THE IMPACT OF IMPROVED STARK-BROADENING WIDTHS ON THE MODELLING OF Cr III LINES IN EARLY-TYPE STARS

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The work

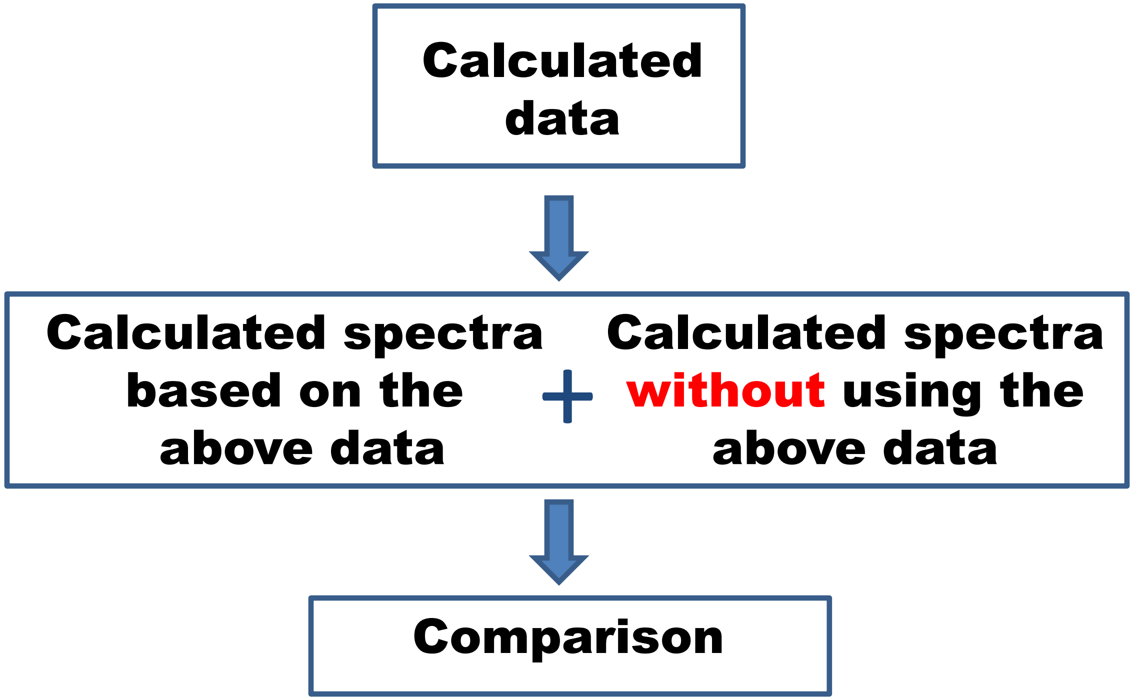
- Calculation of Stark widths for Cr III spectral lines using modified semiempirical formula (MSE)
  - Perturber (electrons) density of 10^{17} cm^{-3} and T = 5000 K-80,000 K

- Their impact on 56 Cr III spectral lines in the UV in:
  - B3 subgiant star Iota Hercules
  - Subdwarf B-star Feige 66

- Theoretical spectra: LTE calculations
  - ATLAS9 model atmospheres and the line formation code SURFACE

- Comparison between:
  - theory-theory… spectra obtained using different approaches
  - theory-observations (HST/STIS… MAST)

The simplified picture



Calculated data

Calculated spectra based on the above data + **Calculated spectra without using the above data**

Comparison

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Motivation

1. Presence of Cr lines in stellar spectra and the lack of Stark broadening data for them

- Cr III is found in the UV spectra of hot B stars

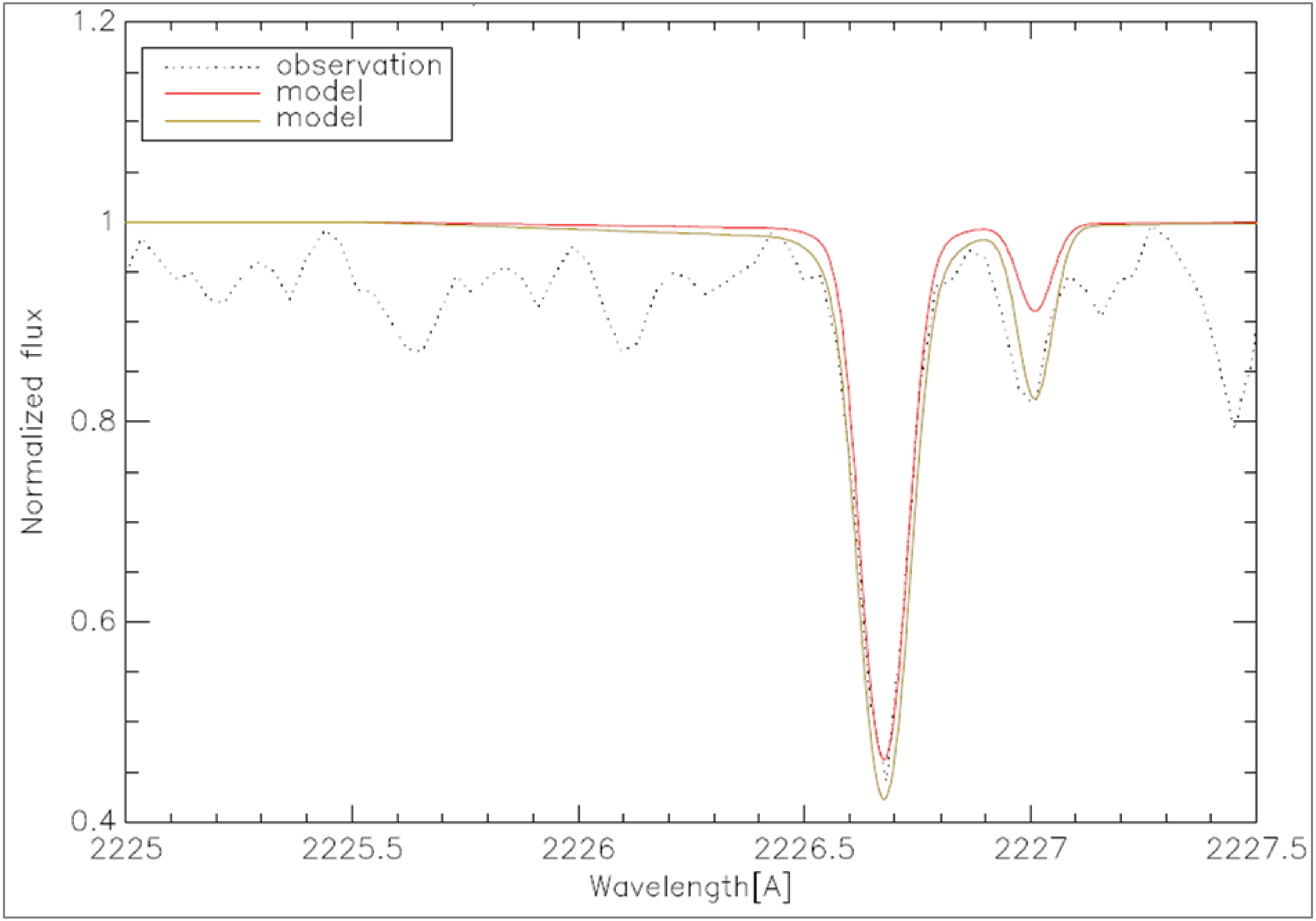
- There was no Stark broadening data of Cr III lines in the literature

- Our calculations for Cr III are the first

Motivation

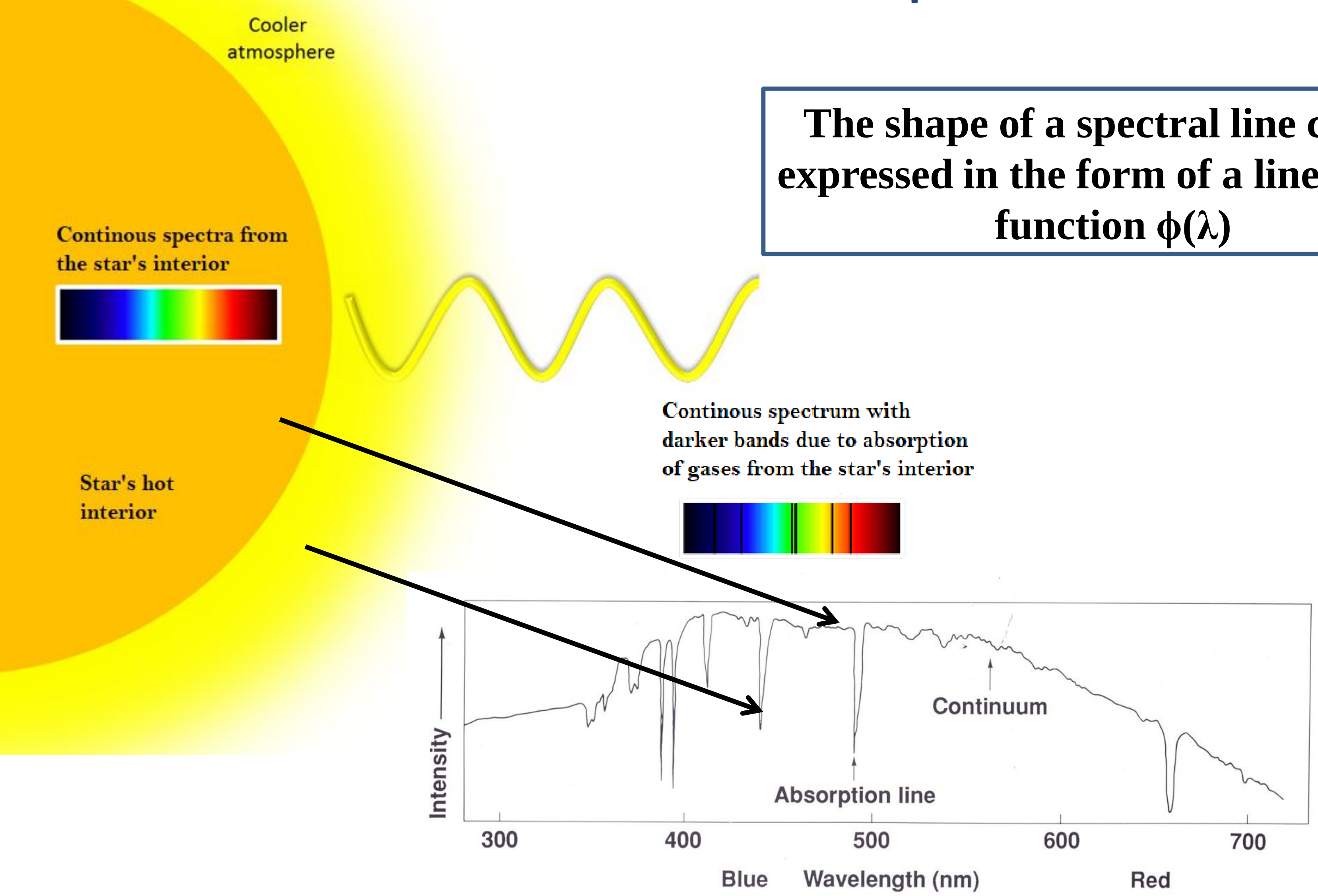
2. Impact of calculated data on stellar spectra and abundance determination:
   - Spectral line shapes are broadened by physical processes
   - Spectral line shapes affect abundance calculation

Motivation


observation
model
model
Normalized flux
1.2
1
0.8
0.6
0.4
2225
2225.5
2226
2226.5
2227
2227.5
Wavelength[A]

The stellar spectra

The shape of a spectral line can be expressed in the form of a line profile function $\phi(\lambda)$



Cooler atmosphere

Continous spectra from the star's interior

Star's hot interior

Continous spectrum with darker bands due to absorption of gases from the star's interior

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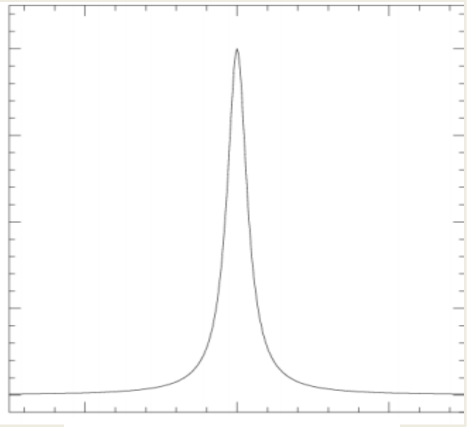
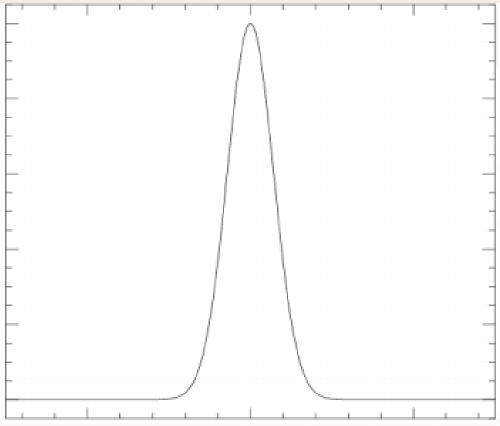
Line broadening



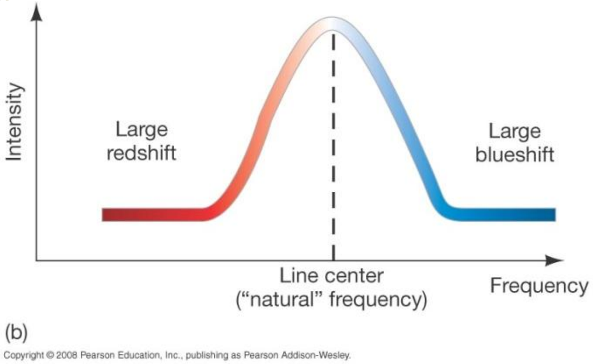
Lorentz profile

1. Natural broadening: result of Heisenberg’s uncertainty principle ~10^{-5} nm
2. Collisional broadening: interaction with other particles

Broadening due to the Doppler effect caused by a distribution of velocities



Gaussian profile



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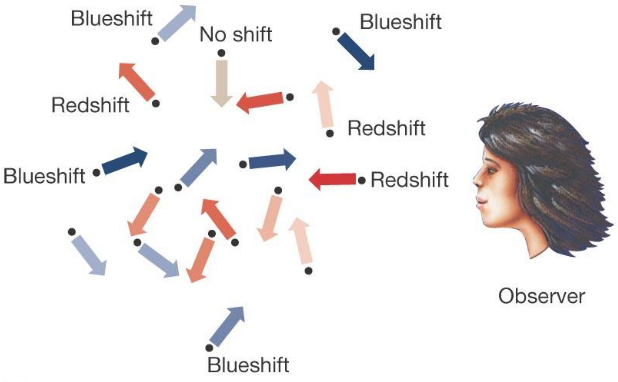

Collisional broadening

1. The presence of nearby particles affect the radiation emitted
2. Transition energy levels are disturbed
3. $\Delta E \propto R^{-p}$
4. $\gamma_{col} \propto R^{-p}$
5. High pressure leads to more collisions and higher broadening

R is distance between absorber and the perturbing particle

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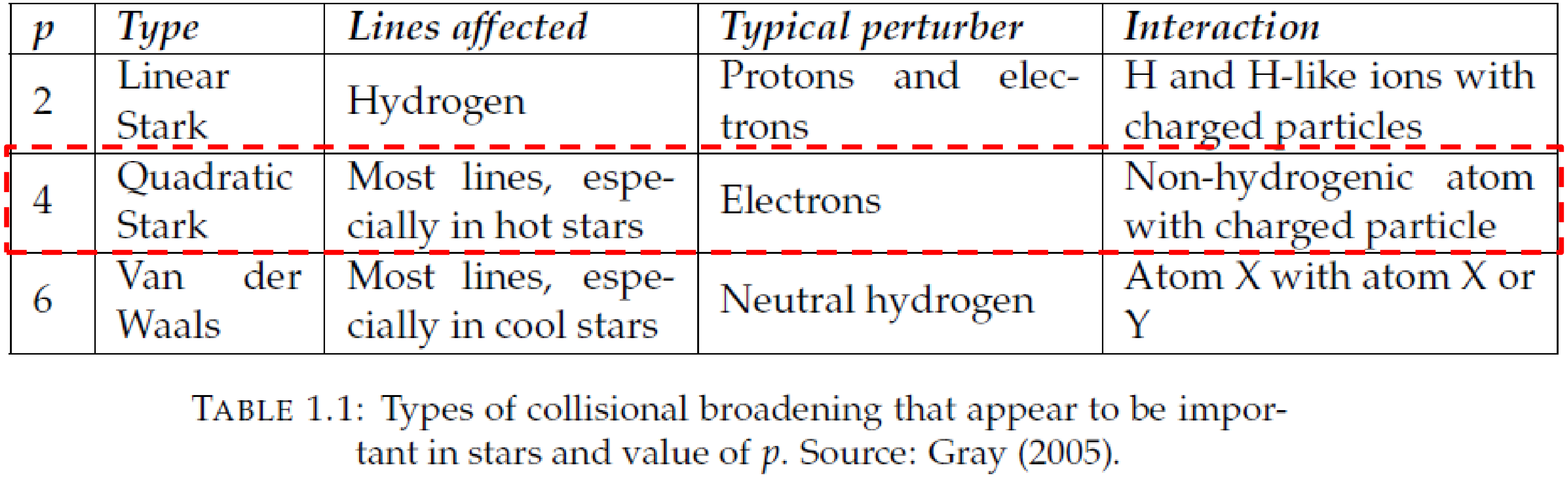
Quadratic Stark broadening



p	*Type*	*Lines affected*	*Typical perturber*	*Interaction*
2	Linear Stark	Hydrogen	Protons and electrons	H and H-like ions with charged particles
4	Quadratic Stark	Most lines, especially in hot stars	Electrons	Non-hydrogenic atom with charged particle
6	Van der Waals	Most lines, especially in cool stars	Neutral hydrogen	Atom X with atom X or Y

TABLE 1.1: Types of collisional broadening that appear to be important in stars and value of p. Source: Gray (2005).

The change in energy of a level due to quadratic Stark broadening

- $\Delta E \propto R^{-4}$
- $\gamma_{col} \propto R^{-4}$

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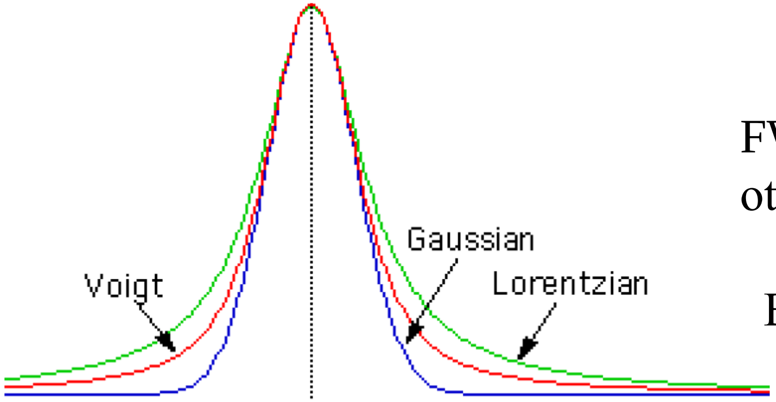
Including all…

φ(υ) → natural broadening * collisonal * thermal Doppler broadening

→ Lorentzian * Lorentzian * Gaussian

Voigt profile = Gaussian core * Lorentzian wings

$$V(\lambda, a) = \frac{constant\,\lambda^2}{c\sqrt{\pi}\Delta\lambda_D} H\left(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma\lambda^2}{4\pi c\Delta\lambda_D}\right)$$



FWHM and γ are related to each other and… they shape the line.

