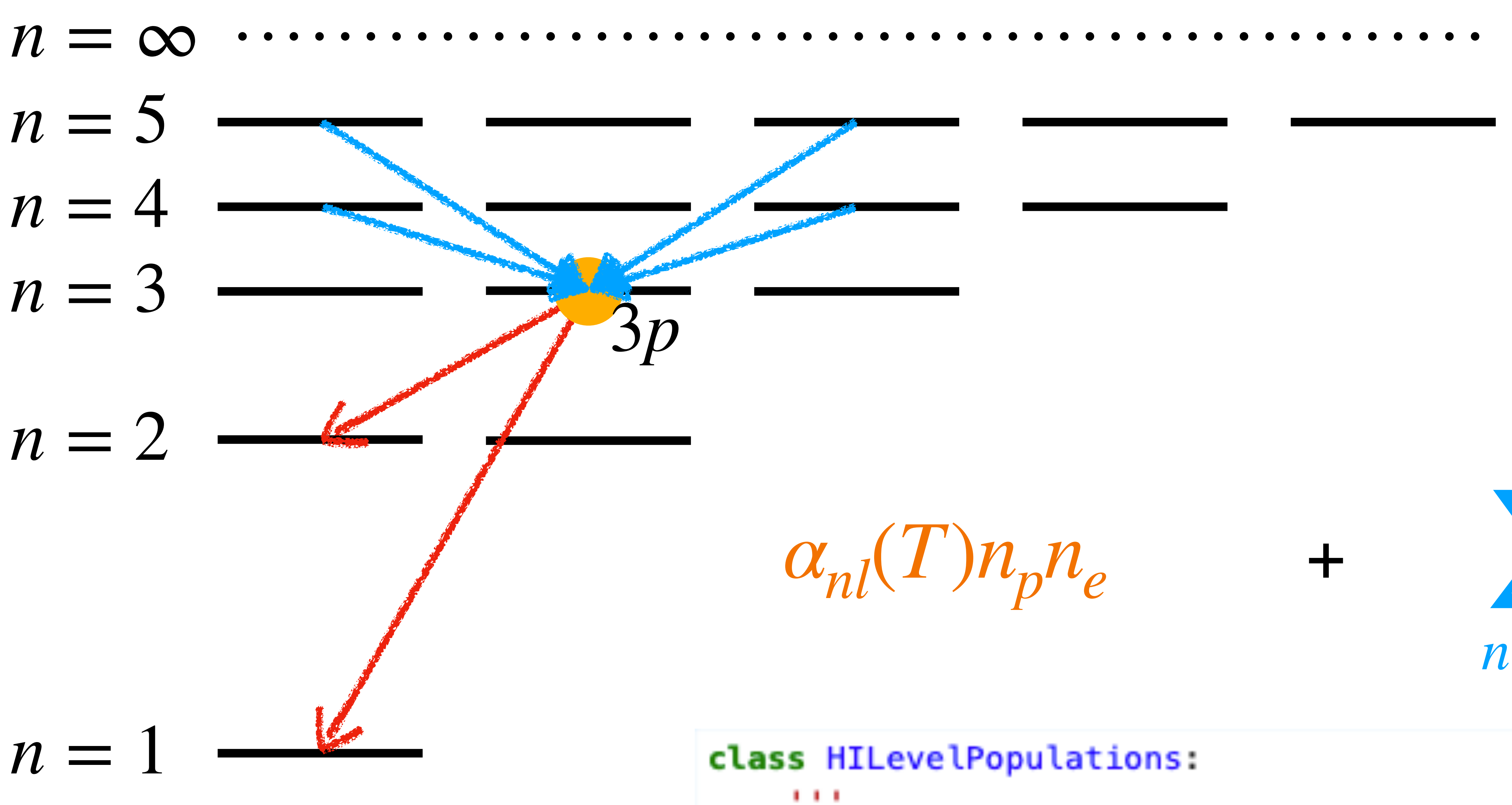
Received April 5, accepted April 25, 1990

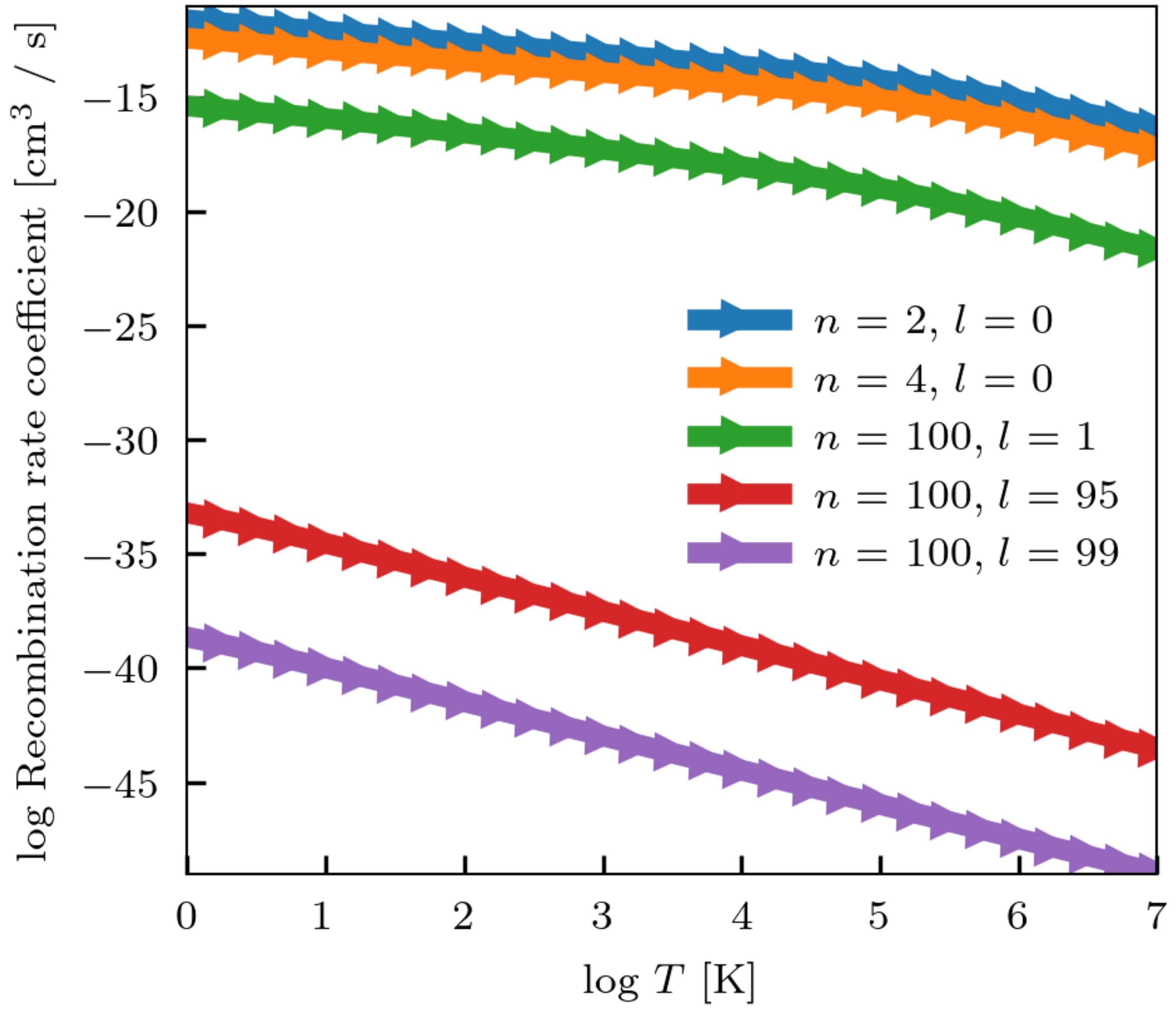
- Solved by Cascade Matrix Formalism (CMF)

https://github.com/YuankangLiu/hypop

Atomic model for hydrogen

Rate equation





$$\alpha_{nl}(T)n_p n_e + \sum_{n'>n}^{\infty} \sum_{L'=L\pm1} n_{n'L'} A_{n'L',nL} = n_{nl} \sum_{n''=n_0}^{n-1} A_{nL,n''L''}$$

```python
class HILevelPopulations:
    '''
    Compute level population for HI using the cascade matrix formalism.
    See Osterbrock & Ferland 2006, section 4.2
    '''
    def __init__(self, nmax=60, TabulatedEinsteinAs = '/cosma/home/dphlss/tt/Codes/EinsteinAs/EinsteinA.dat',
                 TabulatedRecombinationRates = '/cosma/home/dphlss/tt/Data/Recomb/h_iso_recomb.dat',
                 caseB = True, caseBnmax=5, verbose=False):
```

- Solved by Cascade Matrix Formalism (CMF)

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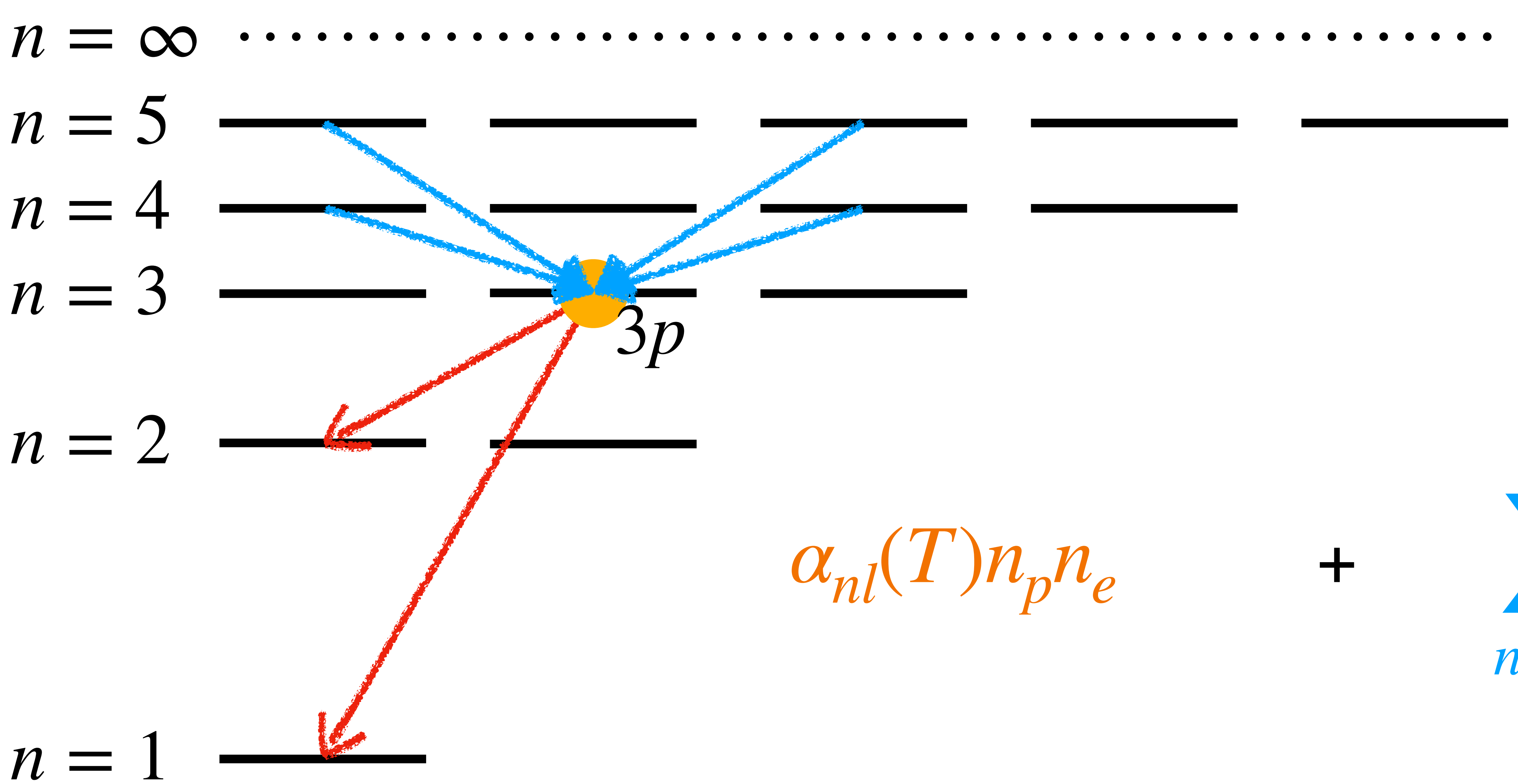
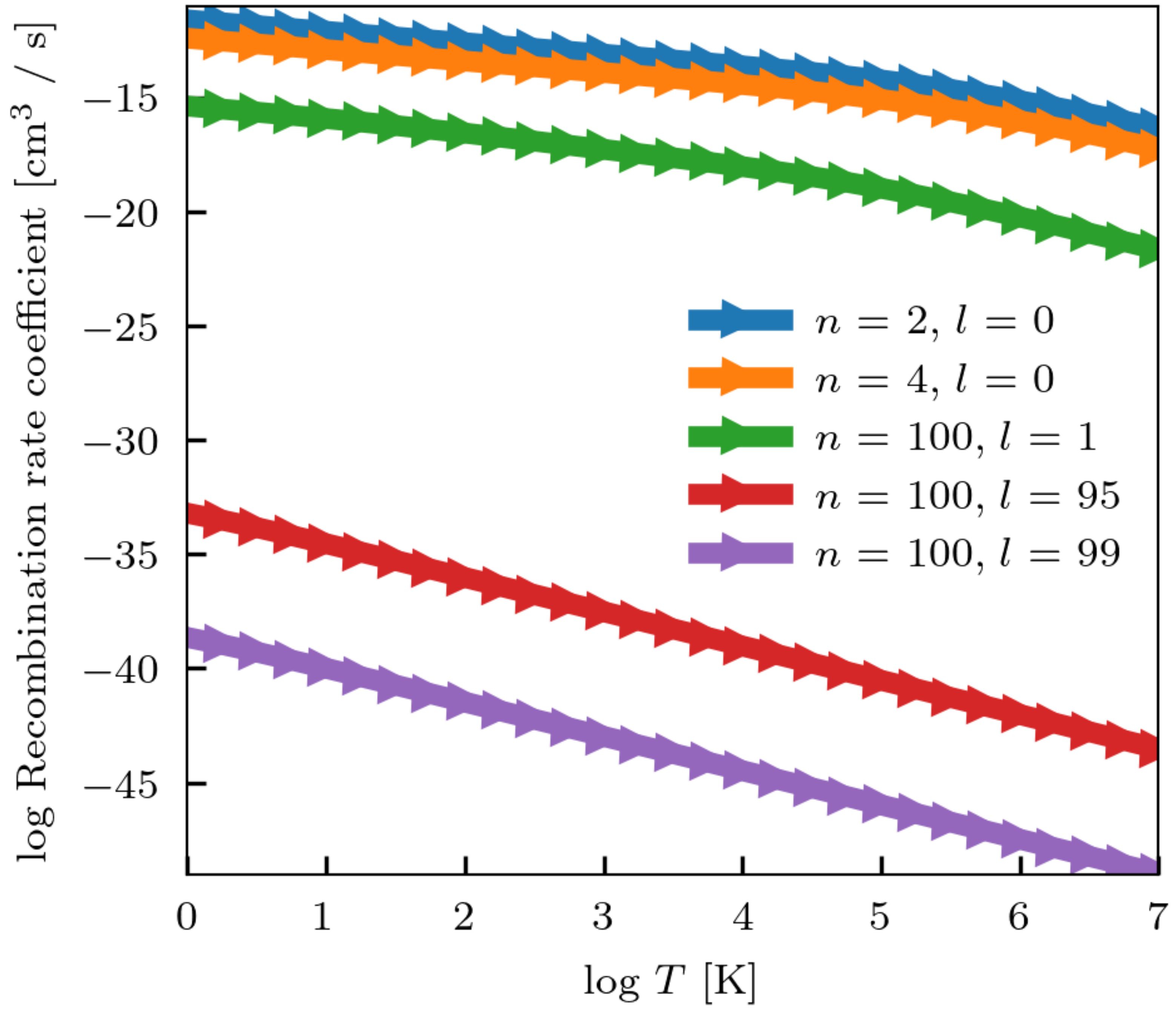
Atomic model for hydrogen