Better values… closer to obs.

$$\gamma = \gamma_n + \gamma_{Stark} + \gamma_{VdW}.$$

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Approximated Stark broadening calculations

- γ_{Stark} used for line computation is a fit by Peytremann (1972) to the detailed calculations of Sahal-Brechot and Segre (1971):

$$\boxed{\gamma_{Stark} = 10^{-8}(n_{eff})^5 N_e \ (s^{-1})}$$

Kurucz 1979

$$n_{eff} = [E_H (Z_{eff})^2/X_{ion} - X_{upper}]$$

If the E_{upper}, $n_{eff} = 5$

- According to Griem and Peach (1975):

$$\boxed{\gamma_{Stark}/N_e = 2\pi c(2W)/N_e \lambda_0^2}$$

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Calculation of the Stark damping constant

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MSE formula
Dimitrijevic and Konjevic, 1980

Data on the energy levels of Cr III are not complete, and it is not possible to perform a more sophisticated semiclassical perturbation calculation.

- Requires a considerably smaller number of atomic data .
- All perturbing levels with Δn ≠ 0, needed for other approaches are lumped together and estimated approximately.
- The accuracy is about ±50% (Dimitrijevic and Popovic, 2001).
- MSE gives very good agreement with experimental measurements (±30%) even for very complex spectra (e.g., XeII and KrII).

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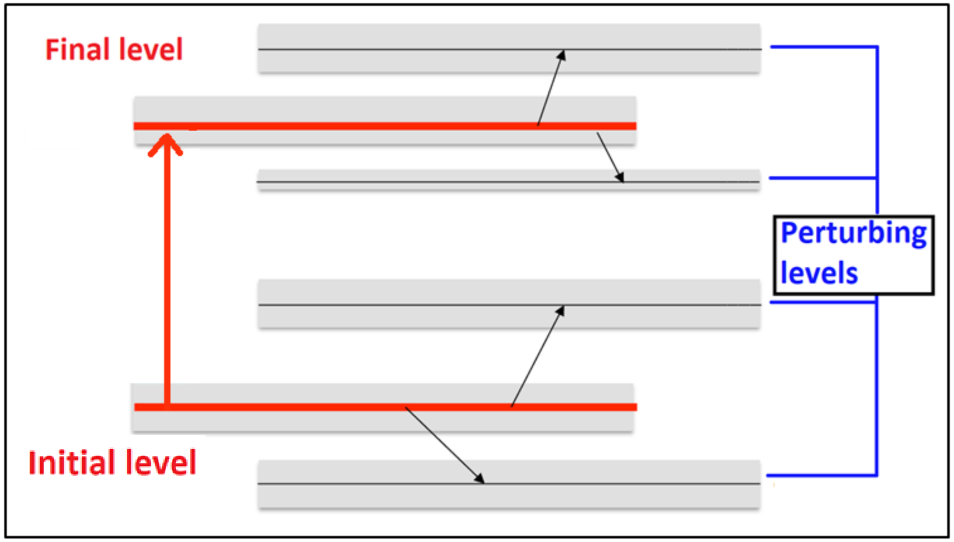
The formula

$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\lambda^2}{\sqrt{3}} \times \left[\underbrace{\boxed{\sum_{\ell_i \pm 1}\sum_{L_{i'}J_{i'}} \overrightarrow{\Re}^2_{\ell_i,\ell_i\pm 1}\tilde{g}\left(x_{\ell_i,\ell_i\pm 1}\right) + \sum_{\ell_f \pm 1}\sum_{L_{f'}J_{f'}} \overrightarrow{\Re}^2_{\ell_f,\ell_f\pm 1}\tilde{g}\left(x_{\ell_f,\ell_f\pm 1}\right)}}_{\mathbf{\Delta n=0\ terms}} + \underbrace{\boxed{\left(\sum_{i'} \overrightarrow{\Re}^2_{ii'}\right)_{\Delta n \neq 0} g\left(x_{n_i,n_i+1}\right) + \left(\sum_{f'} \overrightarrow{\Re}^2_{ff'}\right)_{\Delta n \neq 0} g\left(x_{n_f,n_f+1}\right)}}_{\mathbf{\Delta n \neq 0\ terms}} \right]$$

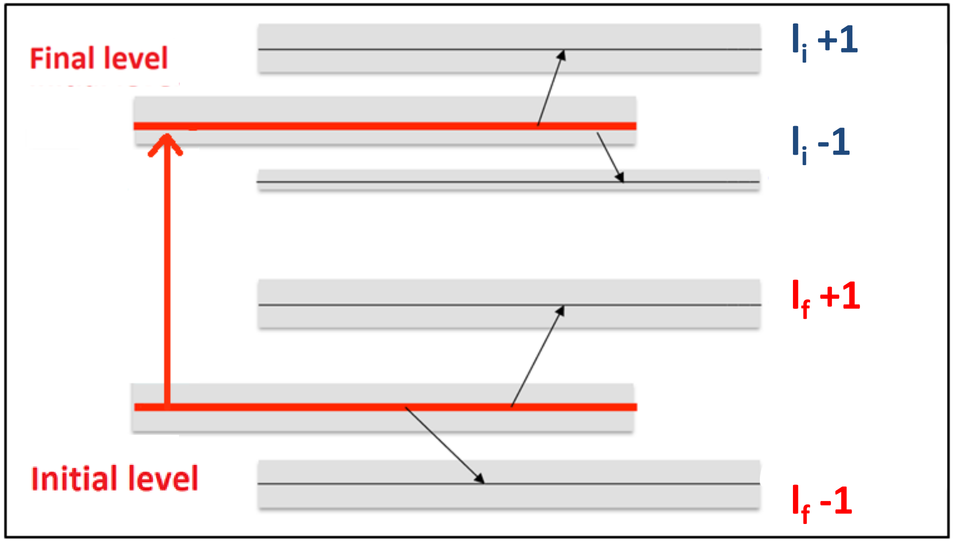


Source: Sahal-Bréchot, 2014

Δn=0 terms

$$\boxed{\sum_{\ell_i\pm1}\sum_{L_{i'}J_{i'}}\overrightarrow{\mathfrak{R}}^{2}_{\ell_i,\ell_i\pm1}\tilde{g}\left(x_{\ell_i,\ell_i\pm1}\right)+\sum_{\ell_f\pm1}\sum_{L_{f'}J_{f'}}\overrightarrow{\mathfrak{R}}^{2}_{\ell_f,\ell_f\pm1}\tilde{g}\left(x_{\ell_f,\ell_f\pm1}\right)}$$

The Gaunt factors are calculated according to Griem, 1968, and Dimitrijević and Konjević, 1980



$\overrightarrow{\mathfrak{R}}^{2}_{\ell_k,\ell_{k'}}$ depends on multiplet and line factors and radial integral (calculated using Coulomb's approximation).

$\overrightarrow{\mathfrak{R}}^{2}_{\ell_k,\ell_{k'}}$ calculated for l+1 and l-1 of initial and final states.

Δn ≠ 0 terms

$$\boxed{\left(\sum_{i'} \overrightarrow{\mathfrak{R}}_{ii'}^{2}\right)_{\Delta n\neq 0} g\left(x_{n_i,n_i+1}\right) + \left(\sum_{f'} \overrightarrow{\mathfrak{R}}_{ff'}^{2}\right)_{\Delta n\neq 0} g\left(x_{n_f,n_f+1}\right)}$$

$$\left(\sum_{k'} \overrightarrow{\mathfrak{R}}_{kk'}^{2}\right)_{\Delta n\neq 0} = \left(\frac{3n_k^*}{2Z}\right)^2 \frac{1}{9}\left(n_k^{*2} + 3\ell_k^2 + 3\ell_k + 11\right)$$

$x_{\ell_k,\ell_{k'}} = E/\Delta E_{\ell_k,\ell_{k'}}$,

$k = i, f$ where $E = \frac{3}{2}kT$ is the electron kinetic energy and

$\Delta E_{\ell_k,\ell_{k'}} = \left|E_{\ell_k} - E_{\ell_{k'}}\right|$,

is the energy difference between levels ℓ_k and $\ell_k \pm 1 (k = i, f)$. Also

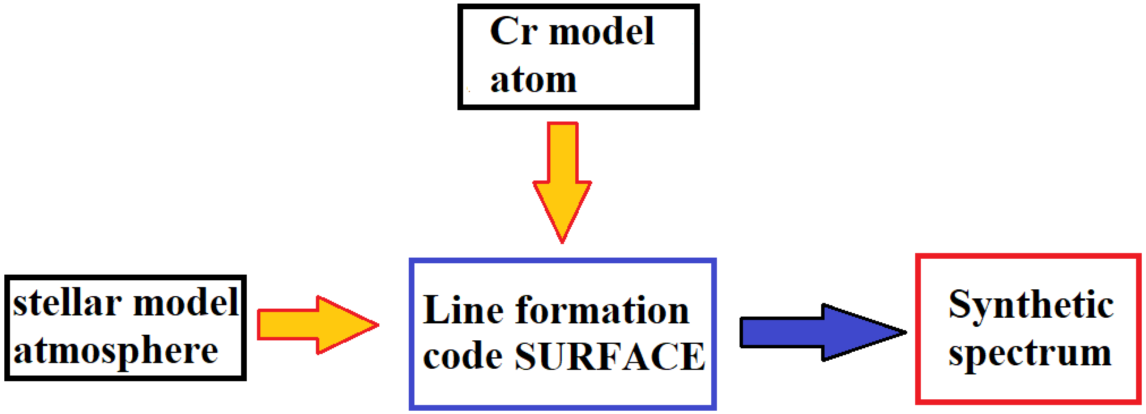
$x_{n_k,n_k+1} \approx E/\Delta E_{n_k,n_k+1}$,

where for $\Delta n \neq 0$ the energy difference between energy levels with n_k and $n_k + 1$, $\Delta E_{n_k,n_k+1}$, is estimated as

$\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H / n_k^{*3}$.

the effective principal quantum number is defined by $n_k^* = \left[E_H Z^2/(E_{ion} - E_k)\right]^{1/2}$

Application



Cr model atom

stellar model atmosphere

Line formation code SURFACE

Synthetic spectrum

Stellar atmosphere: ATLAS9 (Kurucz, 1992)

Synthetic spectrum: line formation code SURFACE (Butler and Giddings, 1985)

Calculated data: Cr model atom

The main objective is to solve the formal solution of RTE

$$I_\nu(\tau_\nu,\mu) = \int_{\tau_1}^{\tau_2} S_\nu(t_\nu) e^{\frac{-(\tau_\nu - t_\nu)}{\mu}} \frac{dt_\nu}{\mu} + I_\nu(0) e^{\frac{-\tau_\nu}{\mu}}$$

The calculations were done assuming LTE

Once I_ν is known the radiative flux coming can be found out

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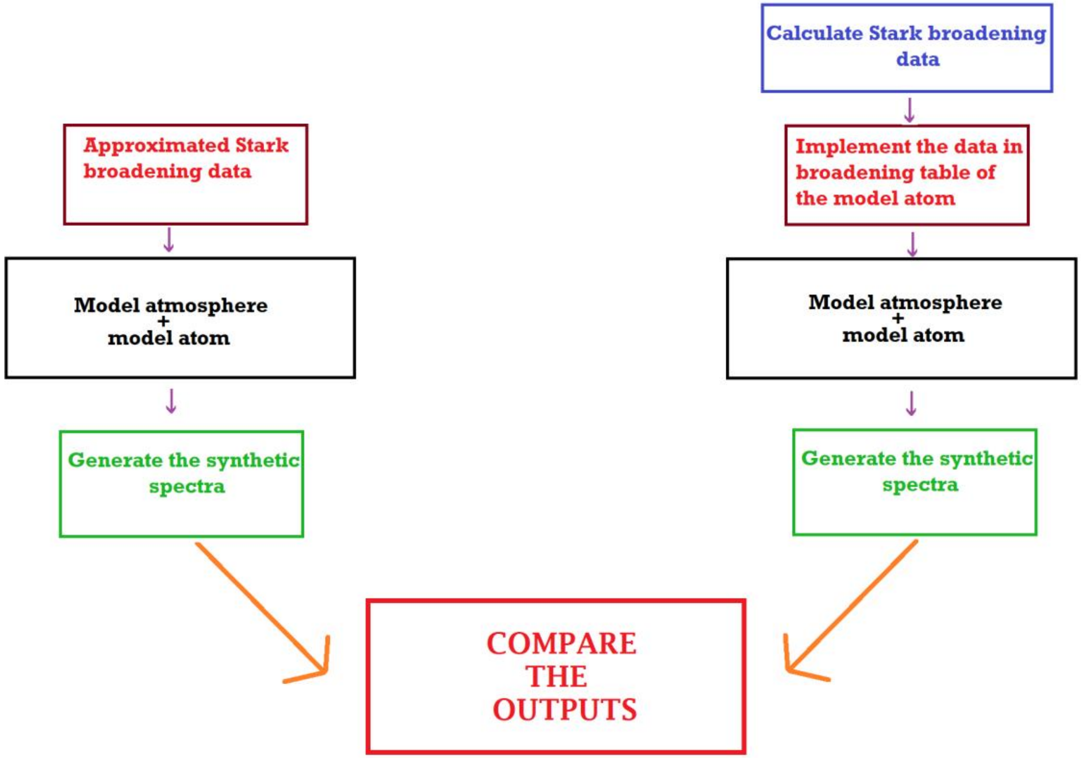


Calculate Stark broadening data

Implement the data in broadening table of the model atom

Model atmosphere + model atom

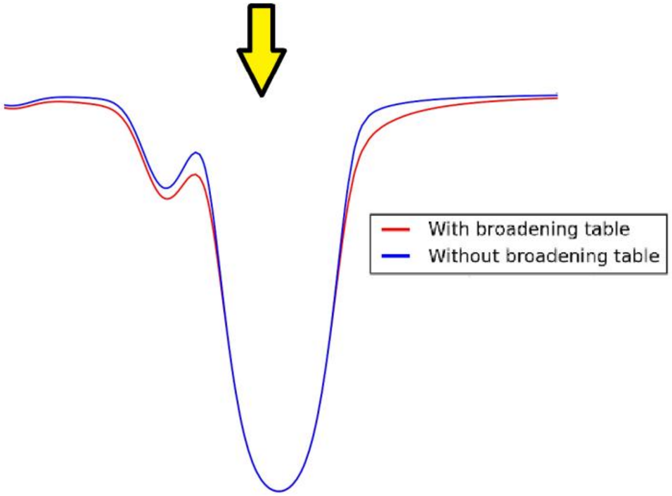
Generate the synthetic spectra

Approximated Stark broadening data

Model atmosphere + model atom

Generate the synthetic spectra

COMPARE THE OUTPUTS



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Results and observations

Results

Transition	T (K)	FWHM (Å)
Cr III 3d^3(^{4}F)4s^{5}F – 3d^3(^{4}F)4p^{5}F^o	5000	0.723E-01
	10,000	0.511E-01
λ = 2121.8 Å	20,000	0.361E-01
3kT/2ΔE = 0.234	40,000	0.256E-01
	80,000	0.181E-01
Cr III 3d^3(^{4}F)4s^{5}F – 3d^3(^{4}F)4p^{5}G^o	5000	0.791E-01
	10,000	0.559E-01
λ = 2241.9 Å	20,000	0.396E-01
3kT/2ΔE = 0.234	40,000	0.280E-01
	80,000	0.198E-01

Source: M. S. Dimitrijevic and A. Chougule, 2018

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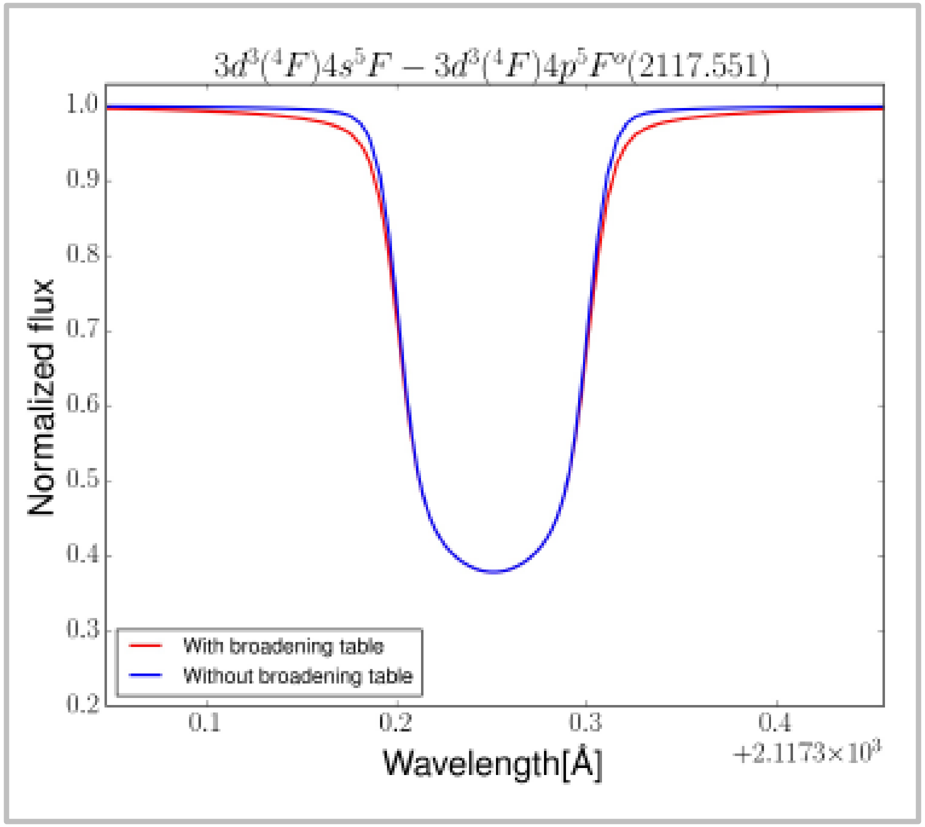
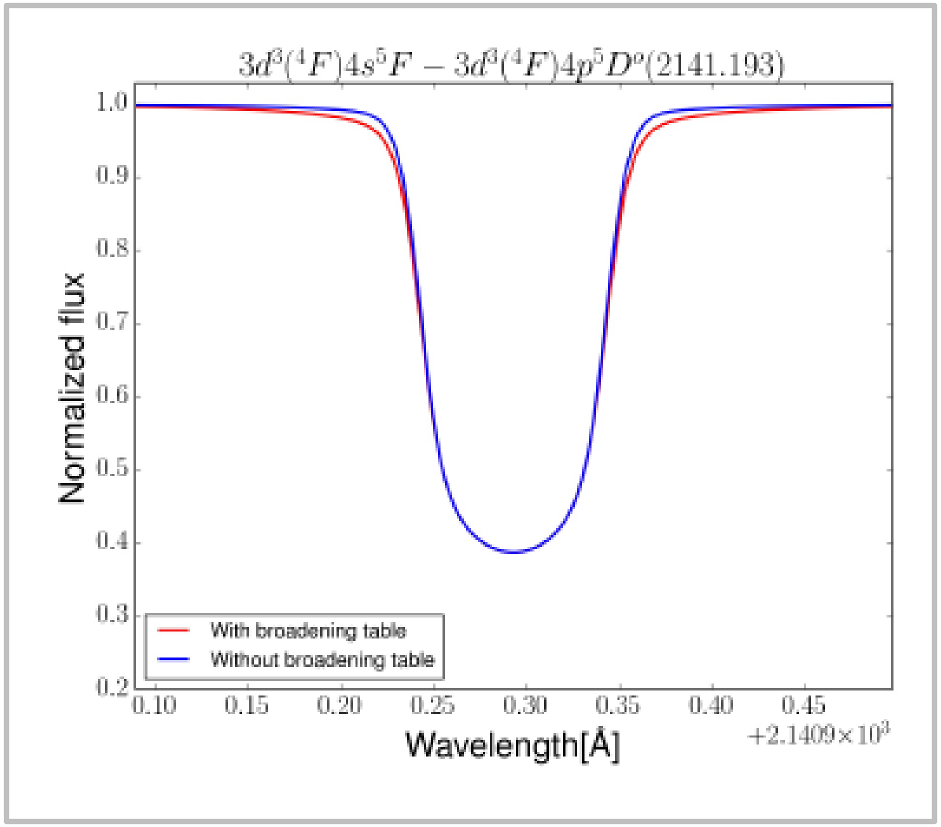
Theoretical Cr III lines in Feige 66



$3d^3(^4F)4s\,^5F - 3d^3(^4F)4p\,^5F^o(2117.551)$



$3d^3(^4F)4s\,^5F - 3d^3(^4F)4p\,^5D^o(2141.193)$

— With broadening table
— Without broadening table

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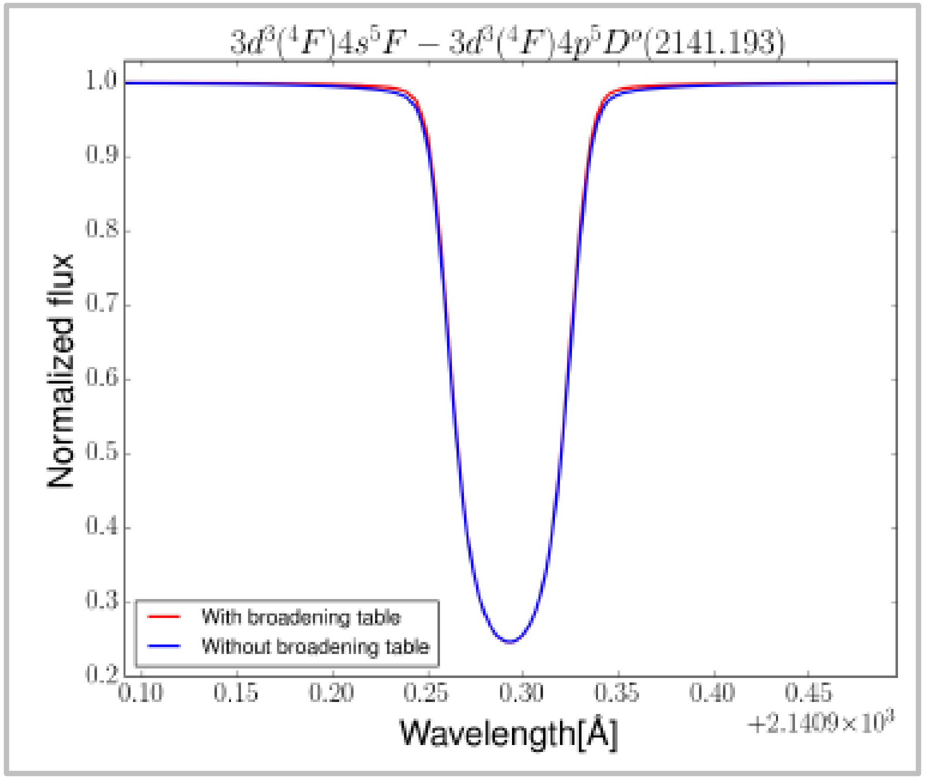
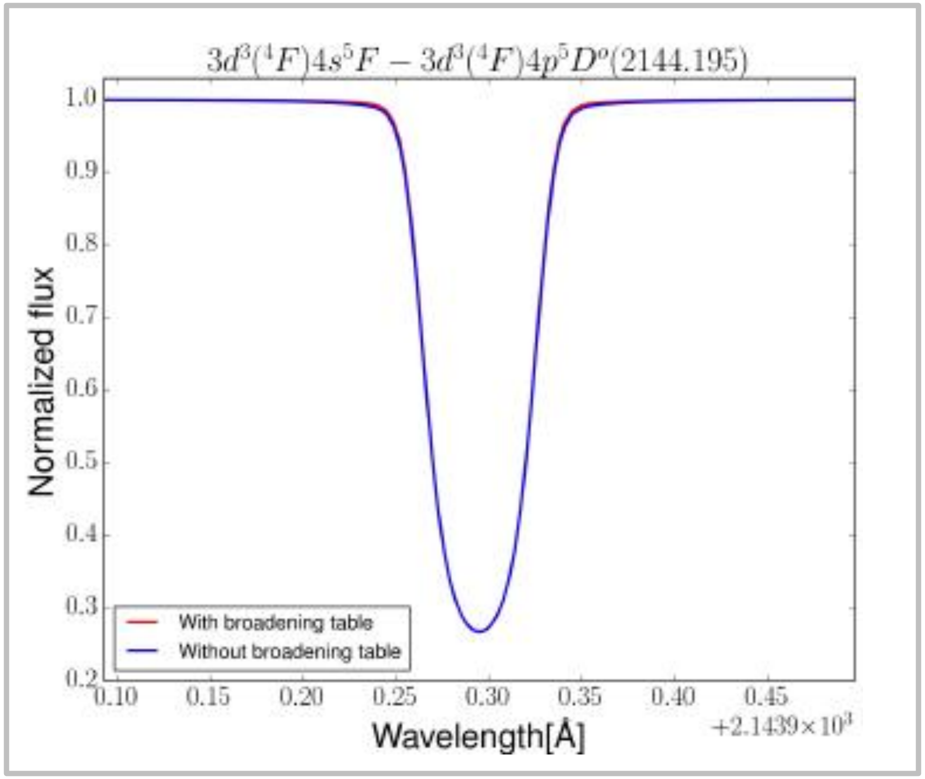
Theoretical Cr III lines in Iota Hercules





🟥 With broadening table
🟦 Without broadening table

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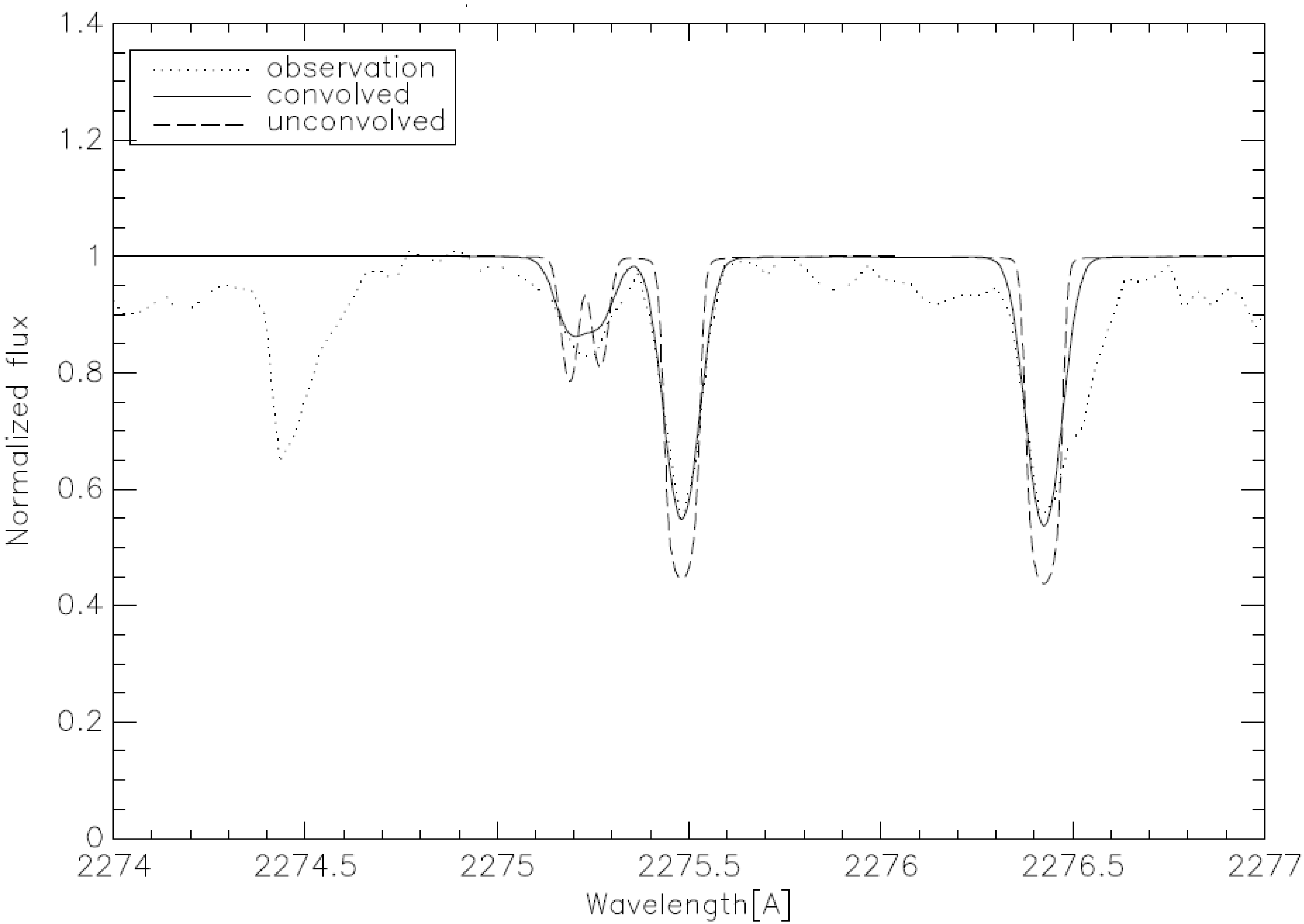
In order to compare with the observations…



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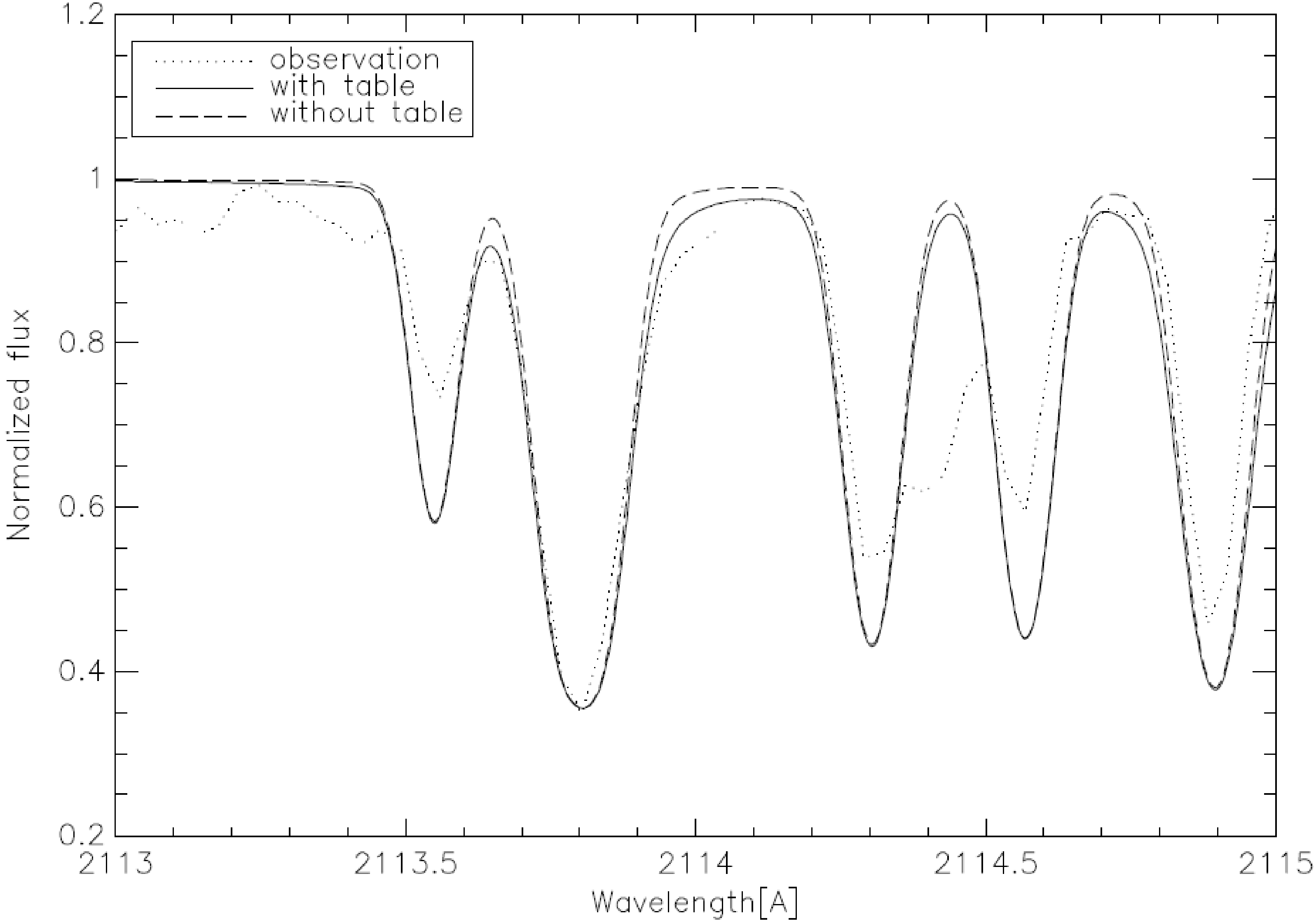
Comparison with the observation: Feige 66



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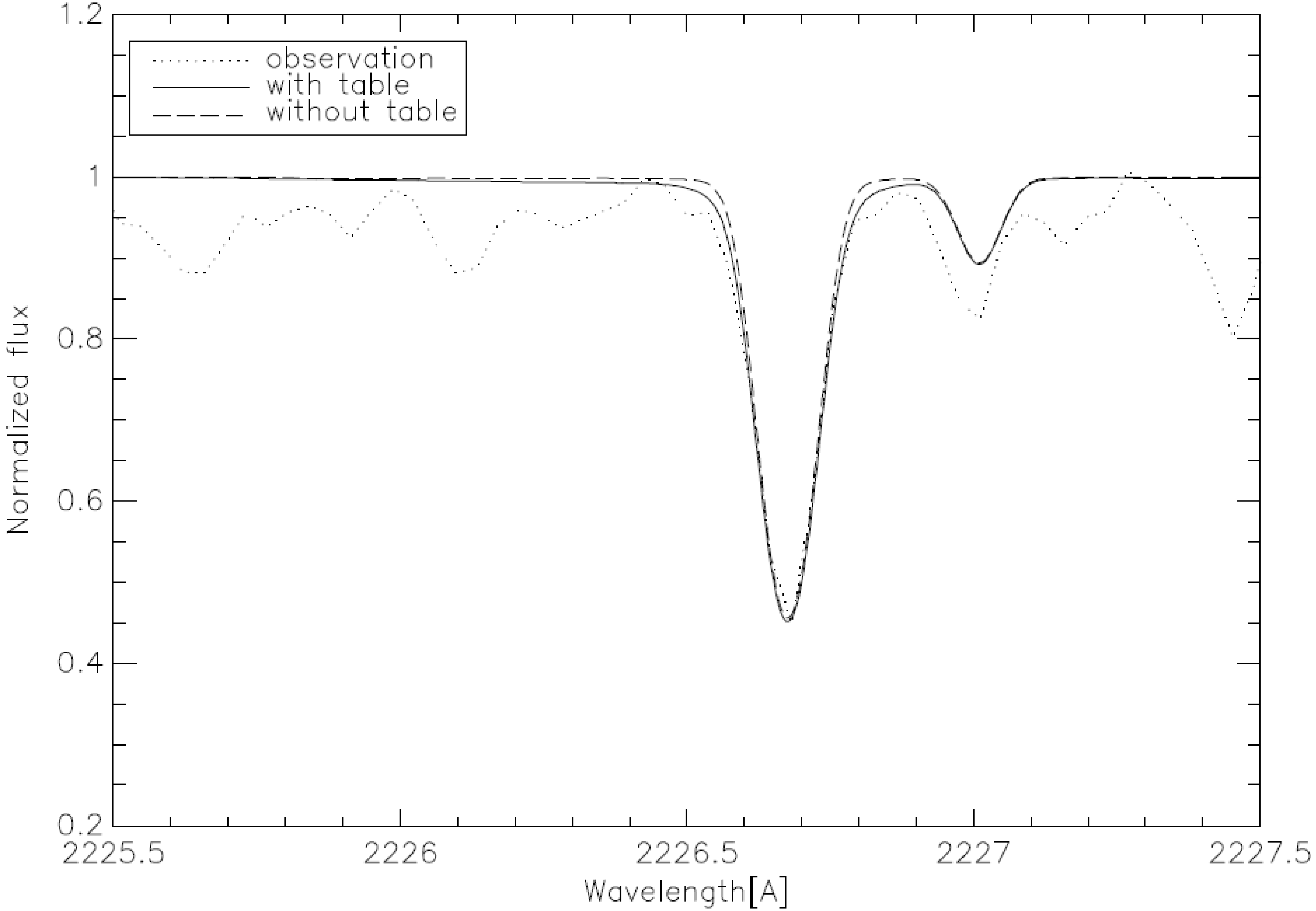
Comparison with the observation: Feige 66