Rate equation





$$\alpha_{nl}(T)n_pn_e + \sum_{n'>n}^{\infty}\sum_{L'=L\pm1} n_{n'L'}A_{n'L',nL} = n_{nl}\sum_{n''=n_0}^{n-1}A_{nL,n''L''}$$

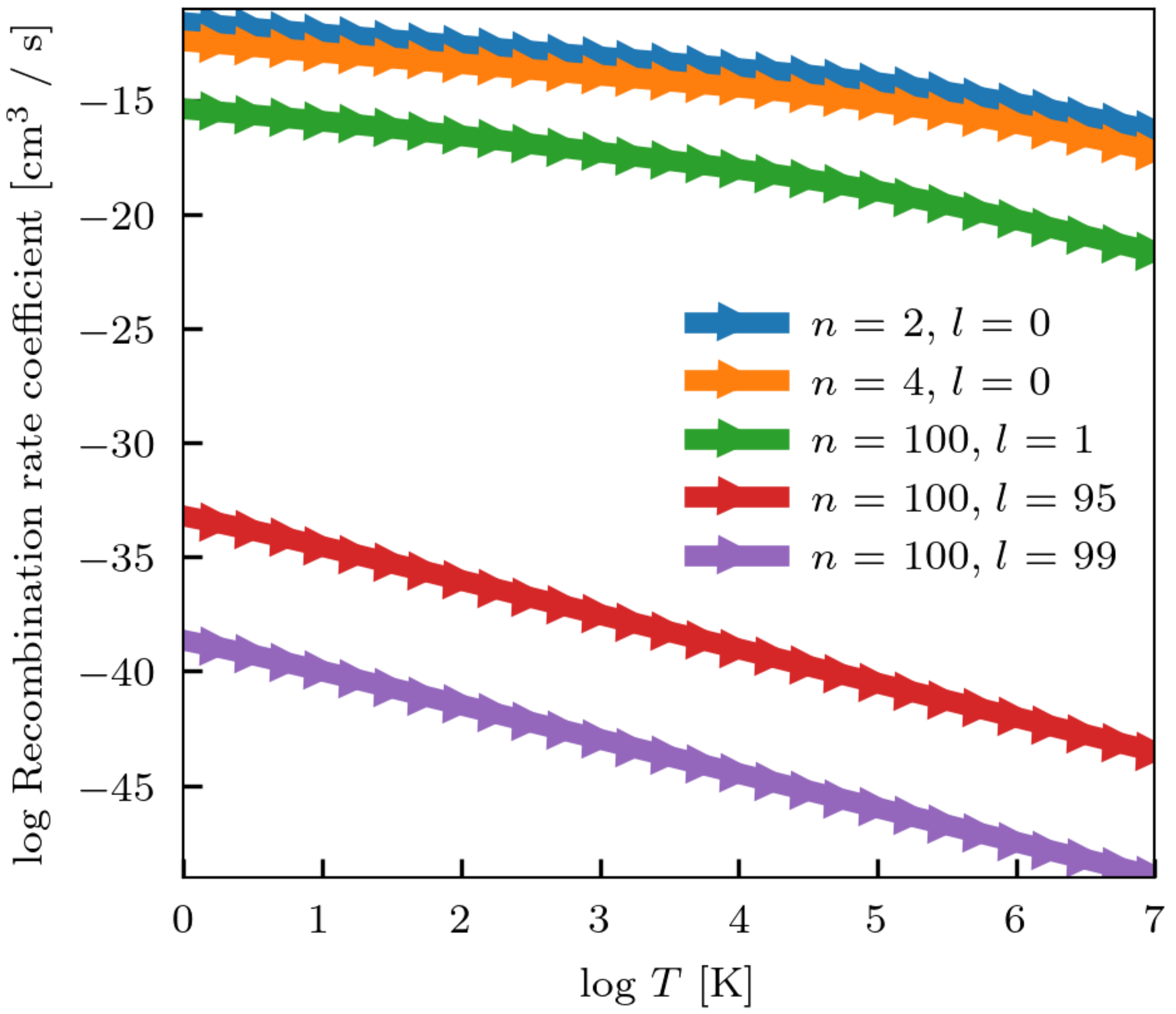
HyPop or **HyLight**

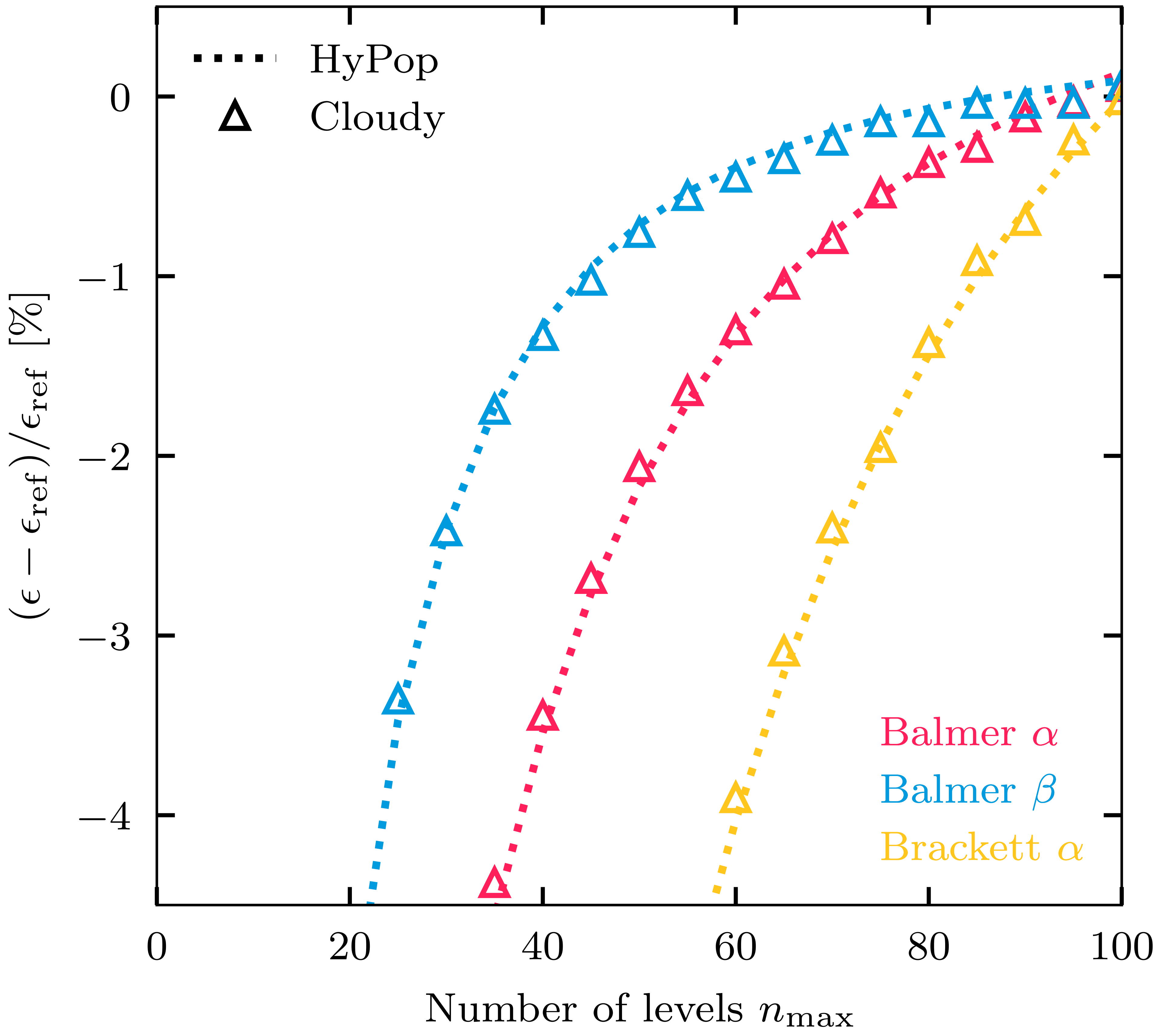
- Solved by Cascade Matrix Formalism (CMF)