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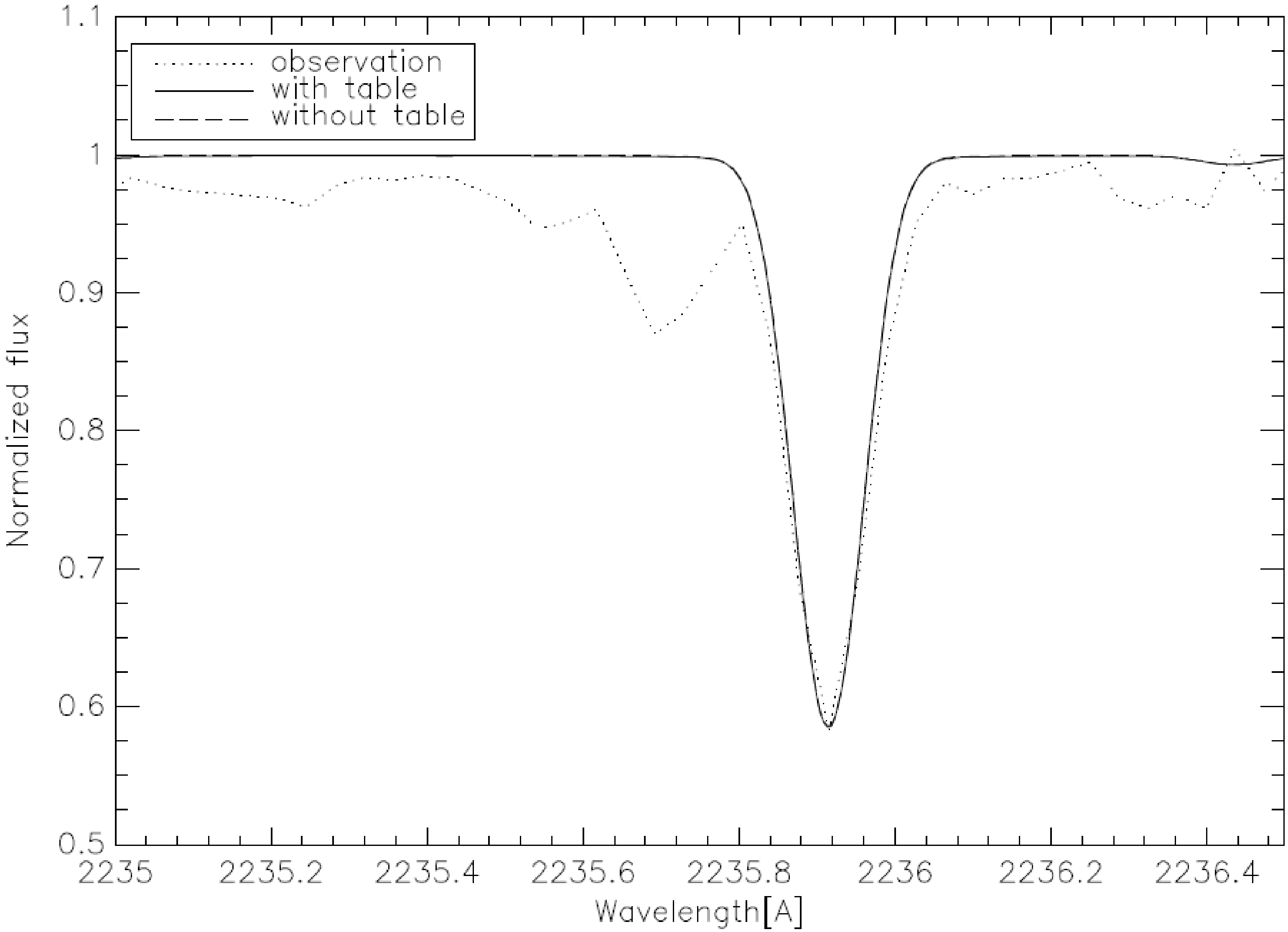
Comparison with the observation: ι Herc.



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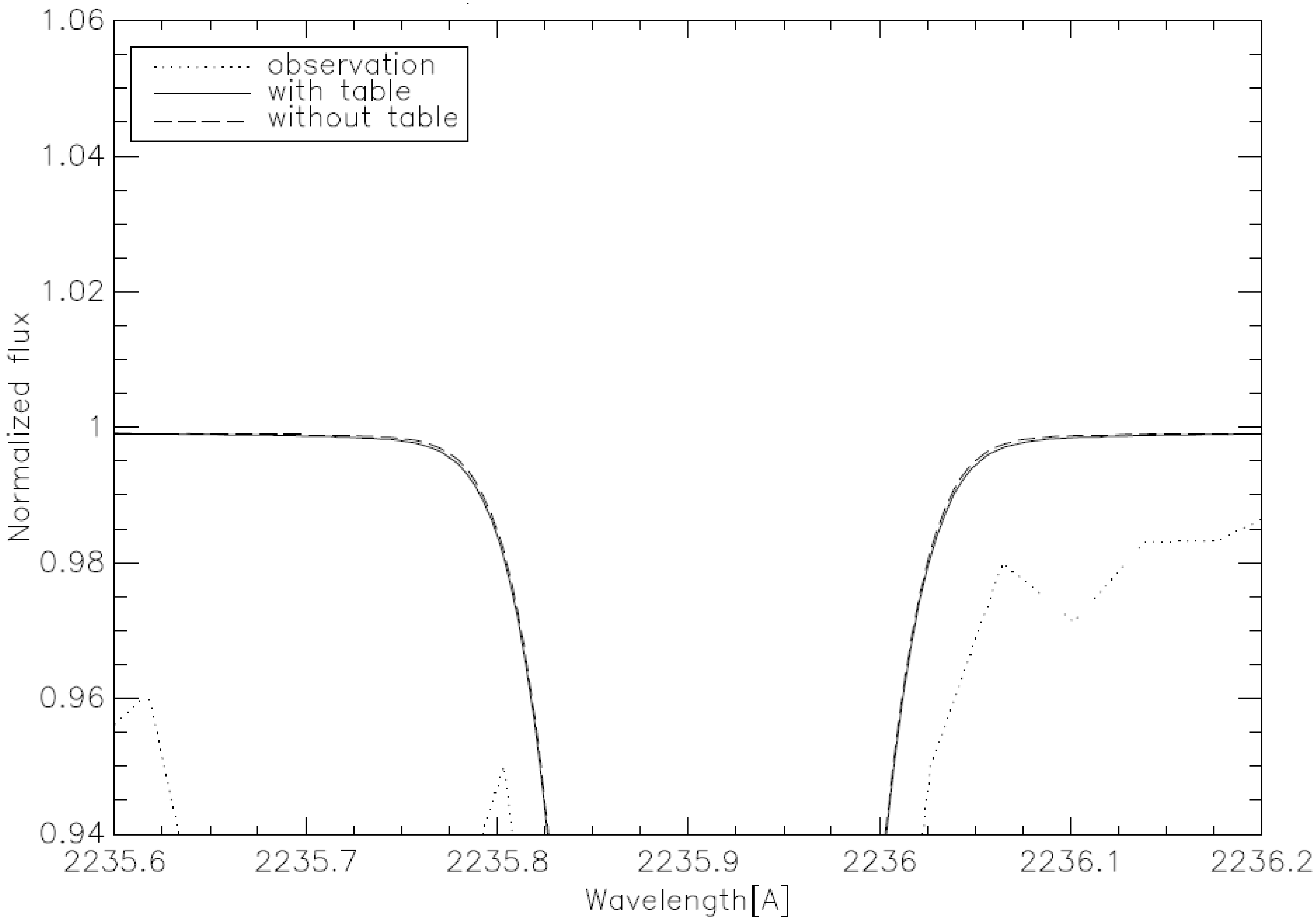
Comparison with the observation: ι Herc.



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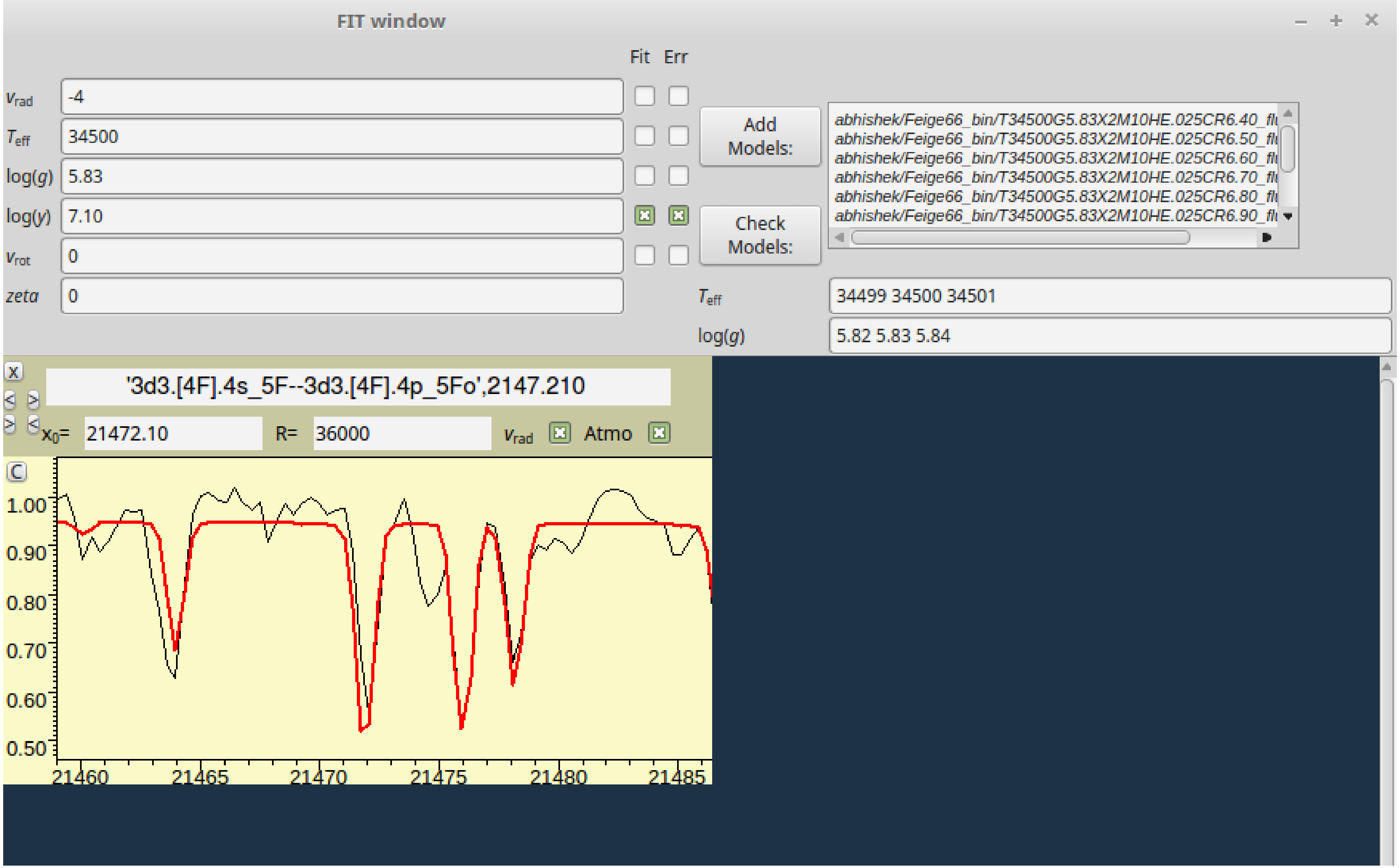
Abundance analysis: Feige 66



FIT window

		Fit	Err
v_{rad}	-4	☐	☐
T_{eff}	34500	☐	☐
log(g)	5.83	☐	☐
log(y)	7.10	☒	☒
v_{rot}	0	☐	☐
zeta	0		

abhishek/Feige66_bin/T34500G5.83X2M10HE.025CR6.40_fl
abhishek/Feige66_bin/T34500G5.83X2M10HE.025CR6.50_fl
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abhishek/Feige66_bin/T34500G5.83X2M10HE.025CR6.70_fl
abhishek/Feige66_bin/T34500G5.83X2M10HE.025CR6.80_fl
abhishek/Feige66_bin/T34500G5.83X2M10HE.025CR6.90_fl

T_{eff} 34499 34500 34501

log(g) 5.82 5.83 5.84

'3d3.[4F].4s_5F--3d3.[4F].4p_5Fo',2147.210

x_0= 21472.10 R= 36000 v_{rad} ☒ Atmo ☒

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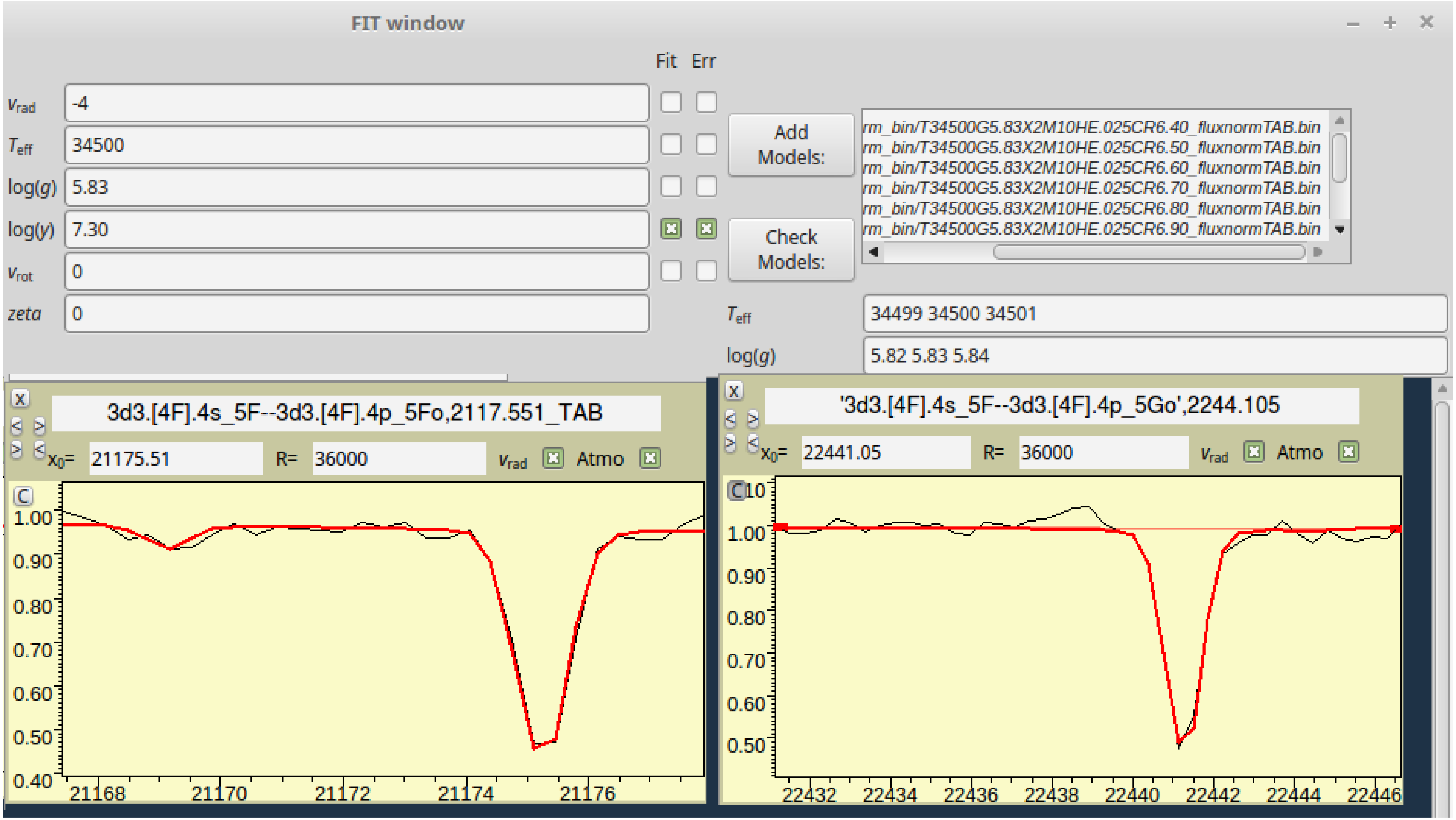
Abundance analysis: Feige 66



	Value	Fit	Err
v_{rad}	-4	☐	☐
T_{eff}	34500	☐	☐
log(g)	5.83	☐	☐
log(y)	7.30	☒	☒
v_{rot}	0	☐	☐
$zeta$	0		

rm_bin/T34500G5.83X2M10HE.025CR6.40_fluxnormTAB.bin
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rm_bin/T34500G5.83X2M10HE.025CR6.90_fluxnormTAB.bin

T_{eff} 34499 34500 34501

log(g) 5.82 5.83 5.84

3d3.[4F].4s_5F--3d3.[4F].4p_5Fo,2117.551_TAB

x_0= 21175.51 R= 36000 v_{rad} ☒ Atmo ☒

'3d3.[4F].4s_5F--3d3.[4F].4p_5Go',2244.105

x_0= 22441.05 R= 36000 v_{rad} ☒ Atmo ☒

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Conclusion

Star	log(g)	T_{eff}	Chromium abundance (model)
Feige 66	5.83	34,500 K	-4.70
Iota Hercules	3.80	17,500 K	-6.40

- Stark broadening is expected to be prominent in the wings of strong lines:

- Appropriate abundance and temperatures are required for their formation. But... the effect strongly depends on surface gravity.
- Subdwarf Feige 66 has a higher value of g, T and ε... hence the effect is visible

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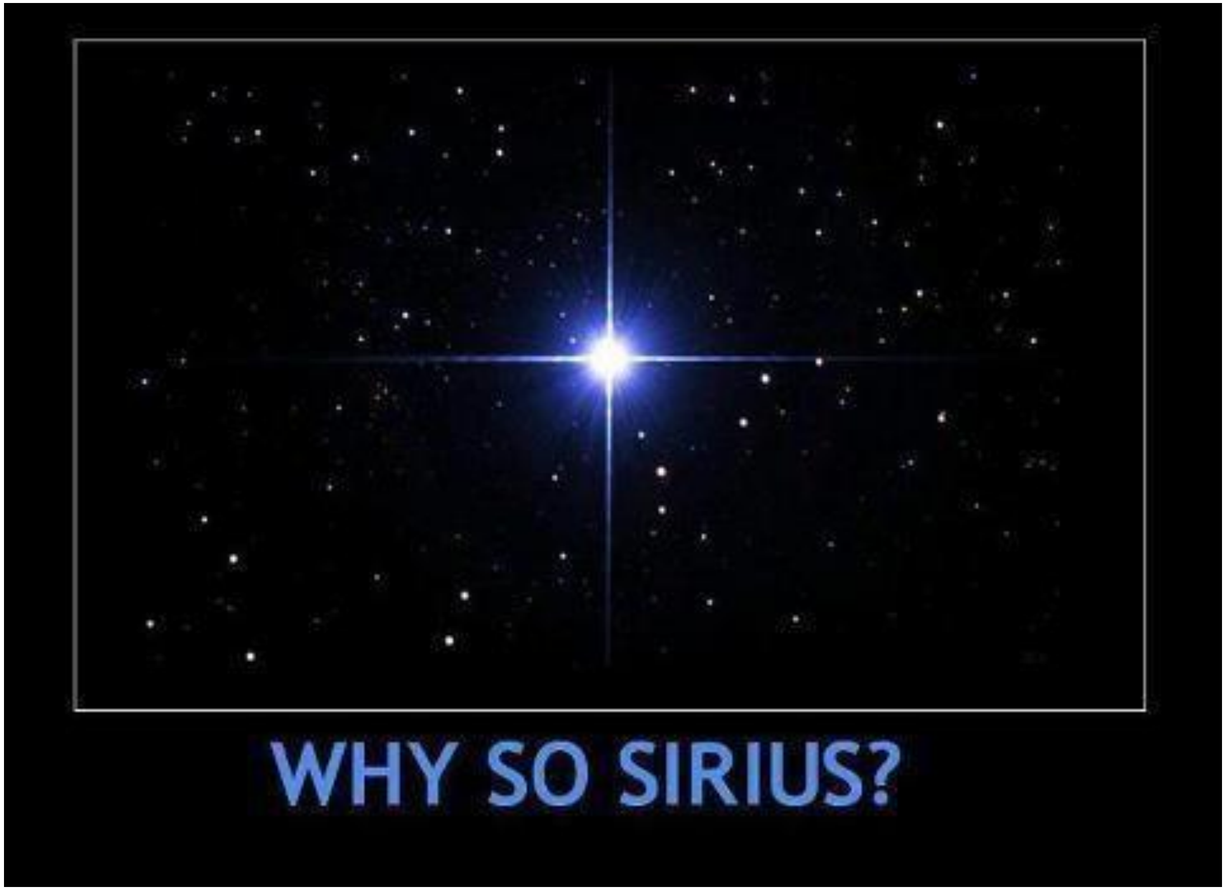
Conclusion

Transition	**Wavelength (Å)**	**Best fit abundance value**	**Mean value (all data)**	**Standard deviation**
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2114.898	7.07		
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2117.551	7.21		
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2147.210	6.85	**7.084**	**0.12986146464598**
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5D^o$	2141.193	7.09		
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5G^o$	2244.105	7.20		

ε = 7.29 ± 0.19 using 65 Cr III lines… S. J. O'Toole and U. Heber, 2006

Hence, in appropriate cases, Stark broadening calculated using MSE affects the line profiles and hence chemical abundance determination (most likely).

Thank you for your attention



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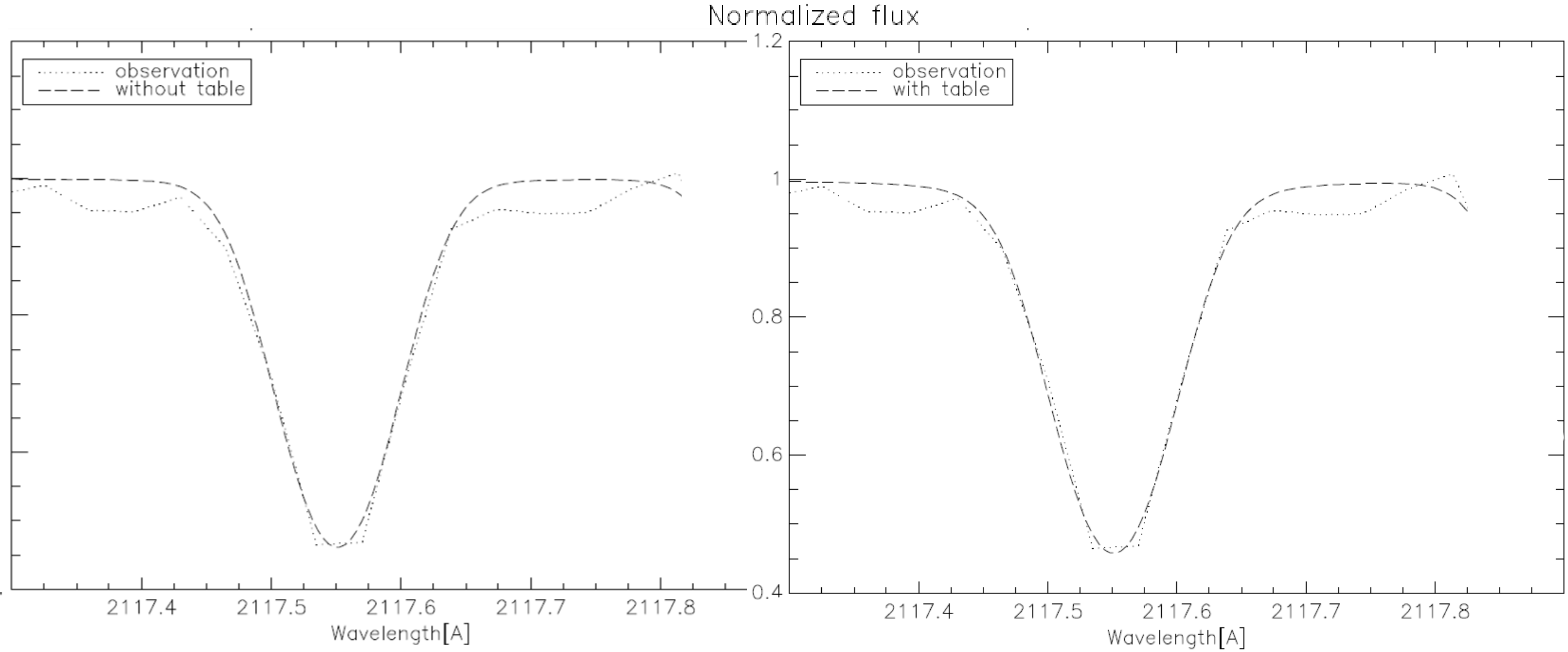
Conclusion

Transition	Wavelength (Å)	Best fit abundance value
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2113.830	-3.80
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2114.898	-4.60
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5F^o$	2117.551	-4.70
$3d^3[^4F]4s^5F$-$3d^3[^4F]4p^5G^o$	2226.676	-4.50

Hence, in appropriate cases, Stark broadening calculated using MSE affects the line profiles and hence chemical abundance determination (most likely).

Comparison with the observation: Feige 66



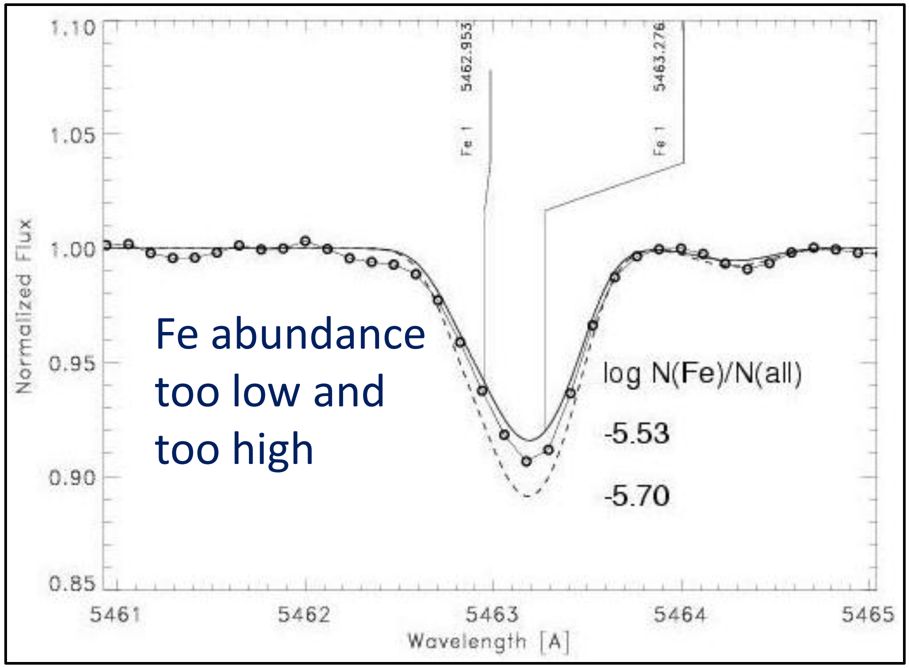
$3d^3[^4F]4s\,^5F—3d^3[^4F]4p\,^5F^o$

λ=2117.551 Å

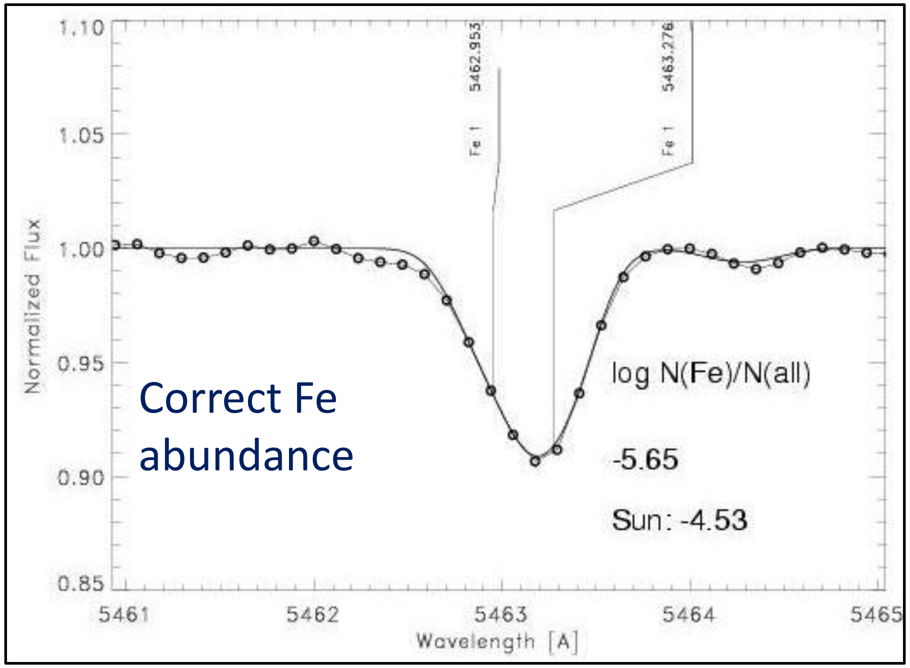
Cr abundance=-4.70

Motivation

2. Impact of calculated data on stellar spectra and abundance determination:
   - Spectral line shapes are broadened by physical processes
   - Spectral line shapes affect abundance calculation



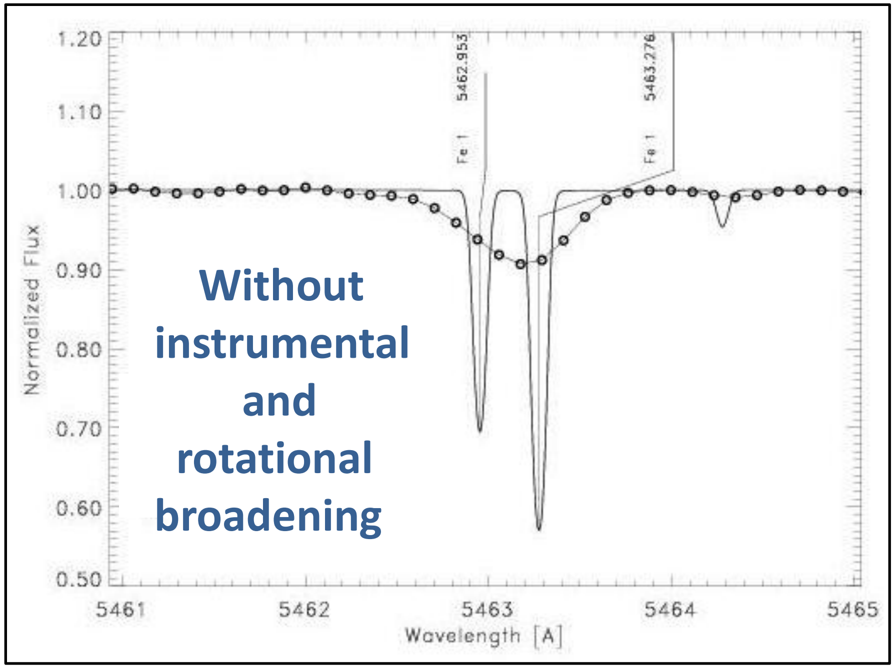
Fe abundance too low and too high



Correct Fe abundance

Image credit: Ulrike Heiter

In order to compare with the observations…



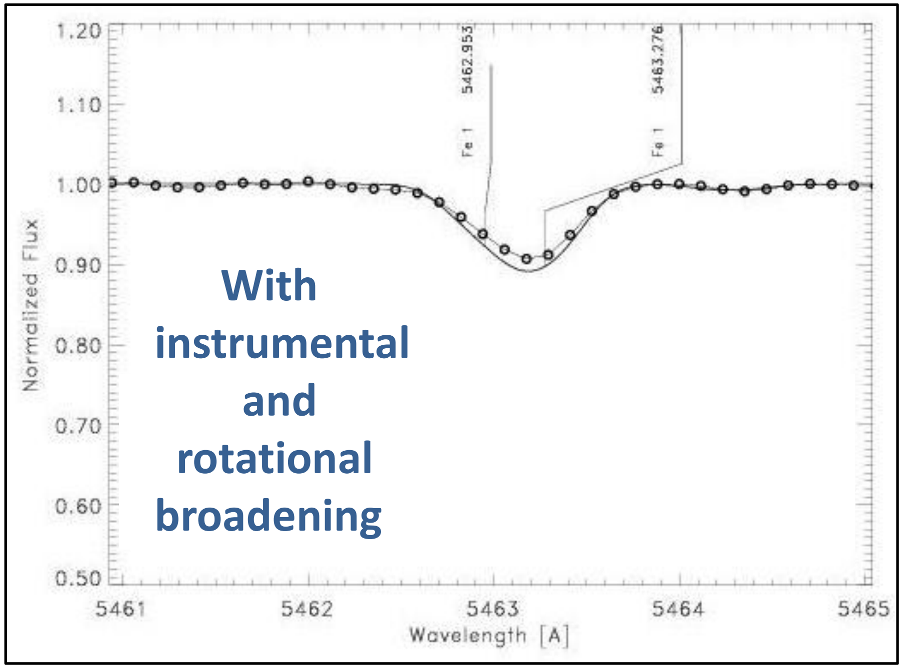


Image credit: Ulrike Heiter

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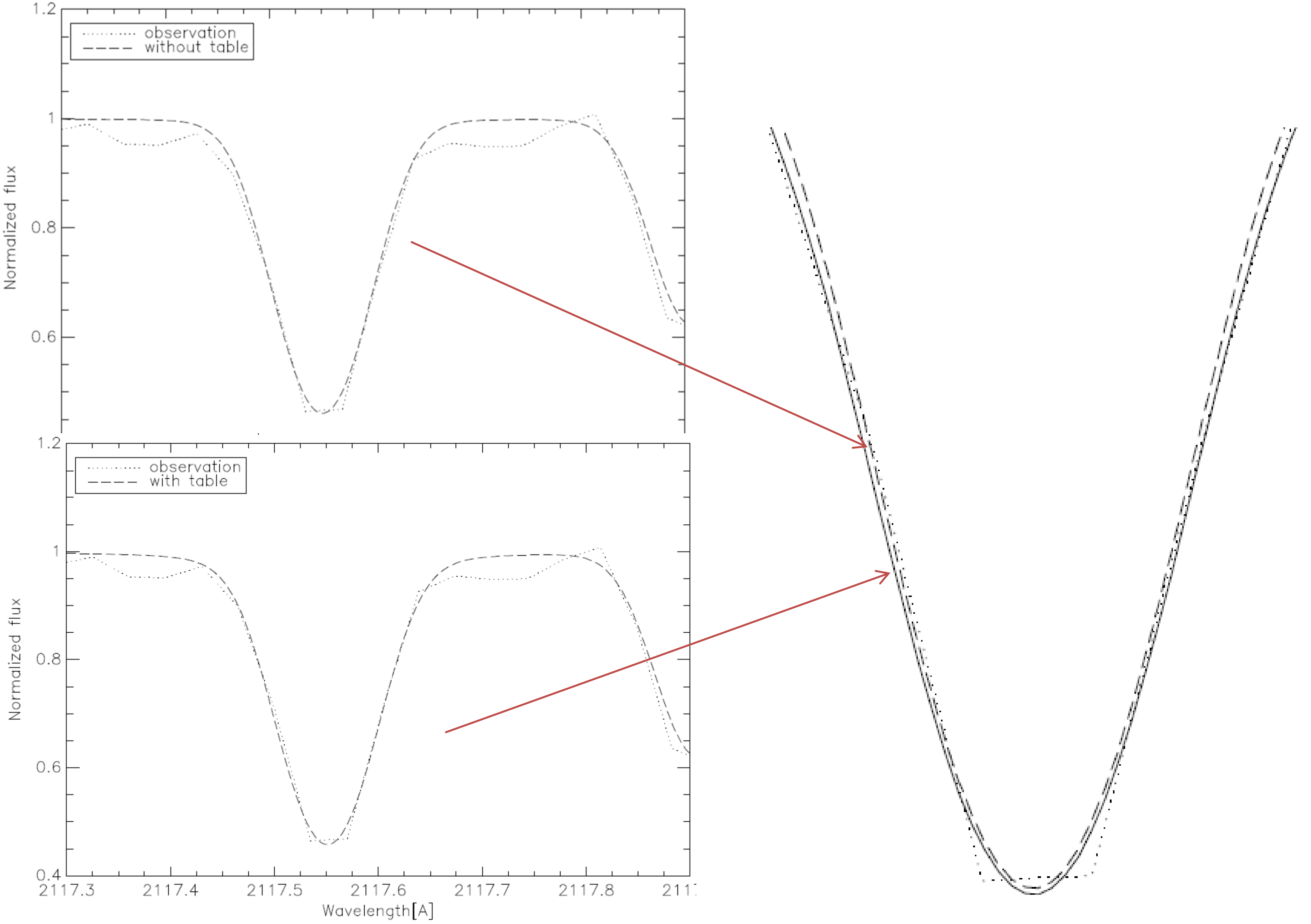
At the core of the line…



Conclusion

Star	log(g)	T_{eff}	Chromium abundance (original model)
Feige 66	5.83	34,500 K	-4.70
Iota Hercules	3.80	17,500 K	-6.40

Stark broadening is expected to be prominent in the wings of strong lin

- appropriate abundance and temperatures are required for their form

But.. The effect strongly depends on surface gravity

Subdwarfs CD 24731 and Feige 66 have higher values of g, T and A → show signatures of SB or any change of it

Hence, in appropriate cases, Stark broadening calculated using MSE affects the line profiles and hence chemical abundance determination.

Abundance value changed from -4.70 to -4.40 : a good fit to the observations was obtained. However, a detailed abundance analysis should be done.

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Comparison with the observation: ι Her

EXTRA SLIDES

Influence of improved Stark broadening data on chromium spectral lines

Joint Master thesis with the University of Innsbruck and the University of Belgrade

Abhishek Chougule

Astromundus edition 7

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- Motivation and approach.

- Stellar spectra

- Line shapes in Astrophysics, types of broadening.

- Stark broadening.

- Why all these steps?

- Calculation of Stark broadening.

- Application: 1. OB-type main sequence stars Iota Hercules and Upsilon Orionis.
  2. Subdwarf B-stars CD-24 731, HD199112, and Feige 66.

- Results and conclusions

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What is the effect of improved Stark broadening data on theoretical stellar spectra? … but why?

- Theoretical stellar spectra: important for abundance determination.

In our case, Cr III and Cr IV spectral lines in the UV.

- Chromium abundance determination may be affected.

Also a bonus!!

Our Stark broadening calculations for Cr III and Cr IV spectral lines are the first.