https://github.com/YuankangLiu/hypop

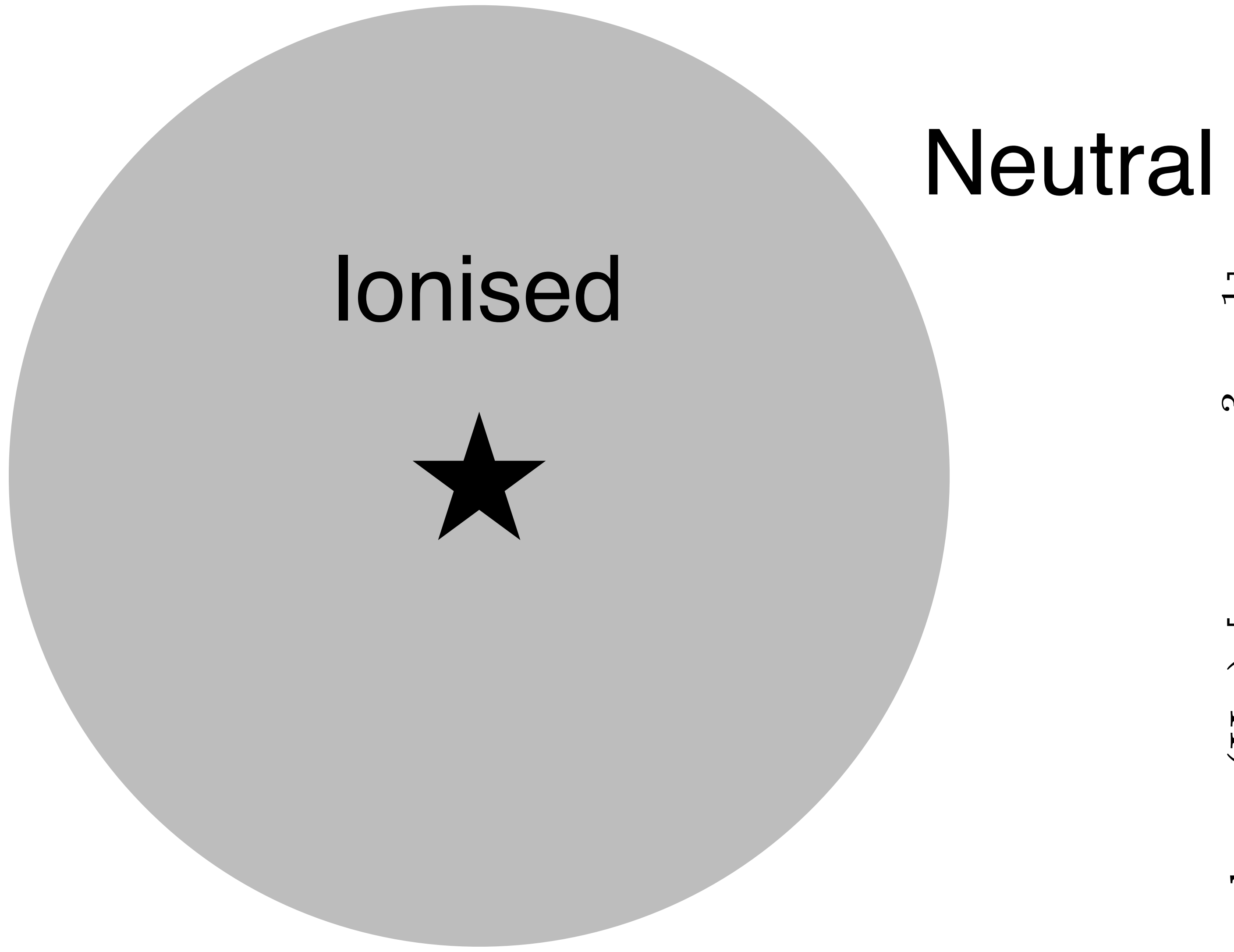
Convergence

$$\alpha_{nl}(T)n_p n_e + \sum_{n'>n}^{\infty}\sum_{L'=L\pm1} n_{n'L'}A_{n'L',nL} = n_{nl}\sum_{n''=n_0}^{n-1} A_{nL,n''L''}$$