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- Calculate Stark broadening for Cr III and Cr IV lines using Modified Semi-Empirical (MSE) approach.

- Include Stark broadening tables into the line formation code SURFACE.

- Obtain the theoretical spectra with and without Stark broadening data for the stars under consideration.

- Compare theoretical spectra…
  with Stark broadening tables vs. without Stark broadening tables.

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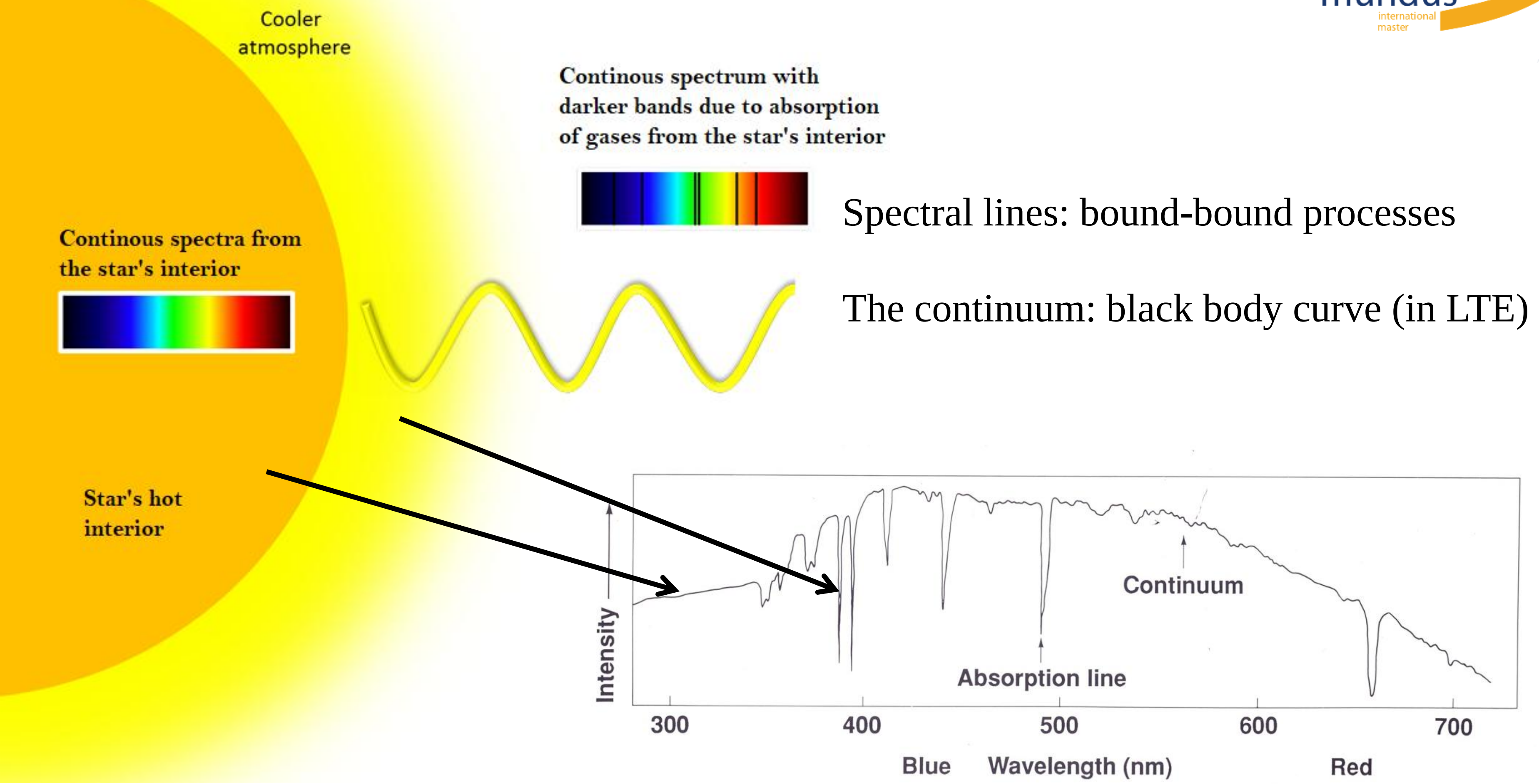
The stellar spectra



Spectral lines: bound-bound processes

The continuum: black body curve (in LTE)

Visual portion of stellar spectrogram

Hartmann/The Cosmic Journey, 4th ed., Fig. 16-5; The Cosmic Voyage, Fig. 16-3

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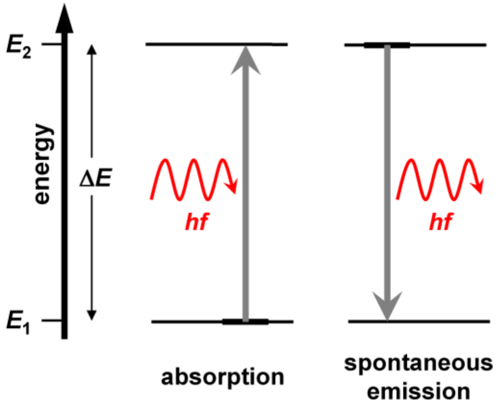
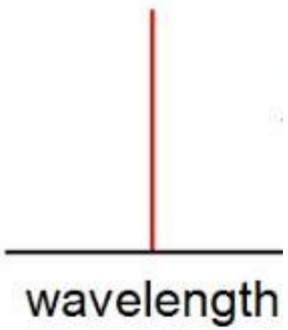
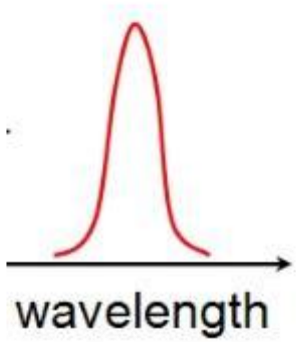
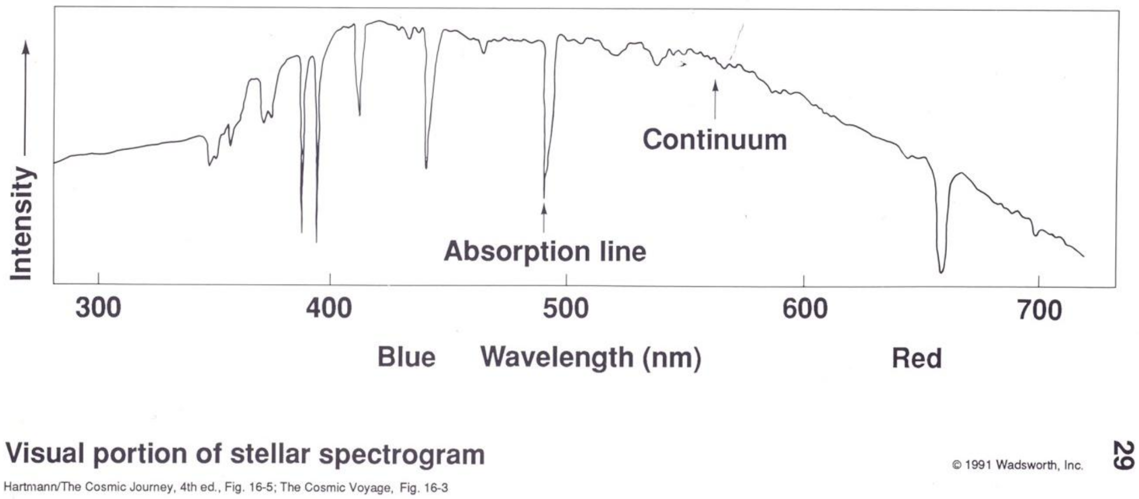
Broadening of stellar spectral lines





But…….





Visual portion of stellar spectrogram

Hartmann/The Cosmic Journey, 4th ed., Fig. 16-5; The Cosmic Voyage, Fig. 16-3

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Broadening of stellar spectral lines

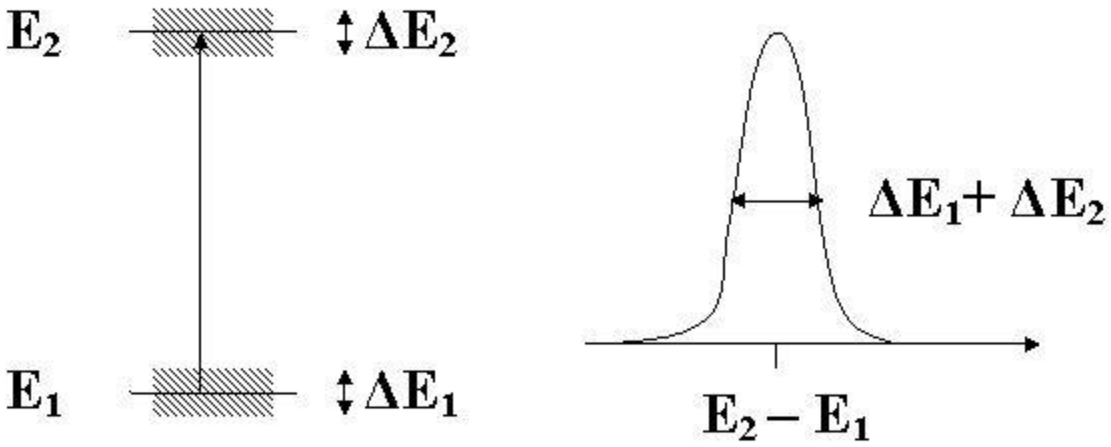
1. **Energy levels are not infinitely sharp.**

2. **Atoms are moving relative to observer.**

The shape of a spectral line can be expressed in the form of a line profile function $\phi(\upsilon)$

Several processes affect the broadening of stellar spectral lines…

Natural broadening



Not due to the interaction with the surrounding

BUT……

$$\Delta E \Delta t \geq \hbar$$

A state's energy and it's lifetime cannot be determined with infinite precision

⇩

lines are not infinitely sharp !

~2-4 x 10^{-5} nm

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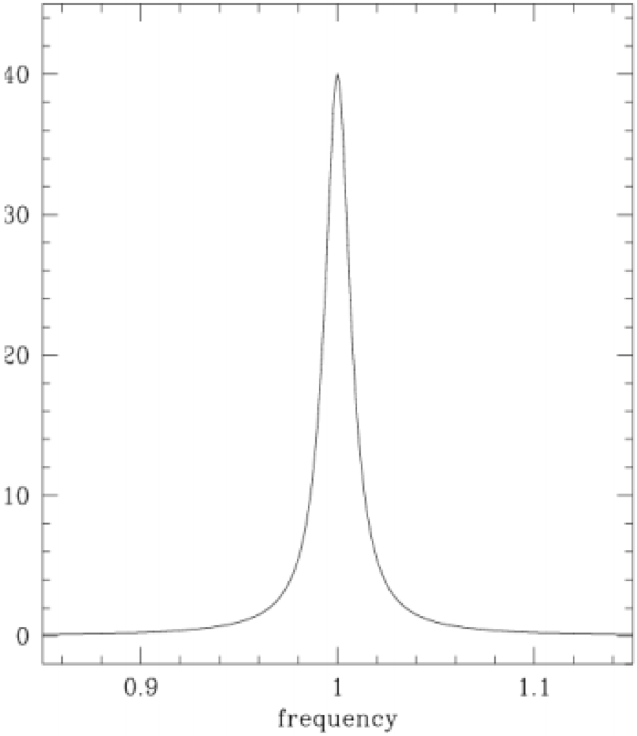
Natural broadening

- This is a Lorentzian or natural line profile.

- Natural line width isn't often directly observed, except in the line wings in low-pressure (nebular) environments. Other broadening mechanisms usually dominate.



$$\phi(\lambda) = \frac{constant\ \lambda^2}{c} \frac{\gamma\lambda^2/4\pi c}{\Delta\lambda^2 + (\frac{\gamma\lambda^2}{4\pi c})^2}$$

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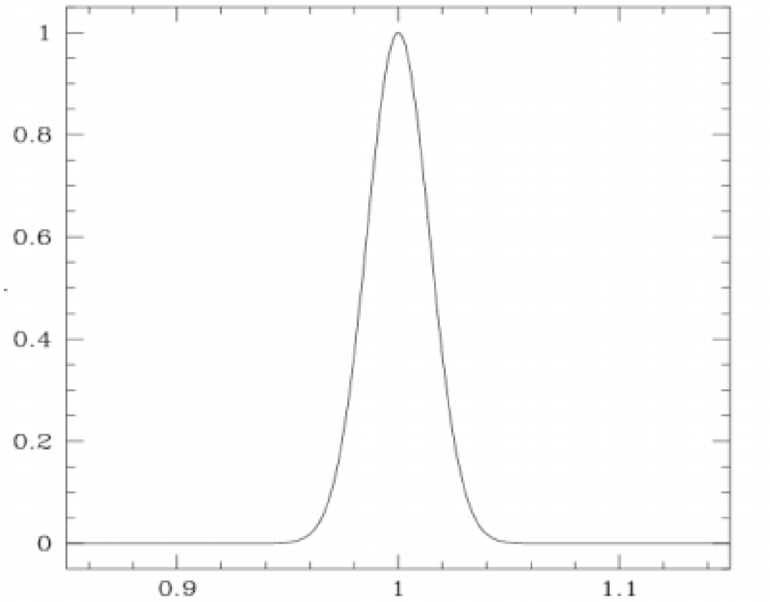
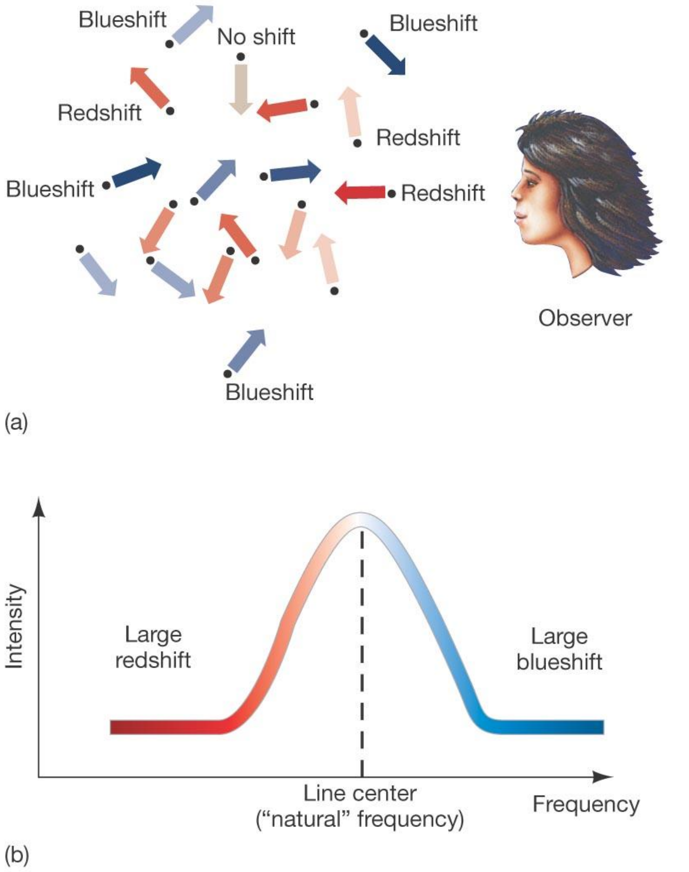
Doppler broadening

Broadening of spectral lines due to the Doppler effect caused by a distribution of velocities



A Gaussian but only for thermal broadening

$$\phi(\lambda) = \frac{constant\ \lambda^2}{c\Delta\lambda_D} \exp\left(-\frac{\Delta\lambda^2}{\Delta\lambda_D^2}\right)$$



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Collisional broadening

The presence of nearby particles will affect the radiation emitted

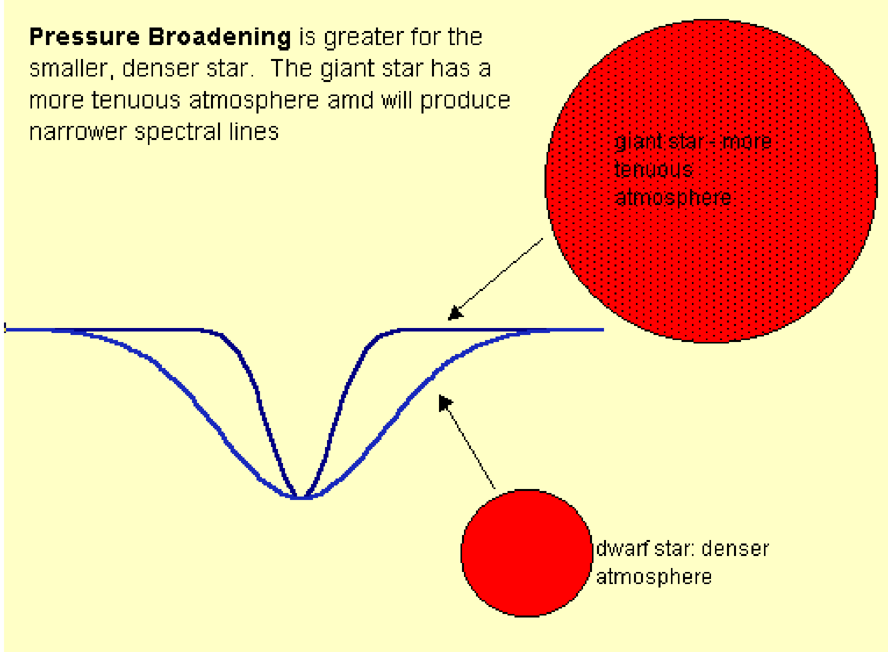
- Transition energy levels are disturbed.

- The perturbation is a function of R (distance between absorber and the perturbing particle).

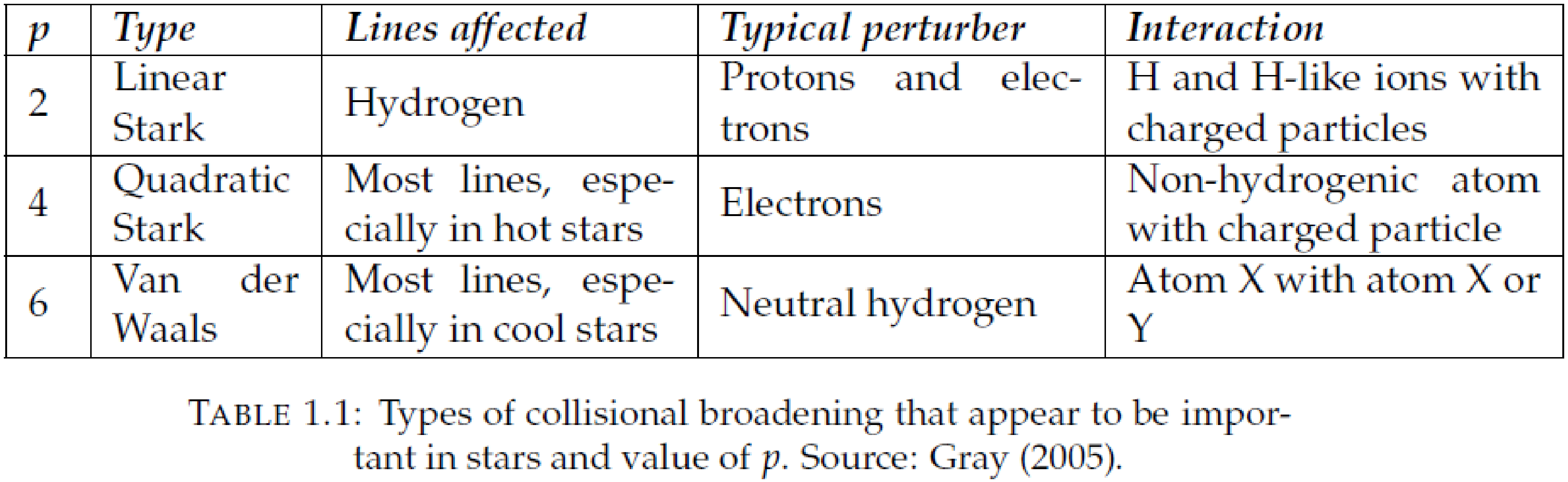
- The change in energy of a level induced by collision : ΔE= constant/R^{p}

- γ_{col} = constant/R^{p}

- High pressure leads to more collisions and higher broadening .



Pressure Broadening is greater for the smaller, denser star. The giant star has a more tenuous atmosphere amd will produce narrower spectral lines



p	*Type*	*Lines affected*	*Typical perturber*	*Interaction*
2	Linear Stark	Hydrogen	Protons and electrons	H and H-like ions with charged particles
4	Quadratic Stark	Most lines, especially in hot stars	Electrons	Non-hydrogenic atom with charged particle
6	Van der Waals	Most lines, especially in cool stars	Neutral hydrogen	Atom X with atom X or Y

TABLE 1.1: Types of collisional broadening that appear to be important in stars and value of *p*. Source: Gray (2005).

Quadratic Stark broadening

- The change in energy of a due to QSB: ΔE= constant/R^4
- γ_{col} = constant/R^4

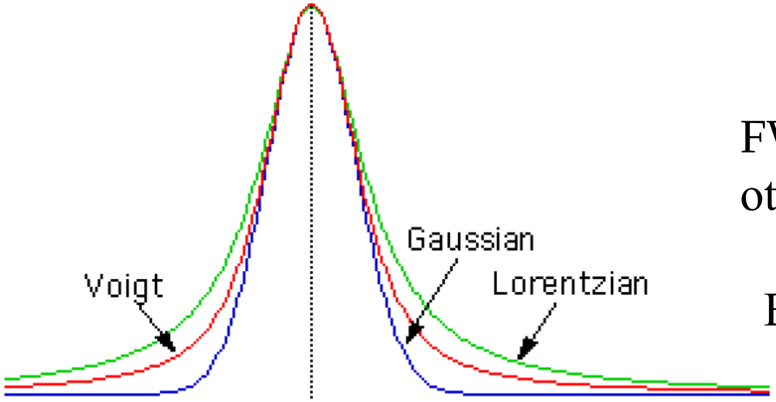
Including all…

ϕ(υ) ⟶ natural broadening + collisonal + thermal Doppler broadening

⟶ Lorentzian + Lorentzian + Gaussian

Voigt profile = Gaussian core + Lorentzian wings

$$V(\lambda, a) = \frac{constant\ \lambda^2}{c\sqrt{\pi}\Delta\lambda_D} H\left(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma\lambda^2}{4\pi c\Delta\lambda_D}\right)$$



FWHM and γ are related to each other and… they shape the line.

Better values… closer to obs.

$$\gamma = \gamma_n + \gamma_{Stark} + \gamma_{VdW}$$

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What is the use?

One of the motivation was Cr abundance determination:

How is it done?

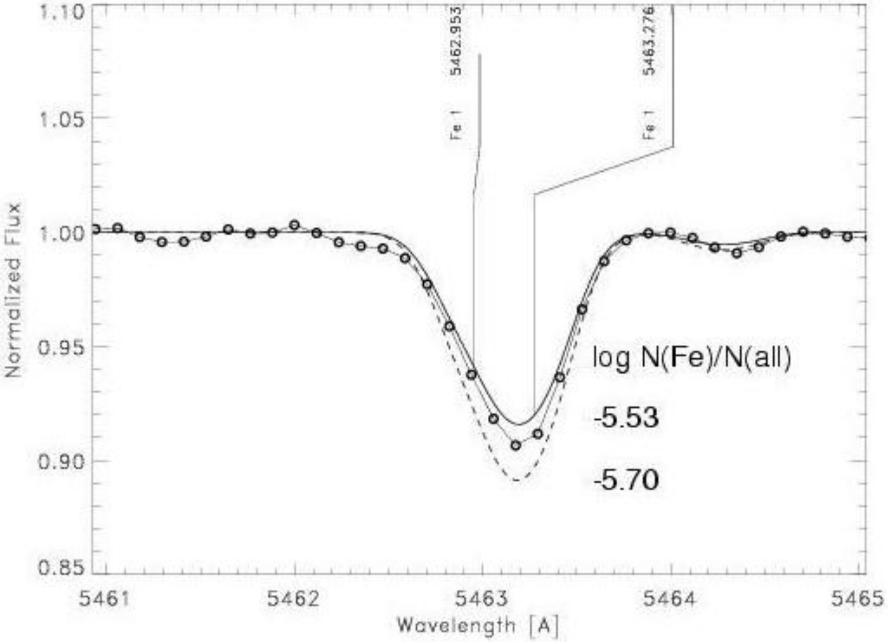
A. Calculation of theoretical spectra

- Calculate stellar model atmosphere.
- Line formation input (calculated Stark broadening data goes here)
- Give them as input into line formation code.

B. Compare theoretical spectrum with observations

- Test how well it fits the observations… tune the theoretical model to get closer to observations.

Have a look at the following example…



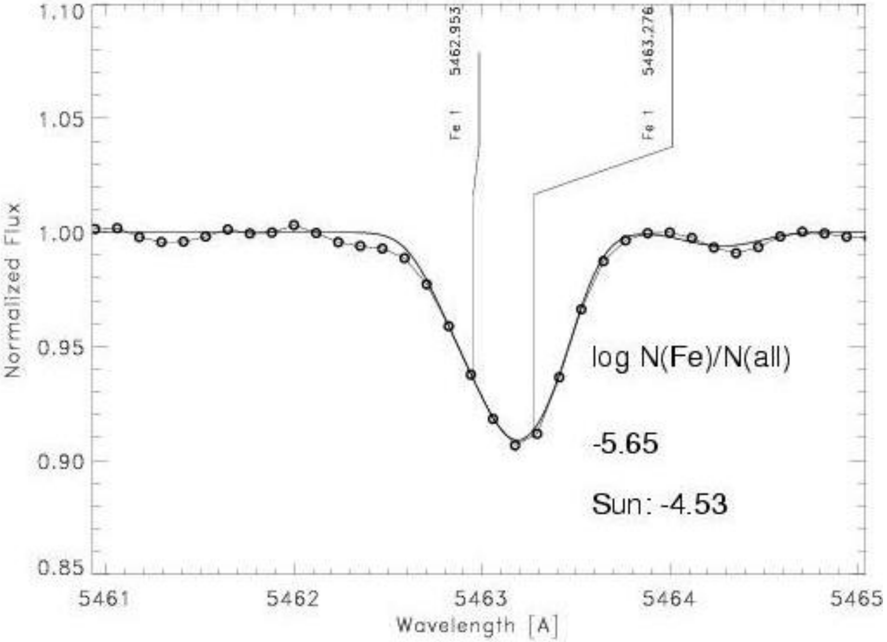


Image credit: Ulrike Heiter

Fe abundance too low and too high

Correct Fe abundance

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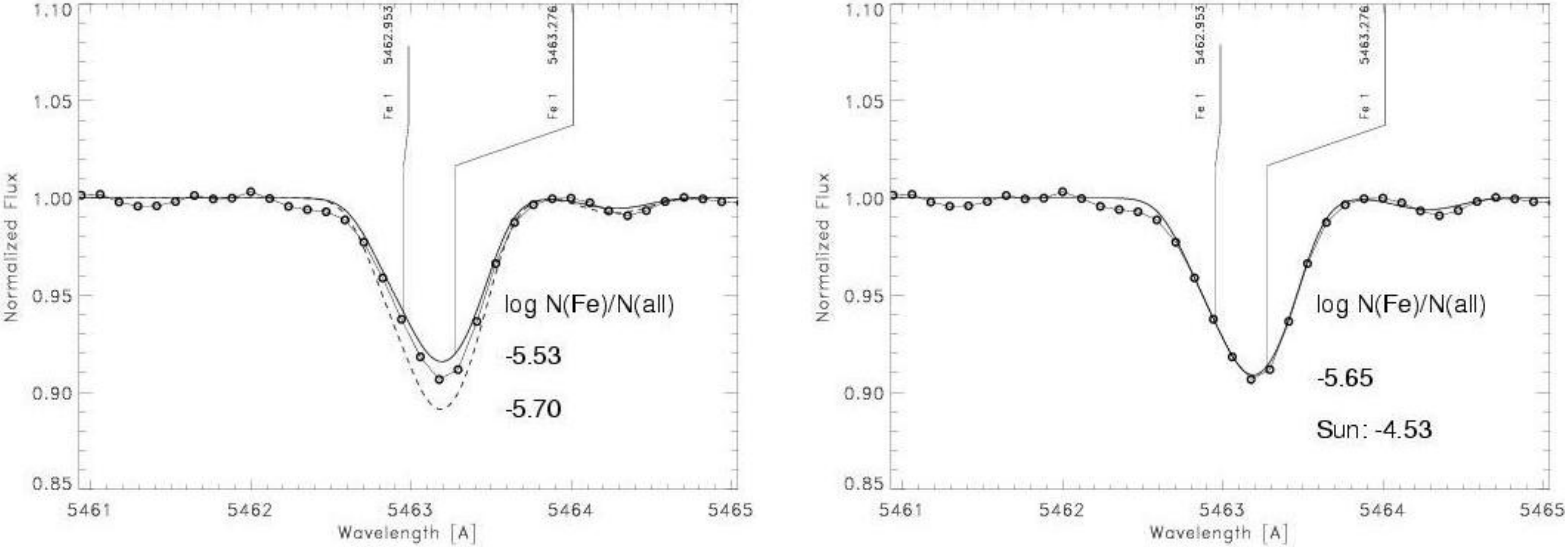
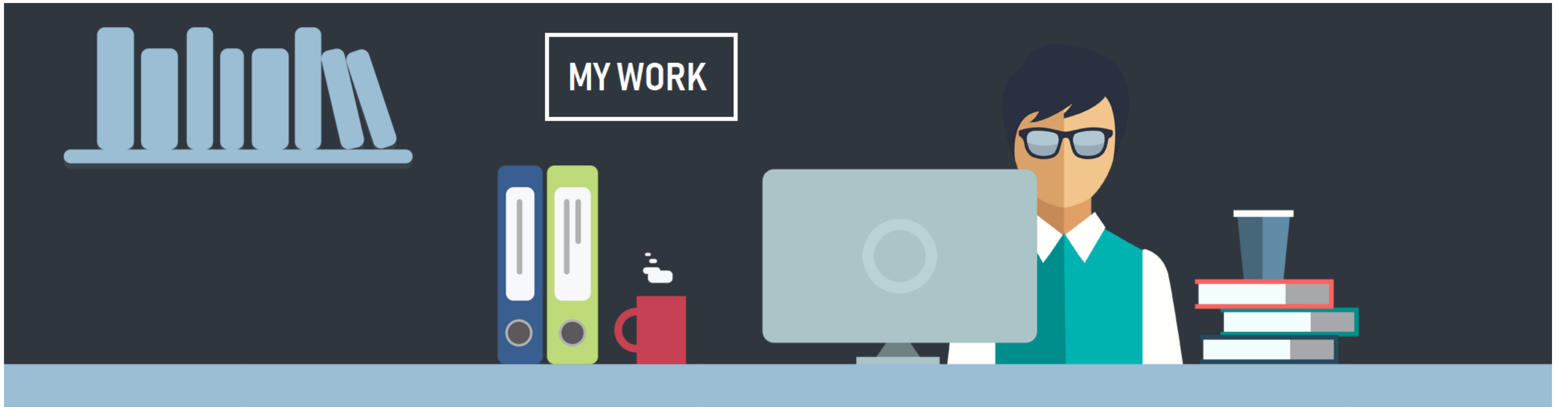


Change in line shapes will effect chemical abundance determination.

But.. line profile depends on damping factor.

Hence, a change in its value will change the line shape and chemical abundance determination.

All that been said……



- Created model ion with the energy levels of interest (input data required for width calculation)
- Calculated Stark broadening (electrons as pert.) for Cr III and Cr IV 4s-4p transitions using modified semi-empirical formula: M.S.Dimitrijevic, N.Konjevic: 1980, JQSRT, 24, 451
- Used the data to calculate theoretical spectrum for stars.
- Compared the spectrum obtained using MSE with those obtained without it.
- Compared with observation

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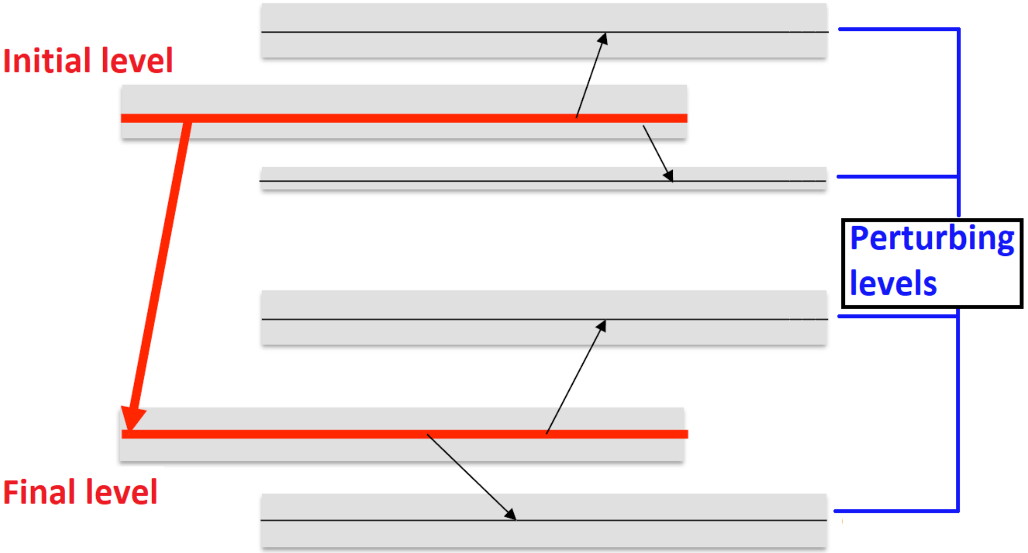
Calculations

The approximations…

1. **The impact approximation:** the interactions are separated in time.

 - the mean duration of an interaction is smaller than the mean interval between two collisions.



Source: Sahal-Bréchot (2014)

2. **The isolated line approximation:** neighboring levels do not overlap.

 - the line profile is a Lorentzian.

Modified Semi-empirical formula

- Requires a considerably smaller number of atomic data (helpful for our case).

- All perturbing levels with $\Delta n \neq 0$, needed for other approaches are lumped together and estimated approximately.

- The accuracy is about ±50% (Dimitrijevic and Popovic, 2001).

- But it has been shown that MSE gives very good agreement with experimental measurements (±30%) even for very complex spectra (e.g., XeII and KrII).

$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\lambda^2}{\sqrt{3}}\cdot\{\sum_{\ell_i\pm1}\sum_{L_{i'}J_{i'}}\vec{\Re}^2_{\ell_i,\ell_i\pm1}\tilde{g}\left(x_{\ell_i,\ell_i\pm1}\right)+$$

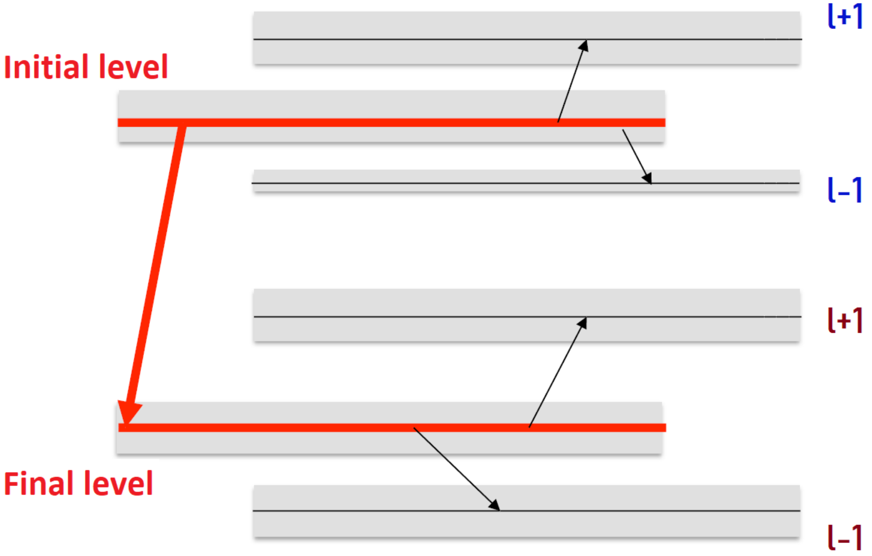
$$\sum_{\ell_f\pm1}\sum_{L_{f'}J_{f'}}\vec{\Re}^2_{\ell_f,\ell_f\pm1}\tilde{g}\left(x_{\ell_f,\ell_f\pm1}\right)+(\sum_{i'}\vec{\Re}^2_{ii'})_{\Delta n\neq0}g\left(x_{n_i,n_i+1}\right)+(\sum_{f'}\vec{\Re}^2_{ff'})_{\Delta n\neq0}g\left(x_{n_f,n_f+1}\right)\}$$

For Δn=0 terms…

$\vec{\Re}^2_{\ell_k,\ell_{k'}}$ depends on multiplet and line factors and radial integral (all are taken from literature).

calculated for l+1 and l-1 of initial and final states.