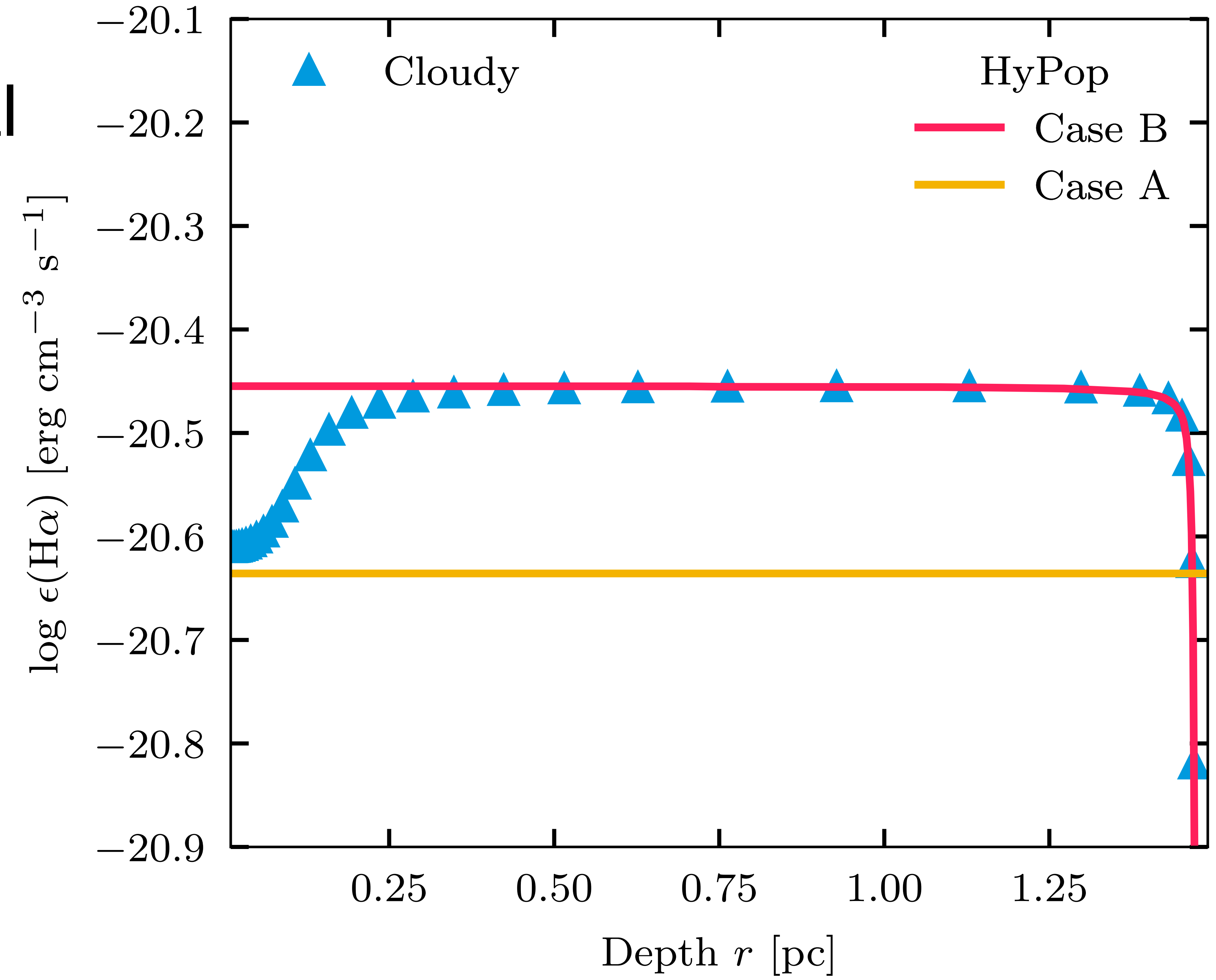


Atomic model for hydrogen

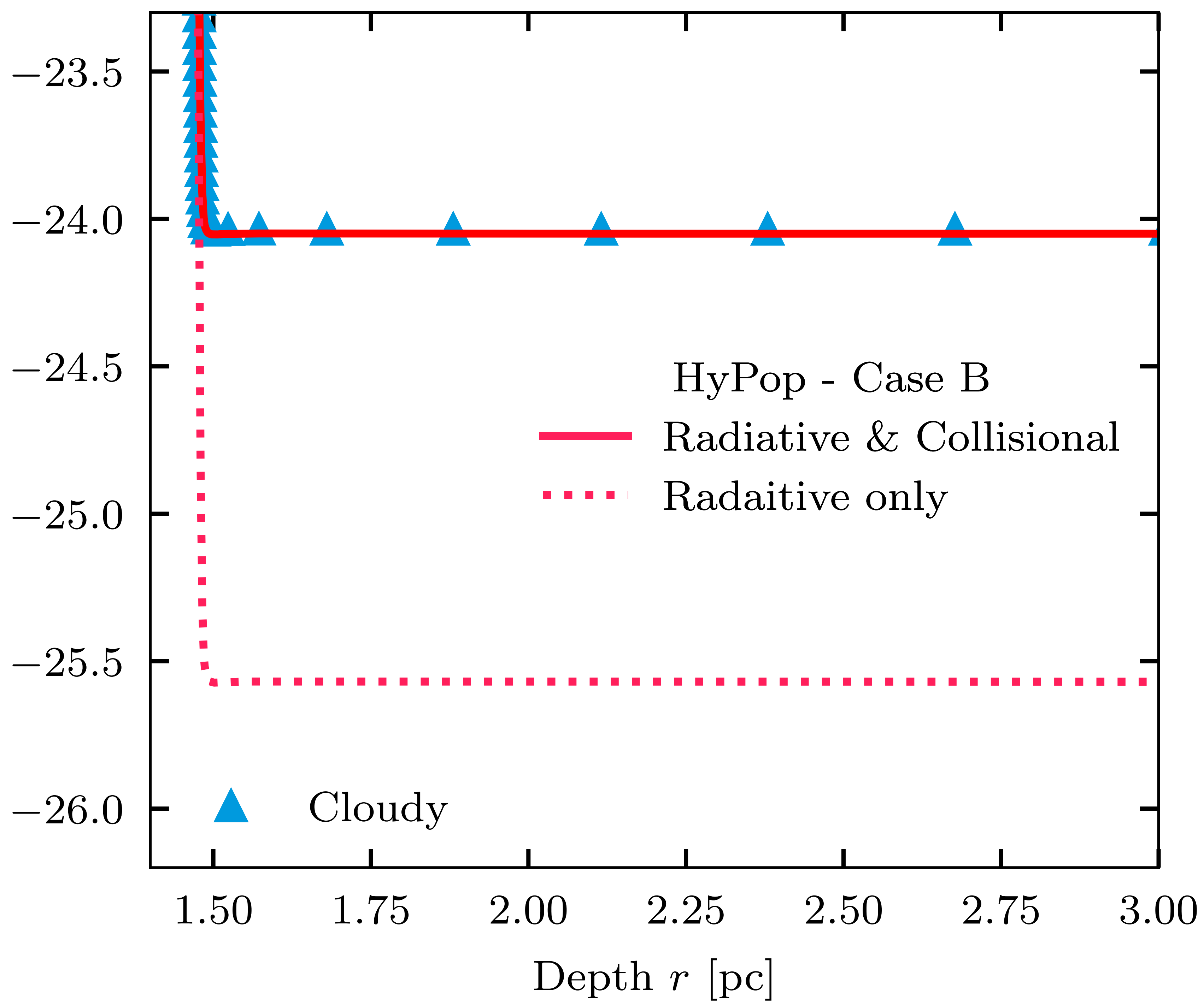


Hα emissivity profile

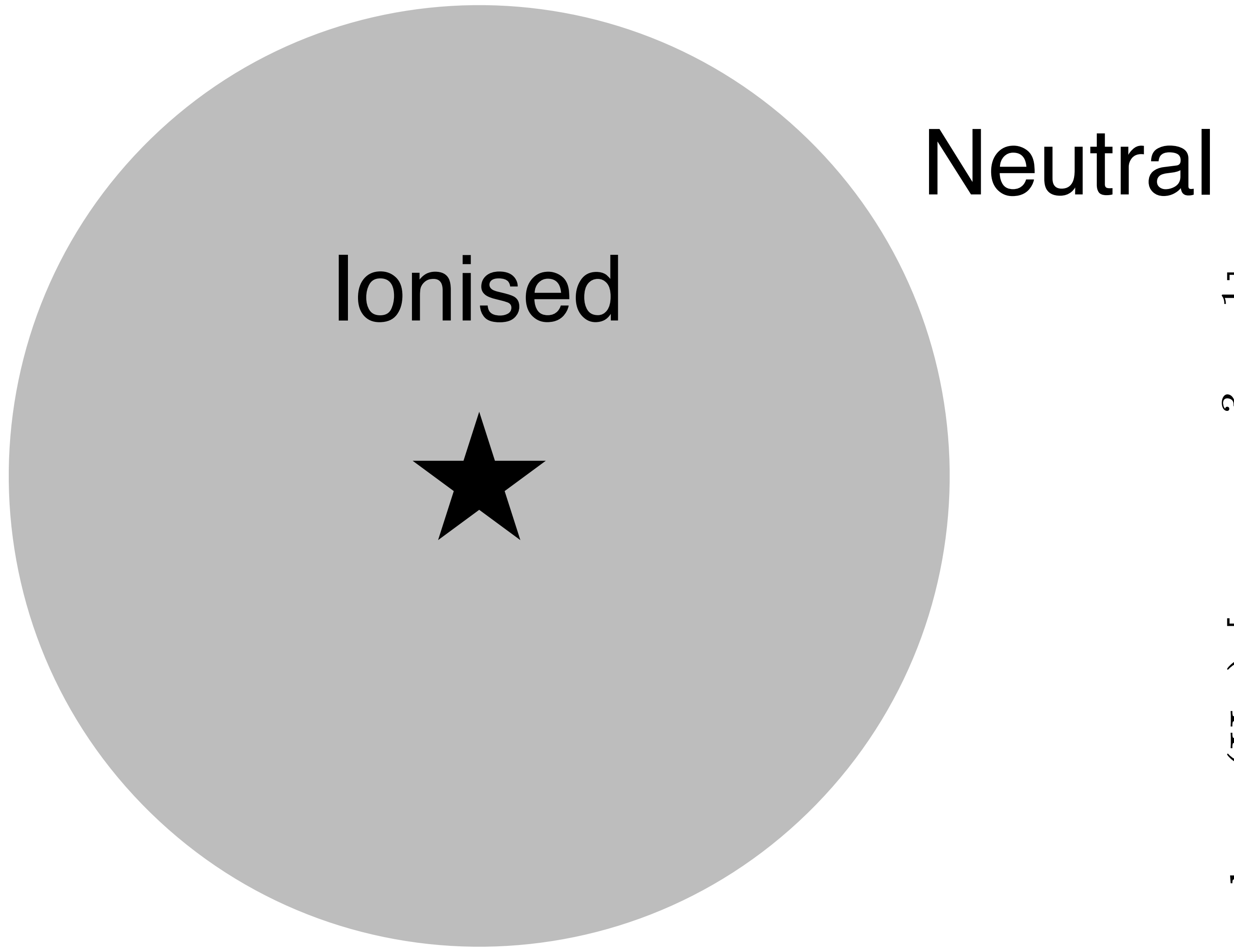
within Strömgren sphere



beyond Strömgren sphere



Atomic model for hydrogen



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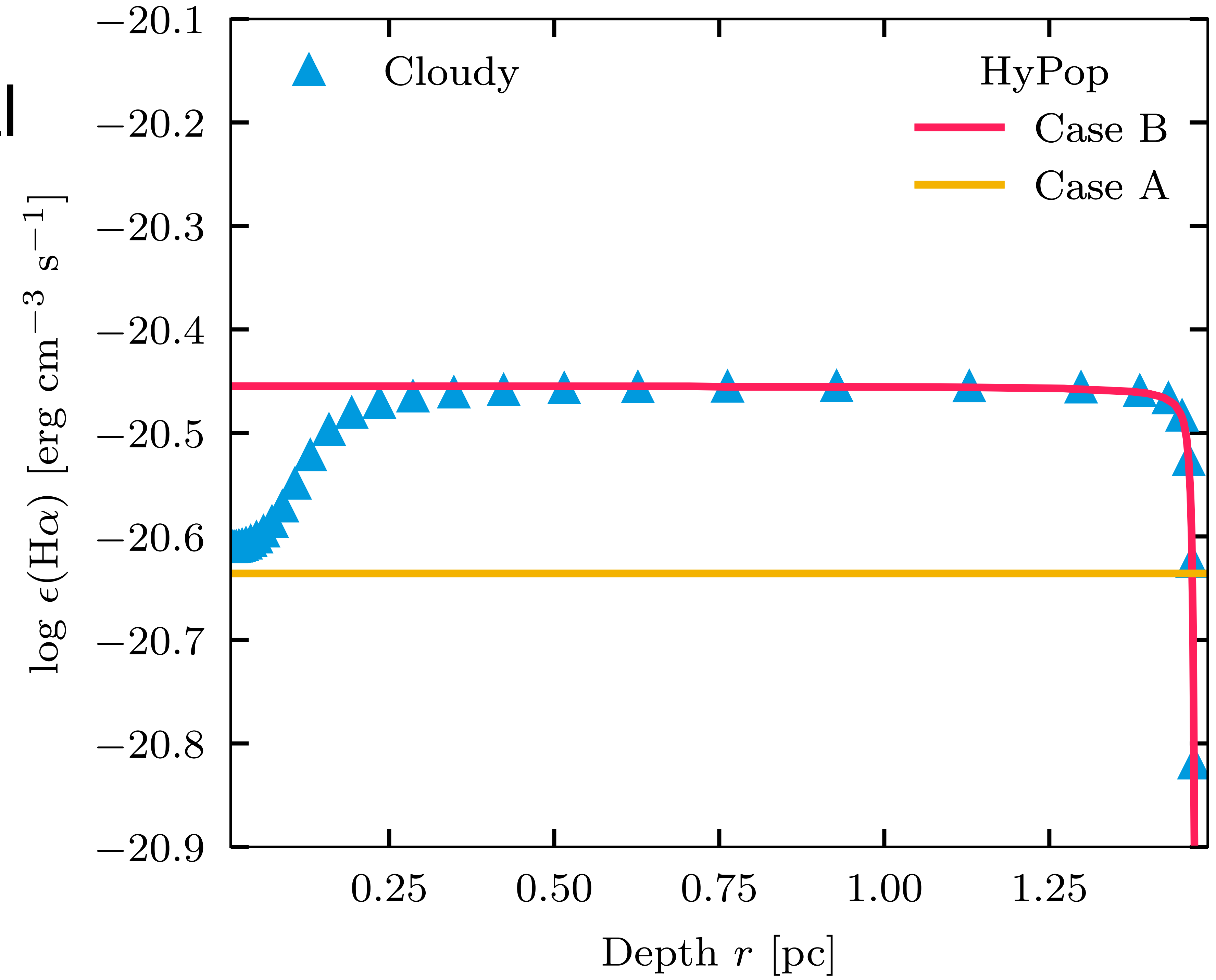
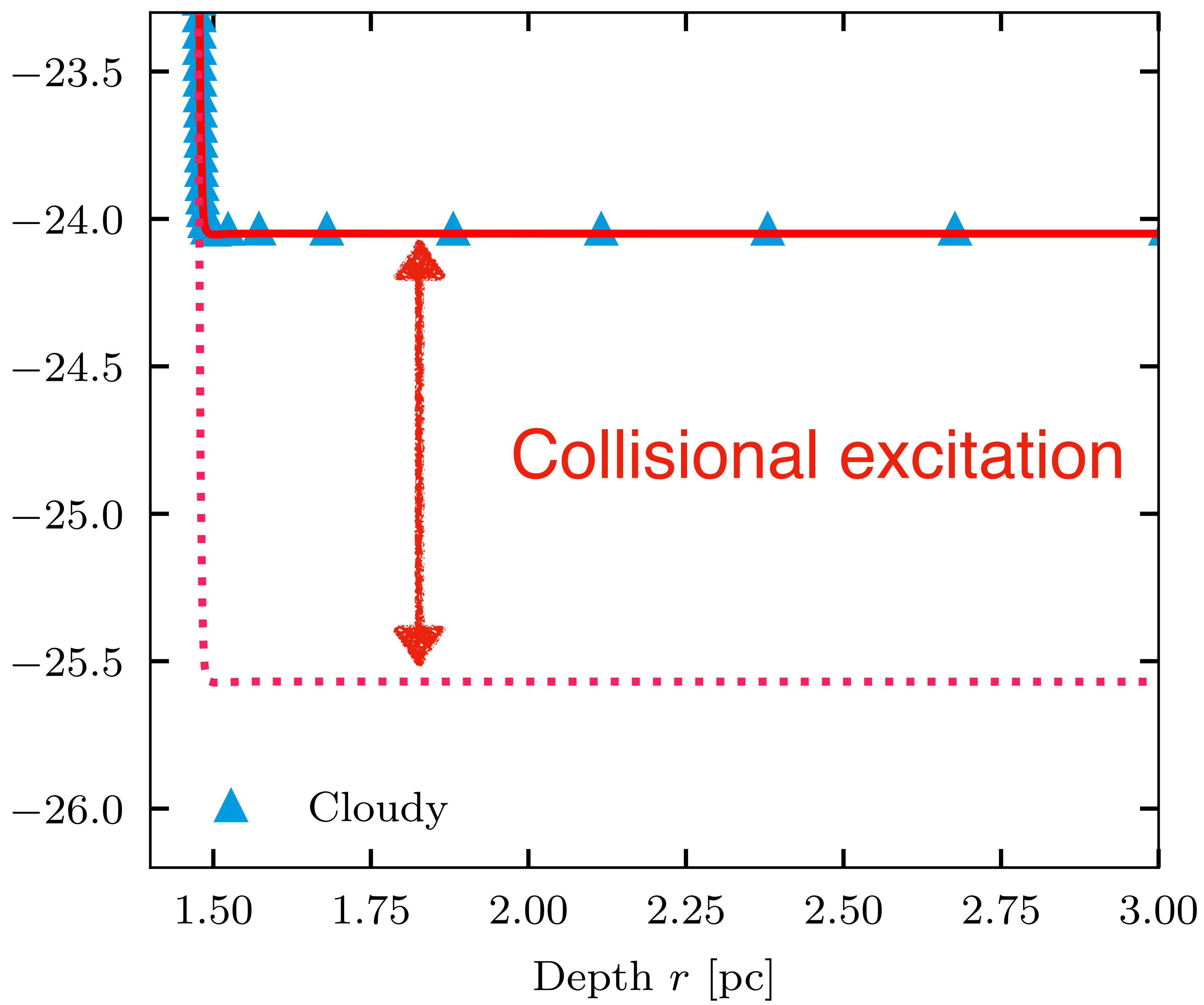
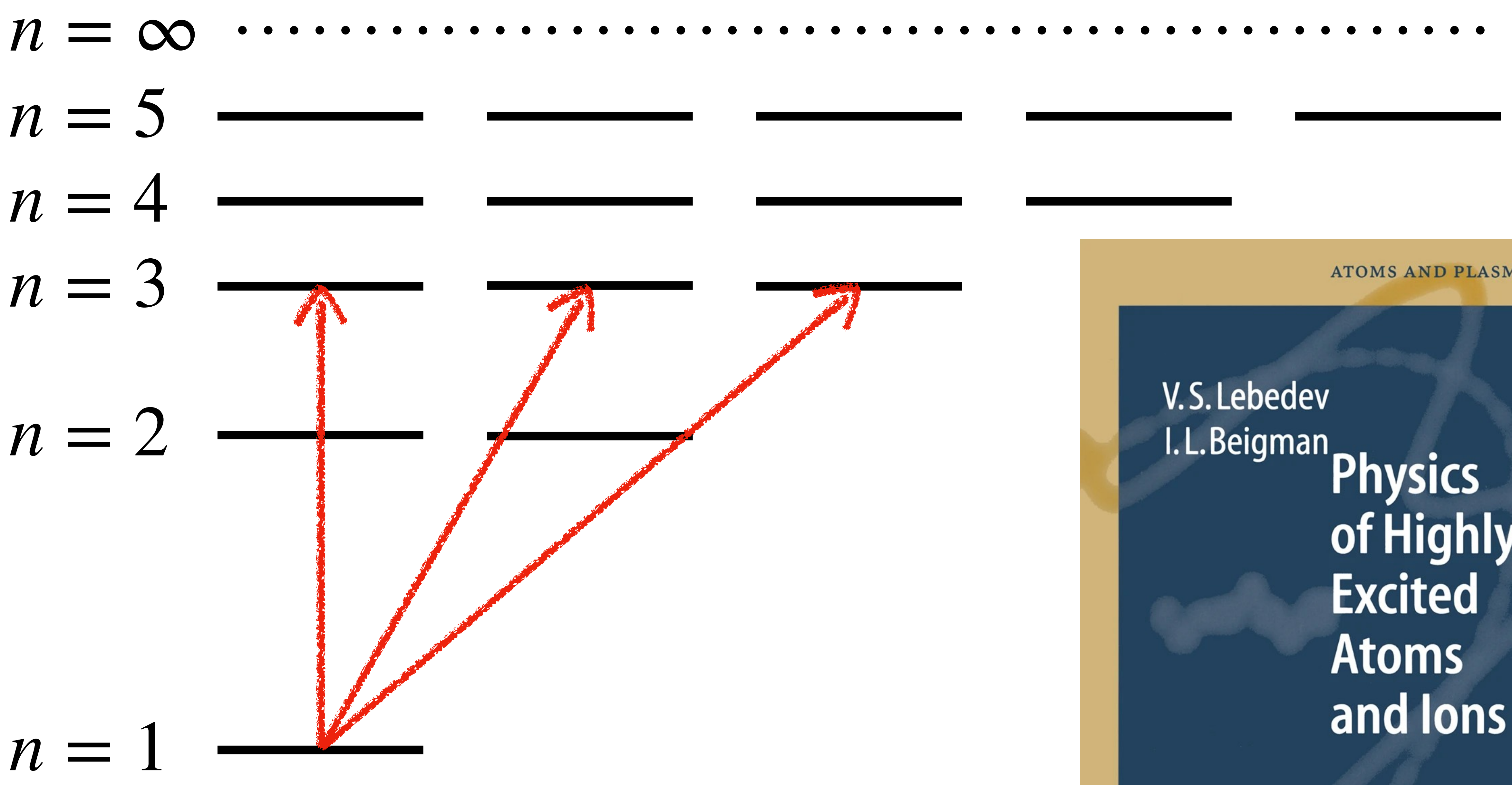


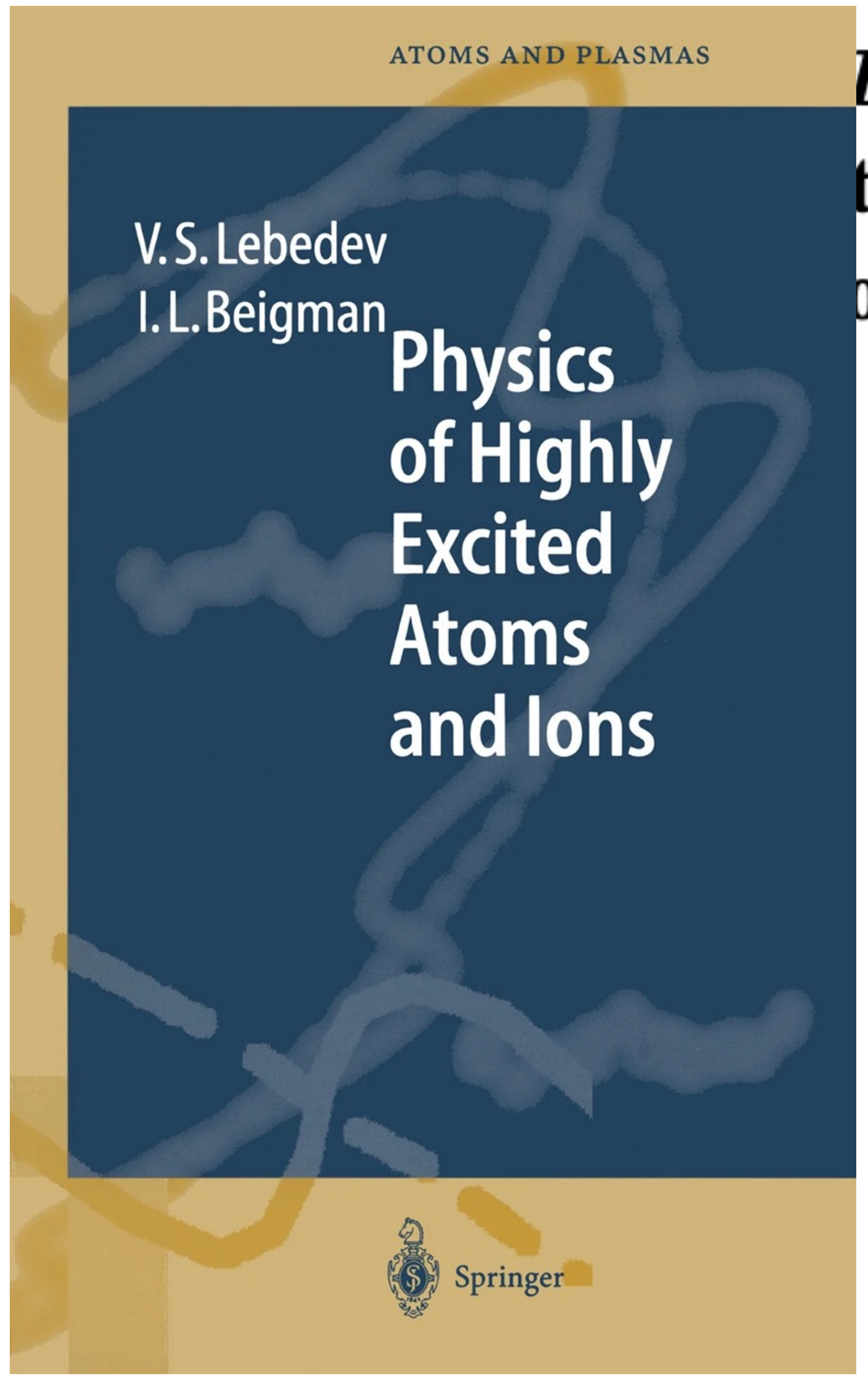
beyond Strömgren sphere



Atomic model for hydrogen

Contribution from collisional excitation





Lebedev & Beigman (1998) use the semiclassical straight-trajectory Born approximation to provide *ab initio* excitation rate coefficients for Rydberg atoms. The de-excitation formula for $n' \to n$ is

$$q_{n'\to n} = \frac{g_n}{g_{n'}} \exp\left(\frac{\Delta E_{nn'}}{kT_e}\right) q_{n\to n'}$$

$$= \frac{g_n}{g_{n'}} 2\sqrt{\pi} a_0^2 \alpha c n \left[\frac{n'}{Z(n'-n)}\right]^3 \frac{f(\theta)\varphi}{\sqrt{\theta}}, \quad (7)$$

where

$$\varphi = \frac{2n'^2 n^2}{(n'+n)^4 (n'-n)^2} [4(n'-n)-1] \exp\left(\frac{E_n}{kT_e}\right) E_1\left(\frac{E_n}{kT_e}\right)$$

$$+ \frac{8n^3}{(n'+n)^2(n'-n)n^2n'^2} (n'-n-0.6)\left(\frac{4}{3} + n^2(n'-n)\right)$$

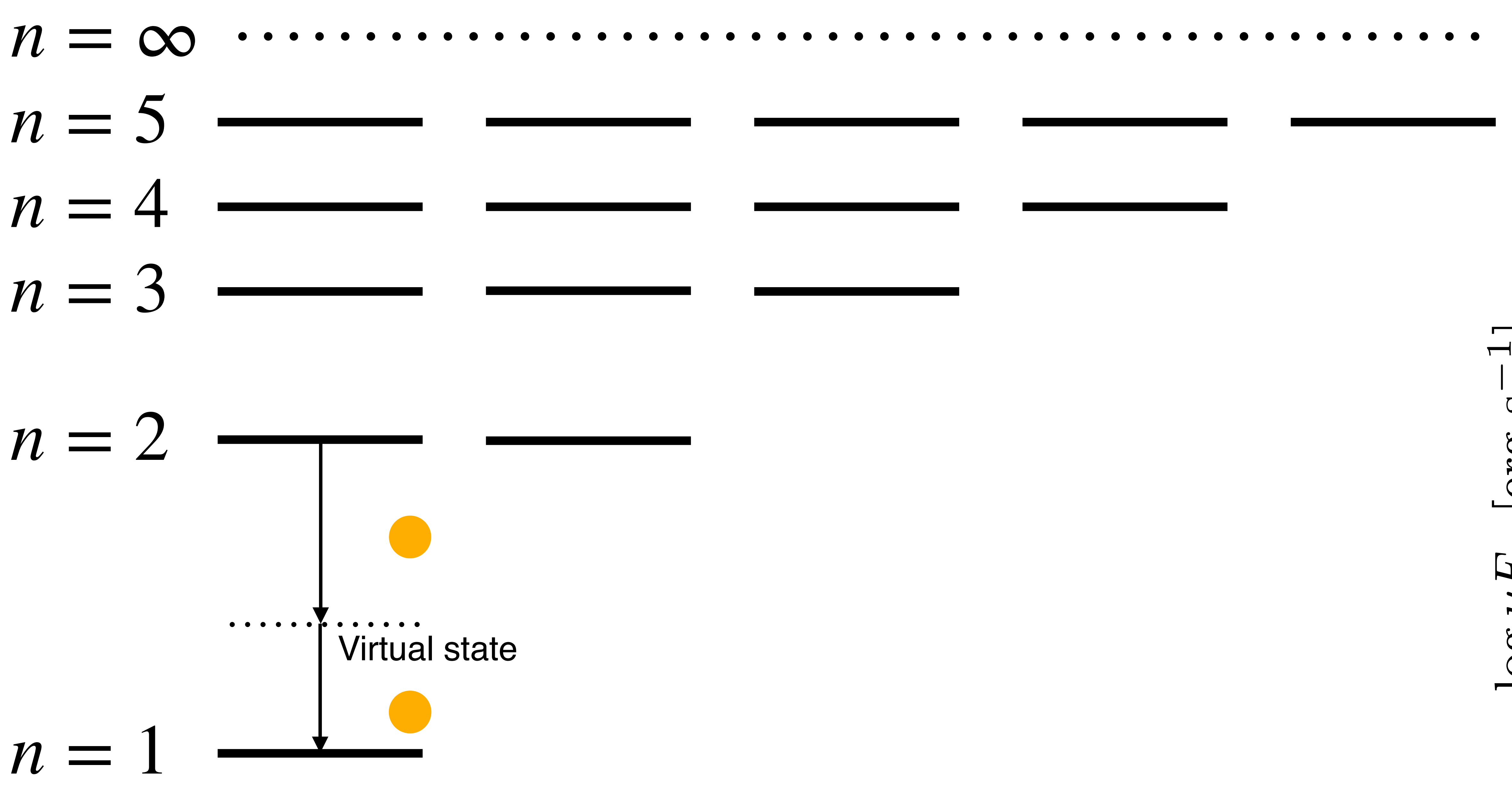
$$\times \left[1 - \frac{E_n}{kT_e} \exp\left(\frac{E_n}{kT_e}\right) E_1\left(\frac{E_n}{kT_e}\right)\right] \quad (8a)$$

$$f(\theta) = \frac{\ln\left(1 + \frac{n\theta}{Z(n'-n)\sqrt{\theta}+2.5}\right)}{\ln\left(1 + \frac{n\sqrt{\theta}}{Z(n'-n)}\right)} \quad (8b)$$

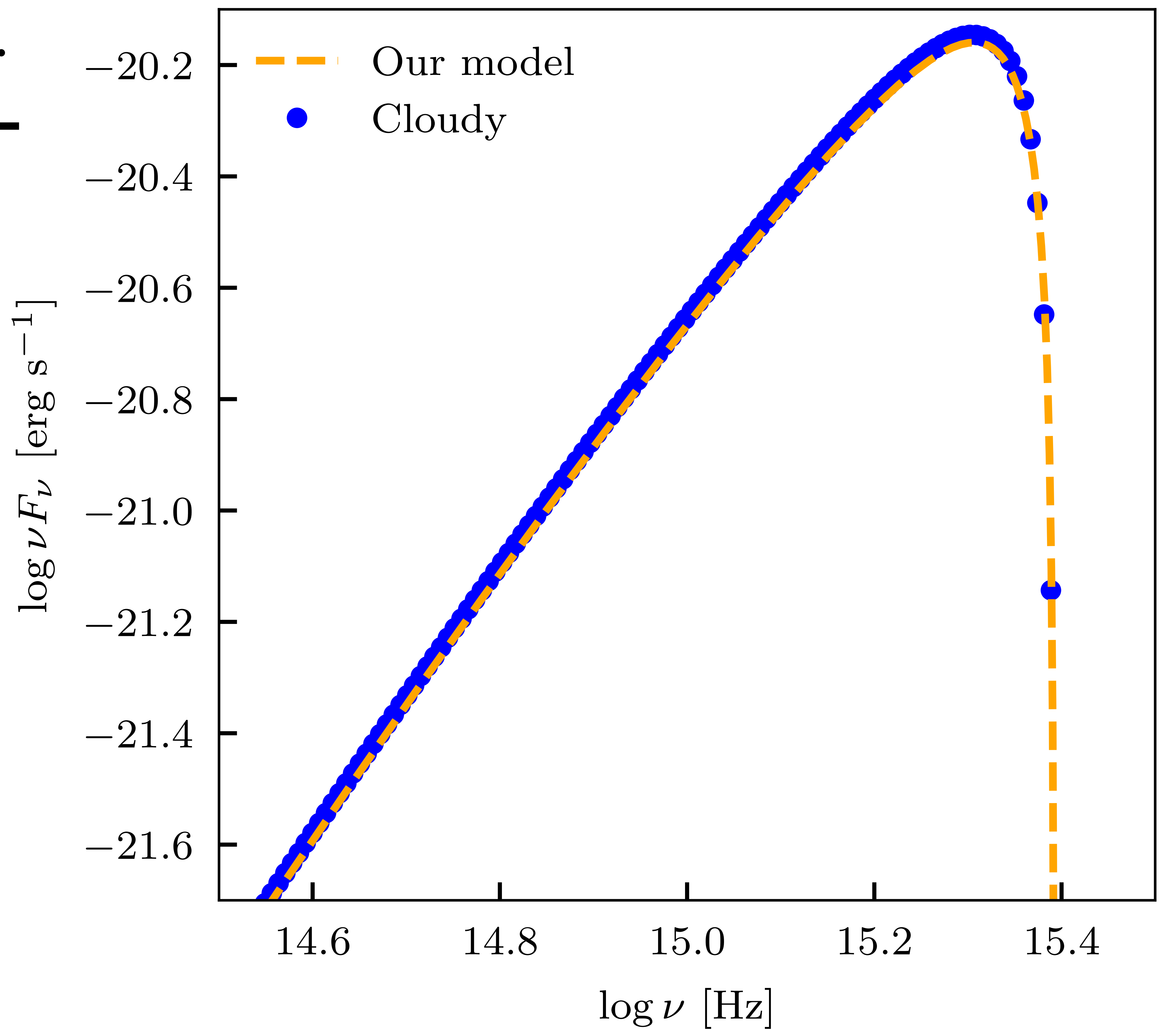
$$\theta = \frac{kT_e}{Z^2 I_H}, \quad (8c)$$

Atomic model for hydrogen

Two-photon continuum



Two-photon continuum spectrum



Application - Mock observables

3D H II region simulation with radiative transfer

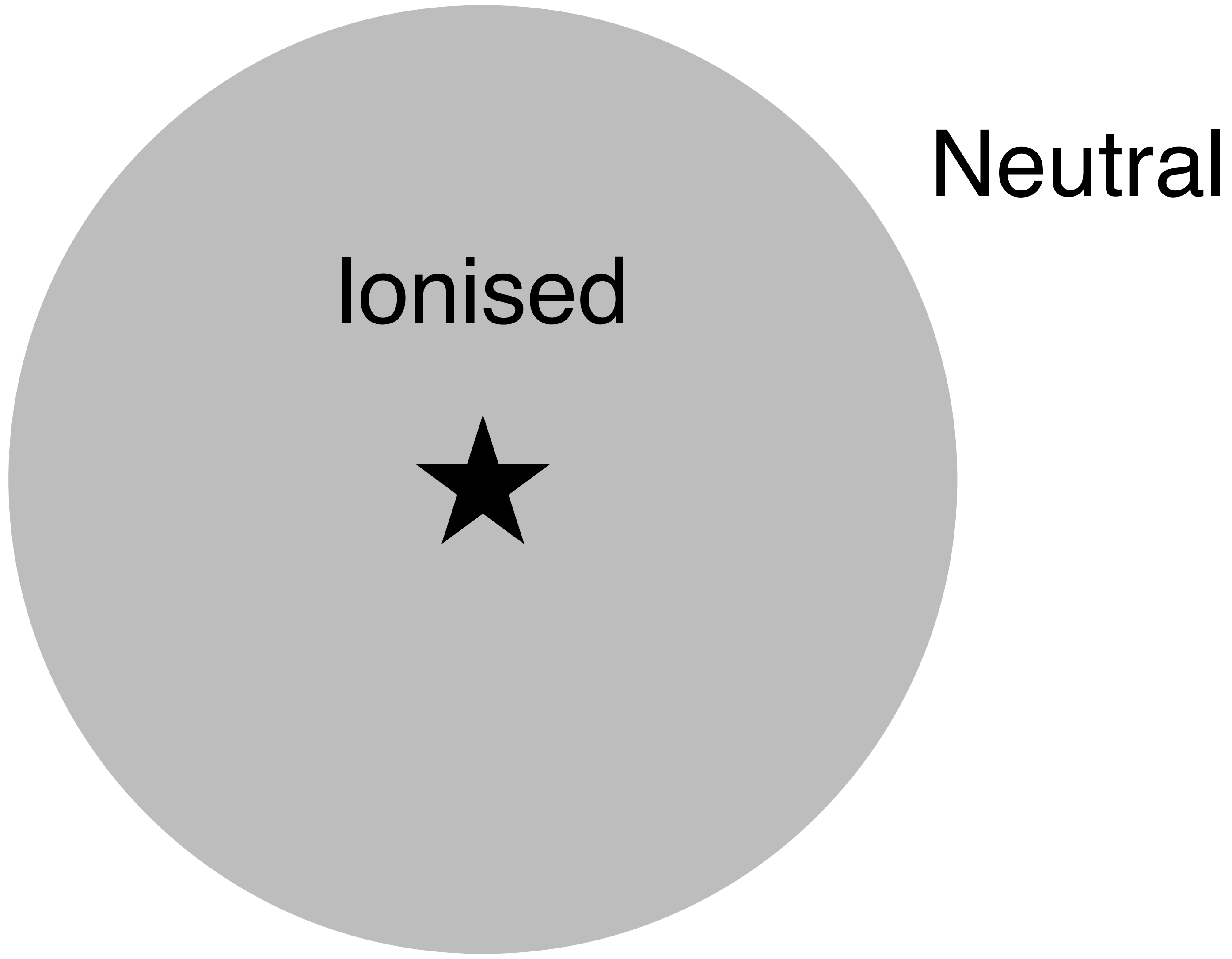
CHIMES + SPHM1RT

CHIMES
CHemistry of the Interstellar Medium and Extragalactic Sources

SWIFT

$n_{\mathrm{H}} = 10$ cm^{-3}

$Q(\mathrm{H}) = 5e47$ s^{-1}



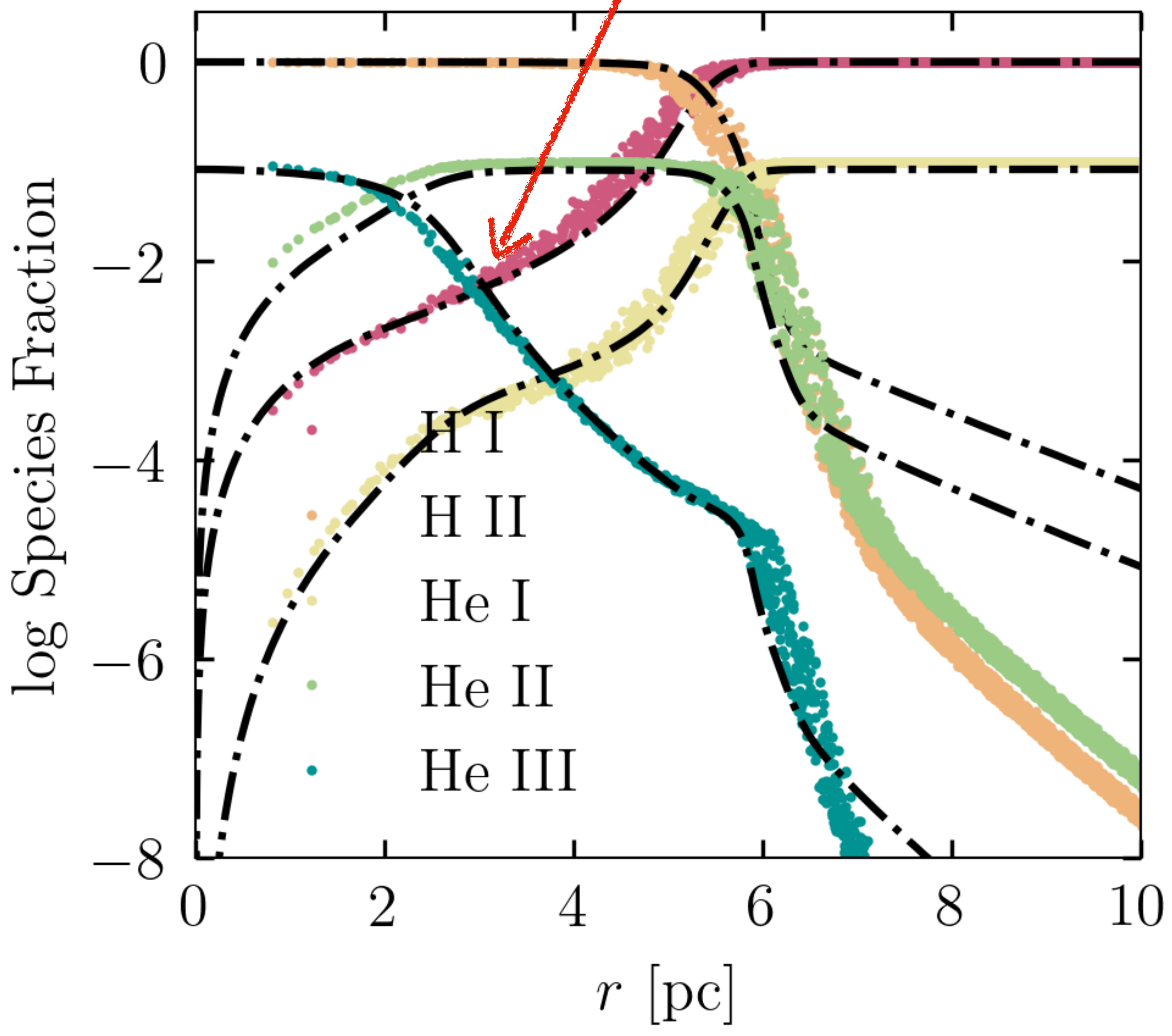
Application - Mock observables

e.g., How many H atoms are in $n = 3$?

3D H II region simulation with radiative transfer

CHIMES + SPHM1RT

Ionisation structure



CHIMES-RT vs. Cloudy

Application - Mock observables

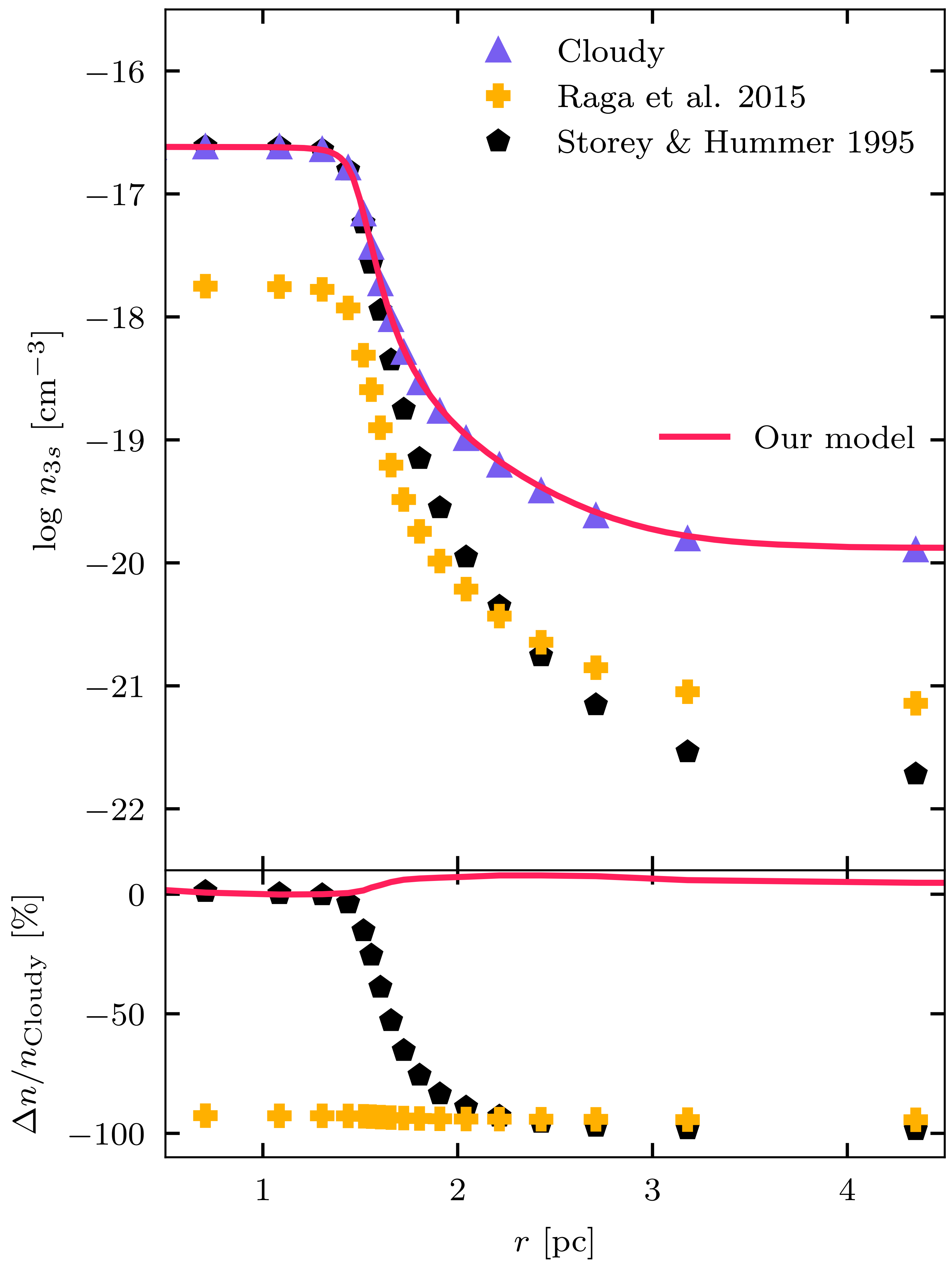
3D H II region simulation with radiative transfer

CHIMES + SPHM1RT ↓

Ionisation structure

Atomic model ↓ n_{nl} for given n_p, n_e, T

Level population



Application - Mock observables

3D H II region simulation with radiative transfer

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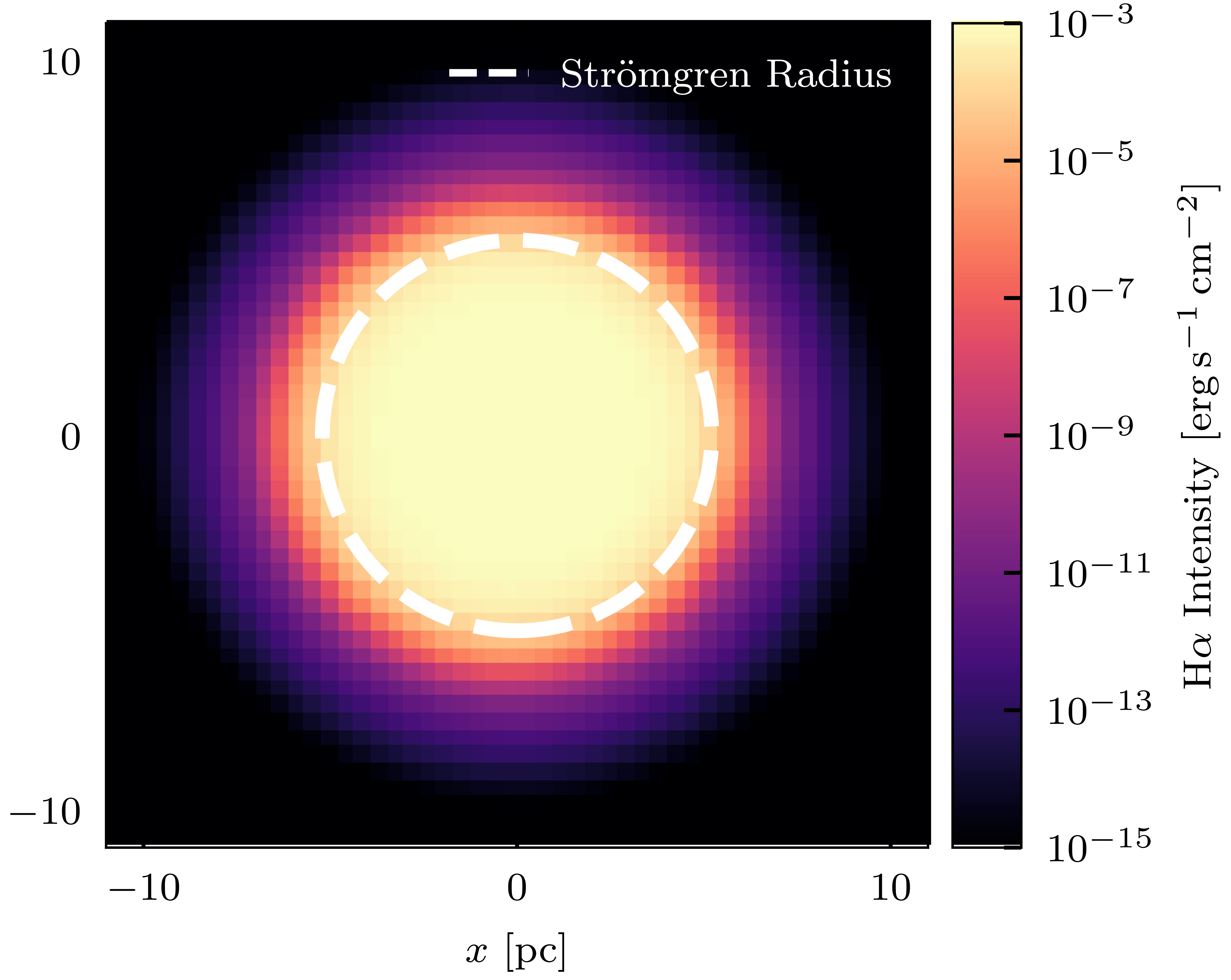
Level population

↓ 

Spectrum & Image



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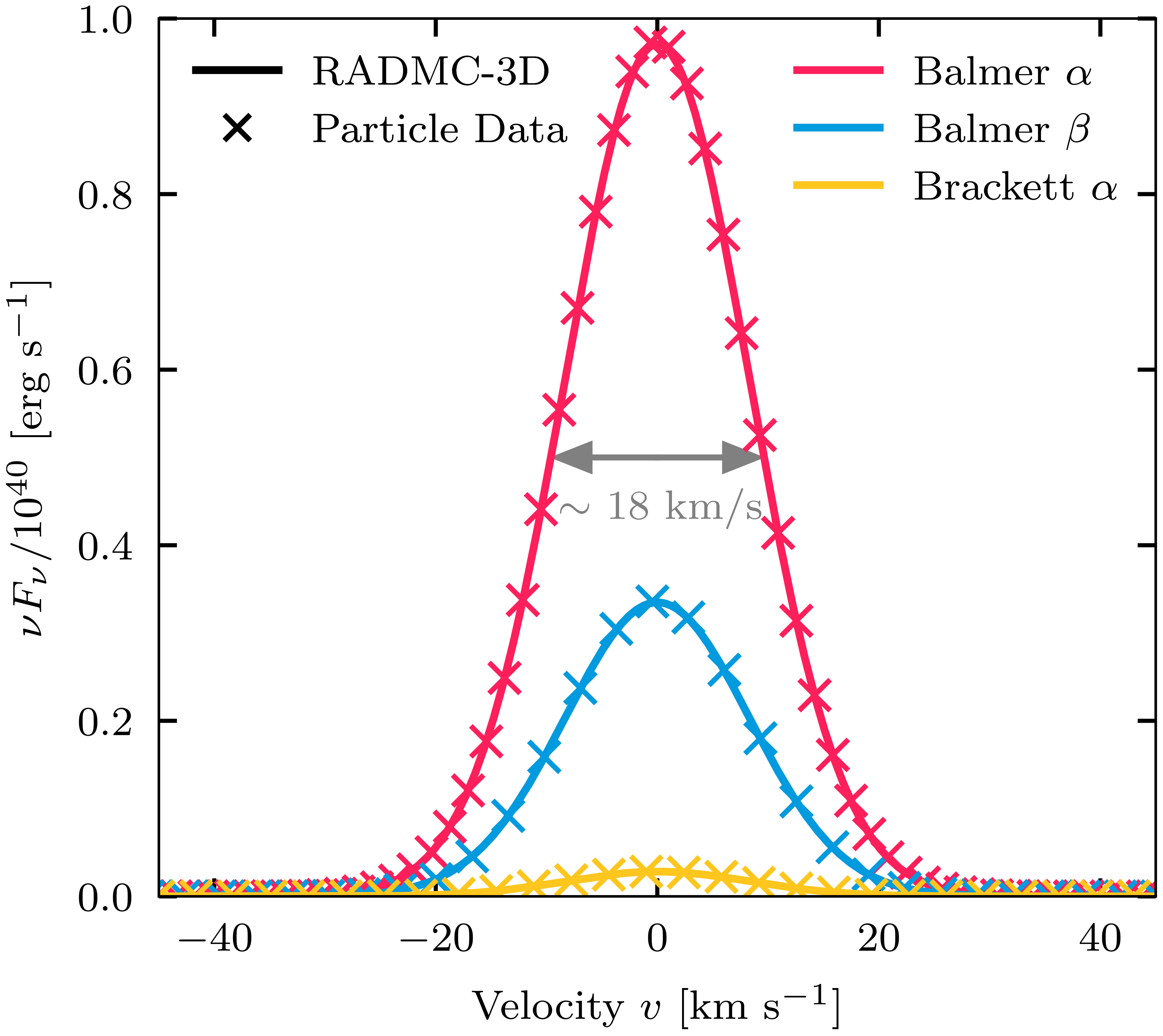
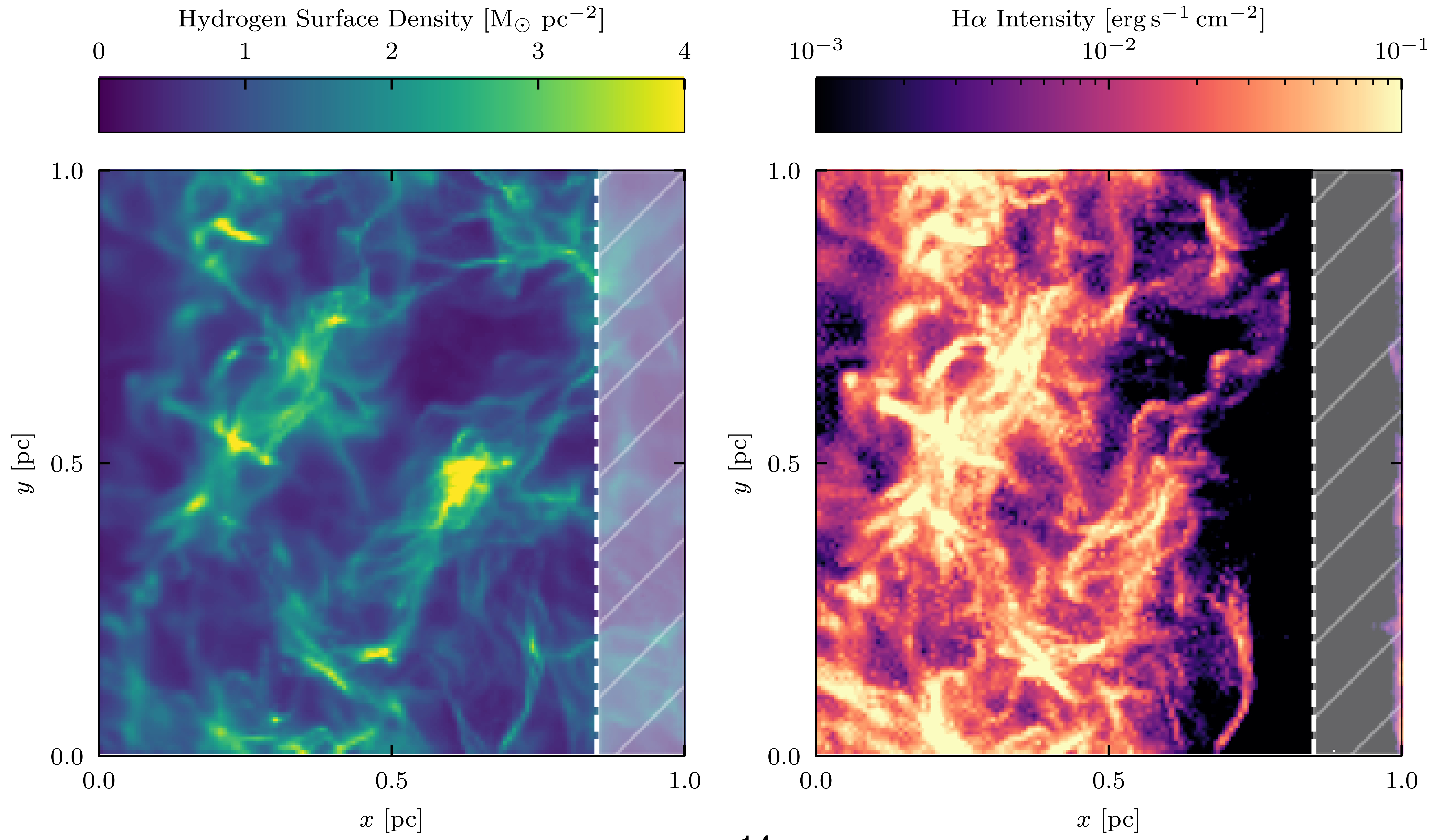
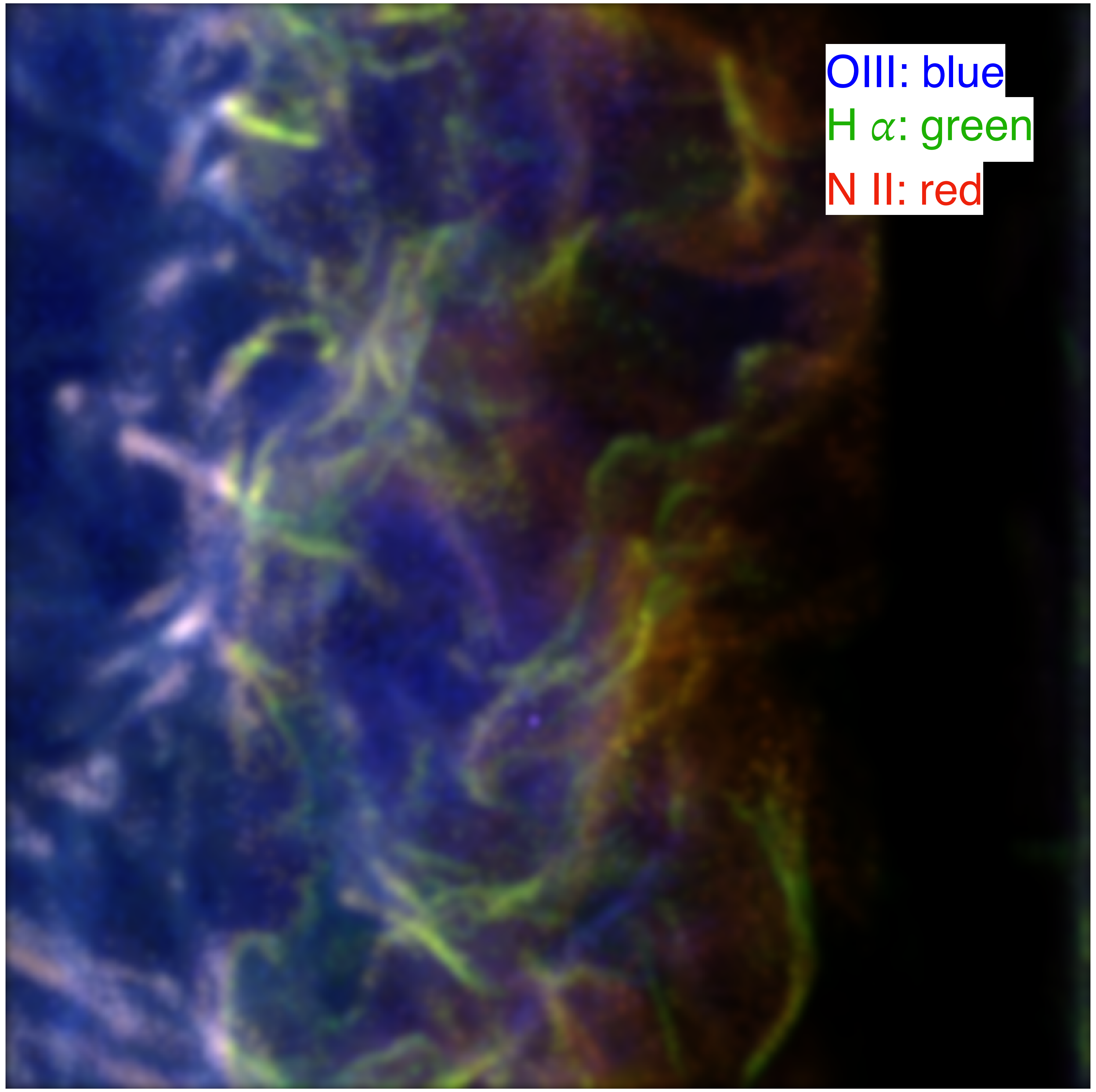


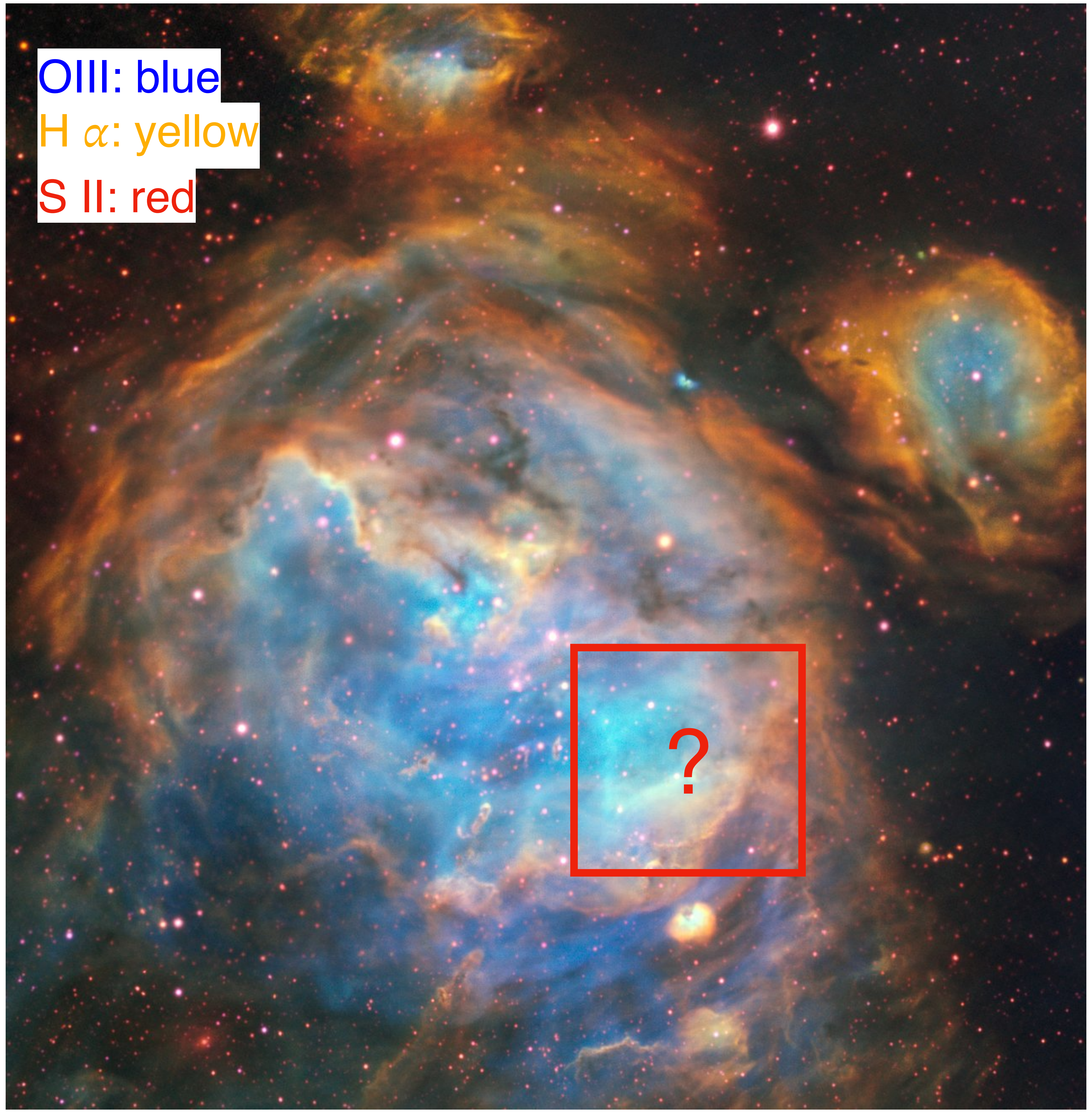
Turbulent Density Field

Not possible with Cloudy!



Example



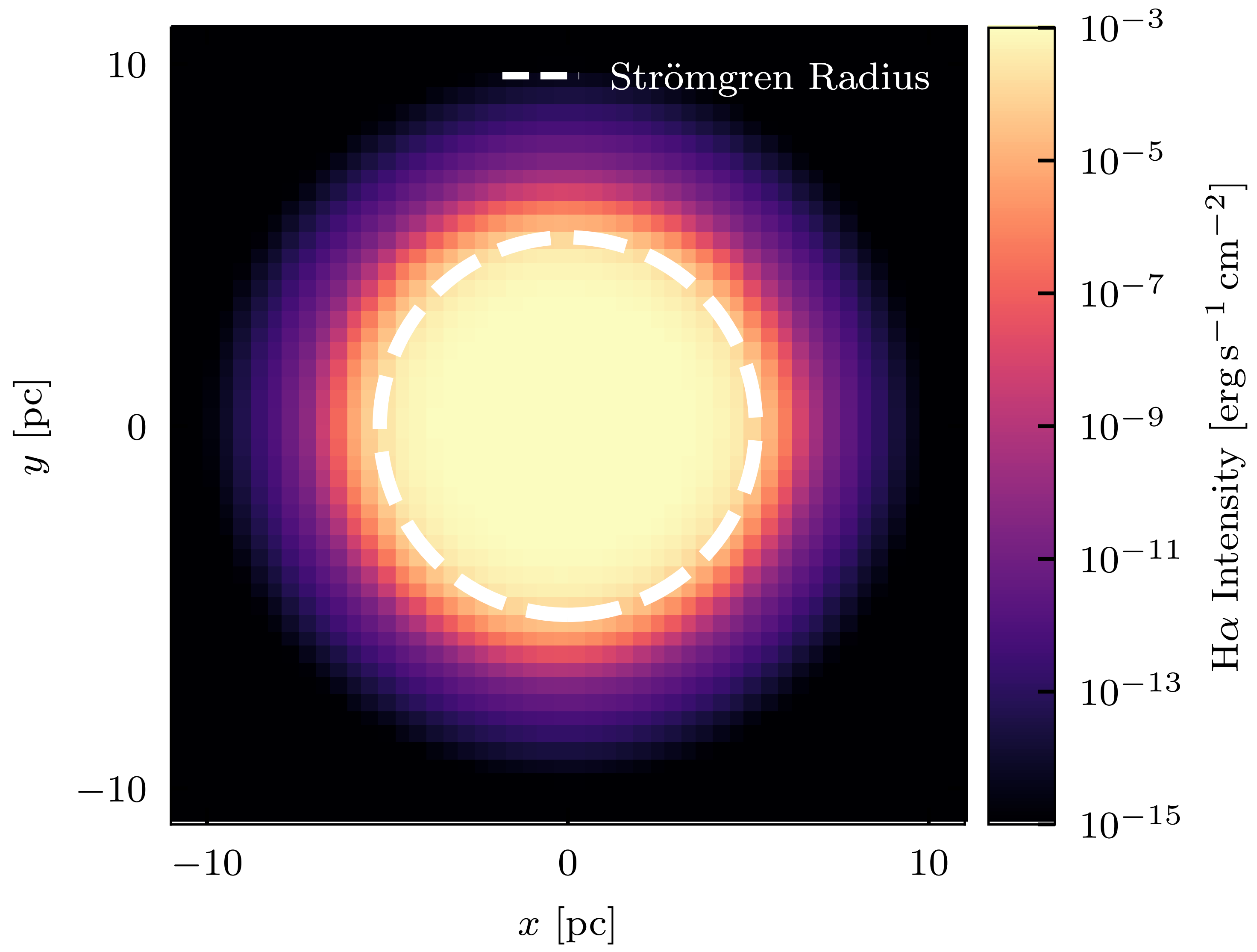


McLeod 2019

Future works & Summary

- Simulations of H II regions and comparison with spatially-resolved observations

- Probing subgrid physics for stellar feedback & non-equilibrium evolution of ISM



- An atomic model for hydrogen recombination line (HyPop)

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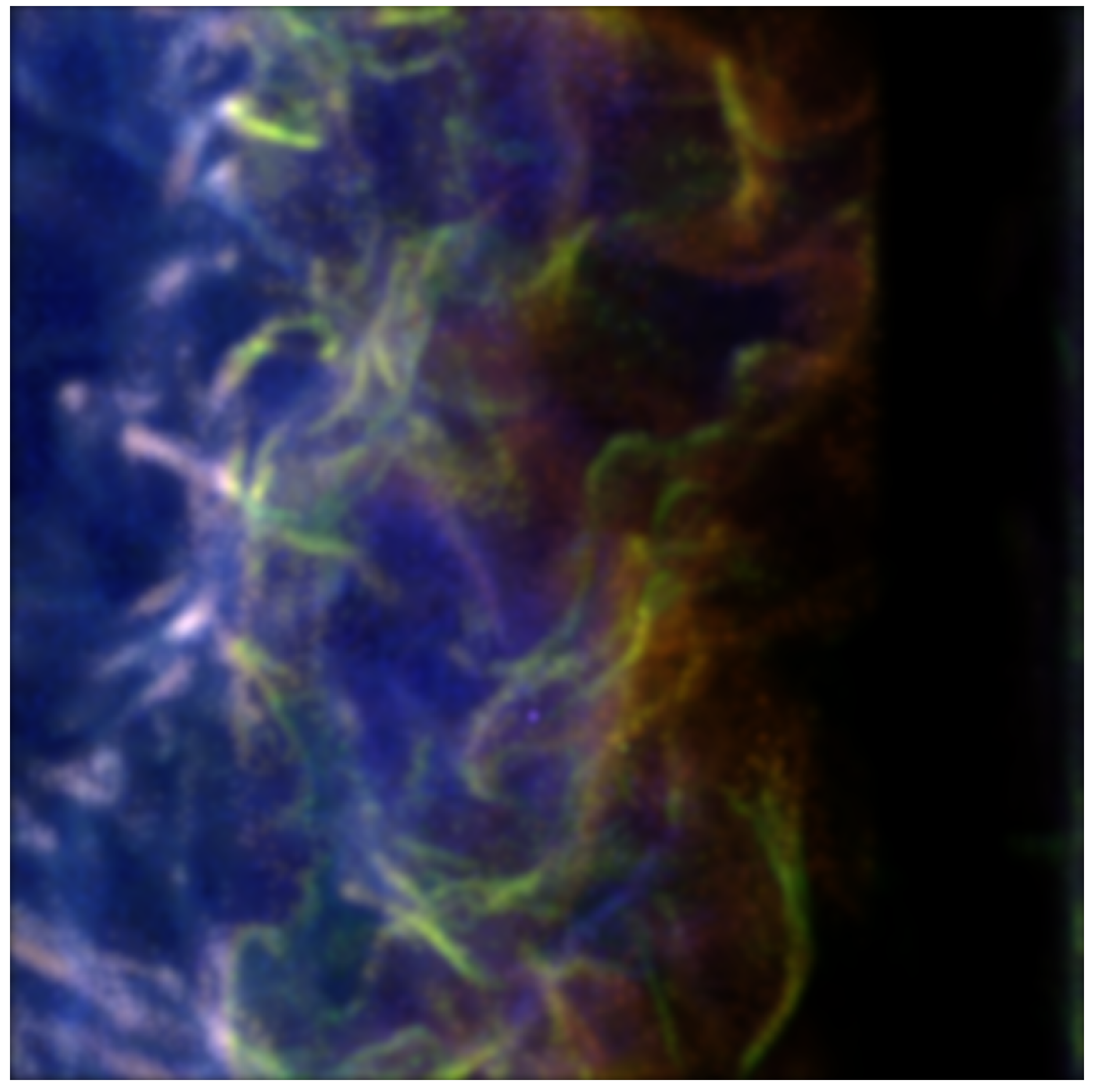
https://github.com/YuankangLiu/hypop



- Applicable for post-processing of radiation-hydrodynamic simulations