The Gaunt factors are taken from literature: Griem(1968), Dimitrijević and Konjević(1980)



$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\lambda^2}{\sqrt{3}}\cdot\{\sum_{\ell_i\pm1}\sum_{L_{i'}J_{i'}}\overrightarrow{\mathfrak{R}}^2_{\ell_i,\ell_i\pm1}\tilde{g}\left(x_{\ell_i,\ell_i\pm1}\right)+$$

$$\sum_{\ell_f\pm1}\sum_{L_{f'}J_{f'}}\overrightarrow{\mathfrak{R}}^2_{\ell_f,\ell_f\pm1}\tilde{g}\left(x_{\ell_f,\ell_f\pm1}\right)+(\sum_{i'}\overrightarrow{\mathfrak{R}}^2_{ii'})_{\Delta n\neq0}g\left(x_{n_i,n_i+1}\right)+(\sum_{f'}\overrightarrow{\mathfrak{R}}^2_{ff'})_{\Delta n\neq0}g\left(x_{n_f,n_f+1},\right.,$$

For Δn ≠ 0 terms…

$$\left(\sum_{k'}\overrightarrow{\mathfrak{R}}^2_{kk'}\right)_{\Delta n\neq0} = (\frac{3n_k^*}{2Z})^2\frac{1}{9}\left(n_k^{*2}+3\ell_k^2+3\ell_k+11\right)$$

$$x_{\ell_k,\ell_{k'}} = E/\Delta E_{\ell_k,\ell_{k'}},$$

$k = i, f$ where $E = \frac{3}{2}kT$ is the electron kinetic energy and

$$\Delta E_{\ell_k,\ell_{k'}} = \left|E_{\ell_k} - E_{\ell_{k'}}\right|,$$

is the energy difference between levels ℓ_k and $\ell_k \pm 1 (k = i, f)$. Also

$$x_{n_k,n_k+1} \approx E/\Delta E_{n_k,n_k+1},$$

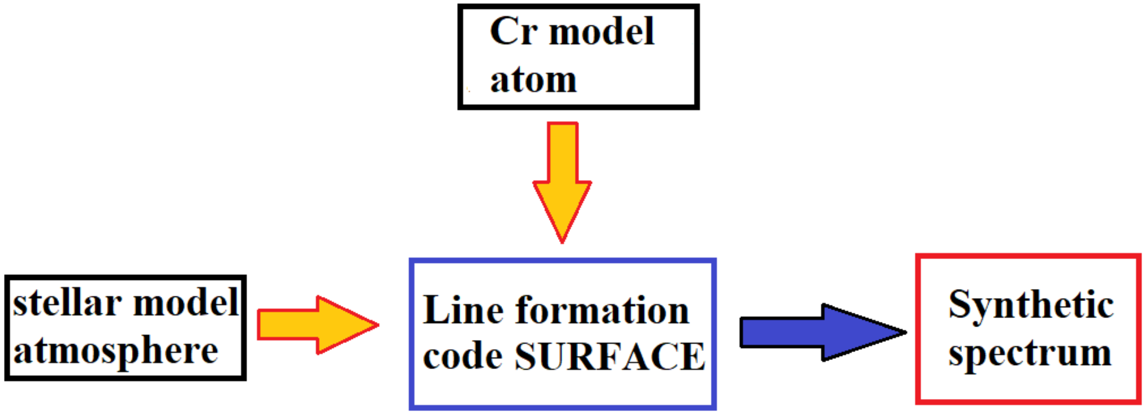
where for $\Delta n \neq 0$ the energy difference between energy levels with n_k and $n_k + 1$, $\Delta E_{n_k,n_k+1}$, is estimated as

$$\Delta E_{n_k,n_k+1} \approx 2Z^2E_H/n_k^{*3}.$$

the effective principal quantum number is defined by

$$n_k^* = [E_HZ^2/(E_{ion} - E_k)]^{1/2},$$

Application



Cr model atom

stellar model atmosphere

Line formation code SURFACE

Synthetic spectrum

Stellar atmosphere: ATLAS9

Synthetic spectrum: line formation code SURFACE

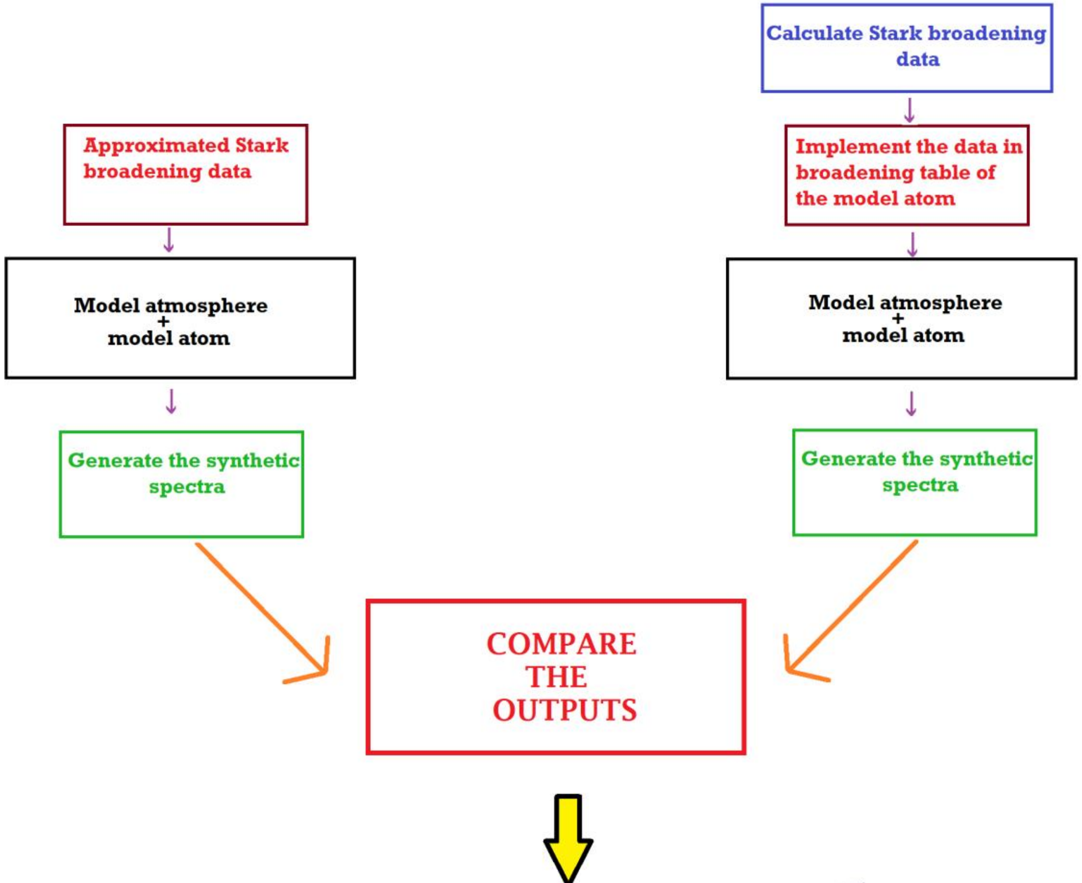
Calculated data: Cr model atom

The main objective is to solve the formal solution of RTE

$$I_\nu(\tau_\nu,\mu) = \int_{\tau_1}^{\tau_2} S_\nu(t_\nu)e^{\frac{-(\tau_\nu - t_\nu)}{\mu}} \frac{dt_\nu}{\mu} + I_\nu(0)e^{\frac{-\tau_\nu}{\mu}}$$

The calculations were done assuming LTE

Once I_ν is known the radiative flux coming can be found out



Approximated Stark broadening data

Model atmosphere + model atom

Generate the synthetic spectra

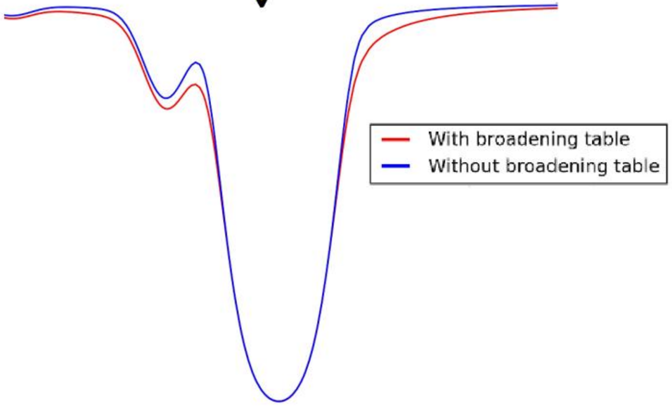
Calculate Stark broadening data

Implement the data in broadening table of the model atom

Model atmosphere + model atom

Generate the synthetic spectra

COMPARE THE OUTPUTS



Results

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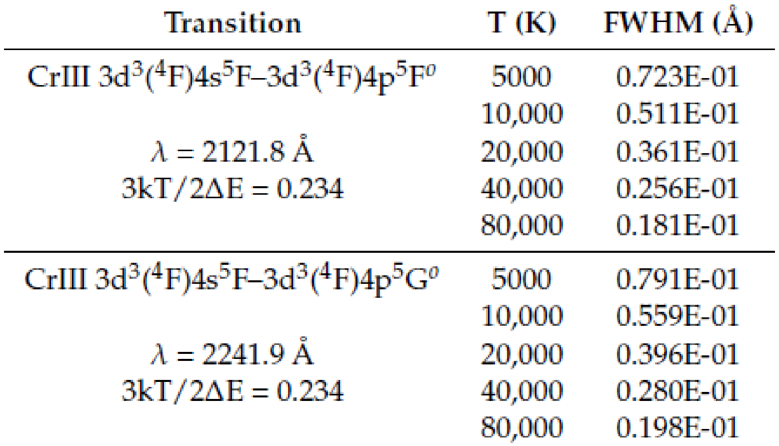
Results



Transition	T (K)	FWHM (Å)
CrIII $3d^3(^4F)4s\,^5F–3d^3(^4F)4p\,^5F^o$	5000	0.723E-01
	10,000	0.511E-01
$\lambda = 2121.8$ Å	20,000	0.361E-01
$3kT/2\Delta E = 0.234$	40,000	0.256E-01
	80,000	0.181E-01
CrIII $3d^3(^4F)4s\,^5F–3d^3(^4F)4p\,^5G^o$	5000	0.791E-01
	10,000	0.559E-01
$\lambda = 2241.9$ Å	20,000	0.396E-01
$3kT/2\Delta E = 0.234$	40,000	0.280E-01
	80,000	0.198E-01

- Stark widths of Cr III and Cr IV spectral lines were calculated by using MSE.

- The obtained results are for a perturber density of 10^{17} cm^3 and temperatures from 5000 K up to 80,000 K.

- 56 Cr III and 47 Cr IV lines in the UV were studied for

  OB-type main sequence stars: Iota Hercules and Upsilon Orionis

  Subdwarf B-stars CD-24 731, HD199112, and Feige 66

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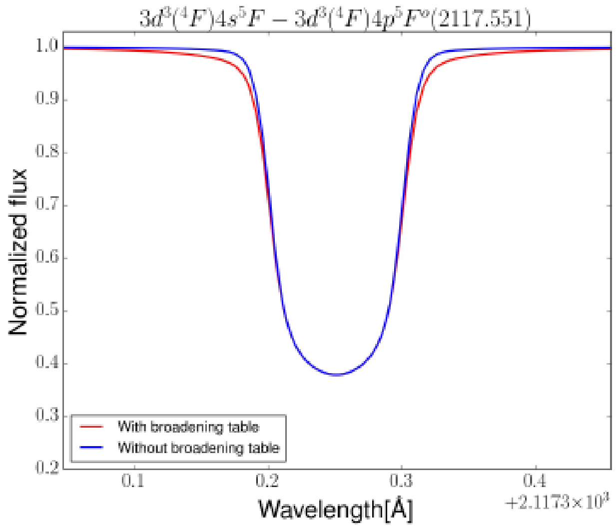
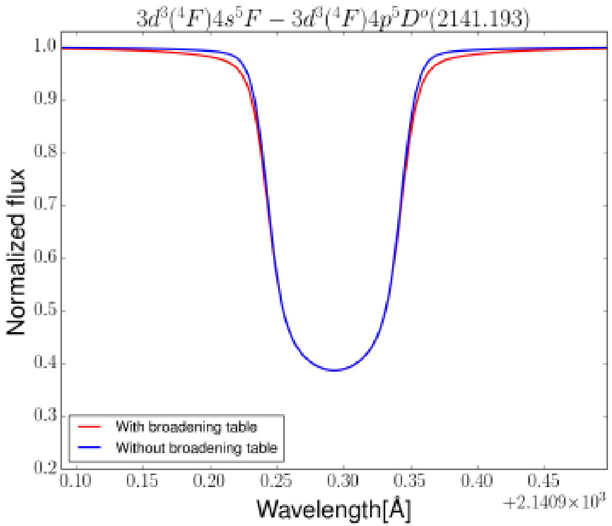
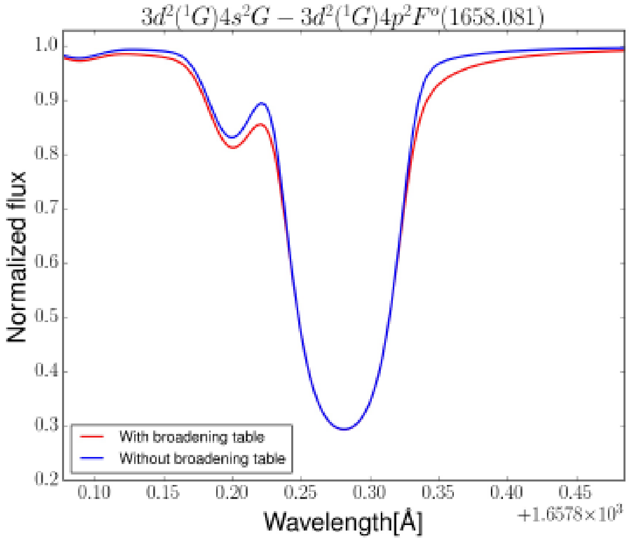
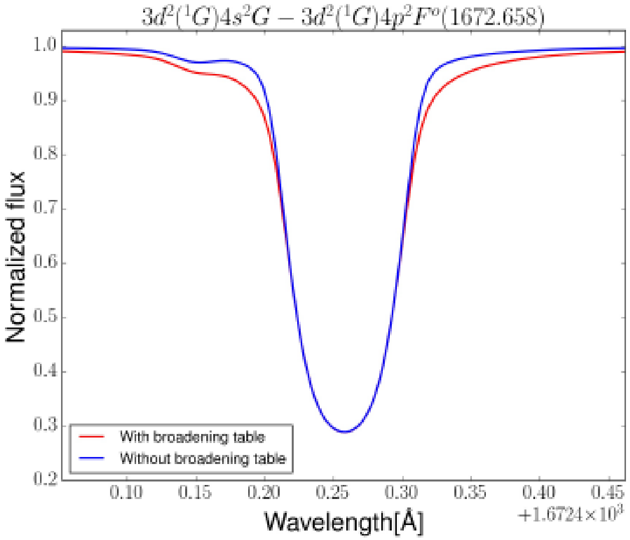
Stark broadening comparison of Cr III lines in Feige 66



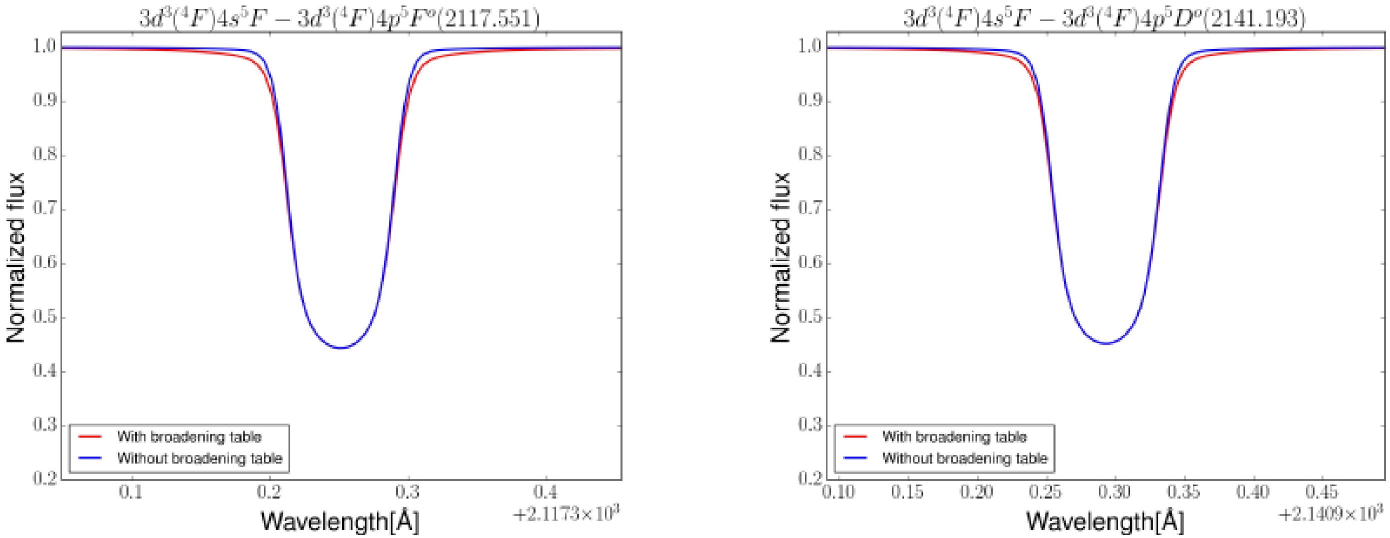


Stark broadening comparison of Cr IV lines in Feige 66

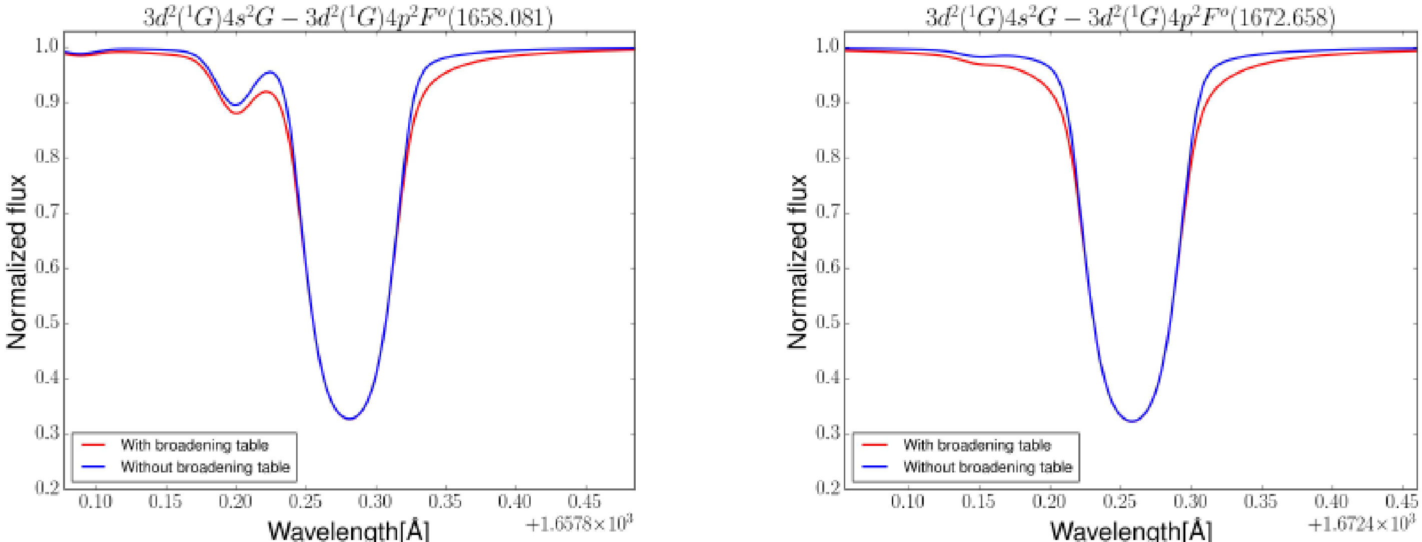




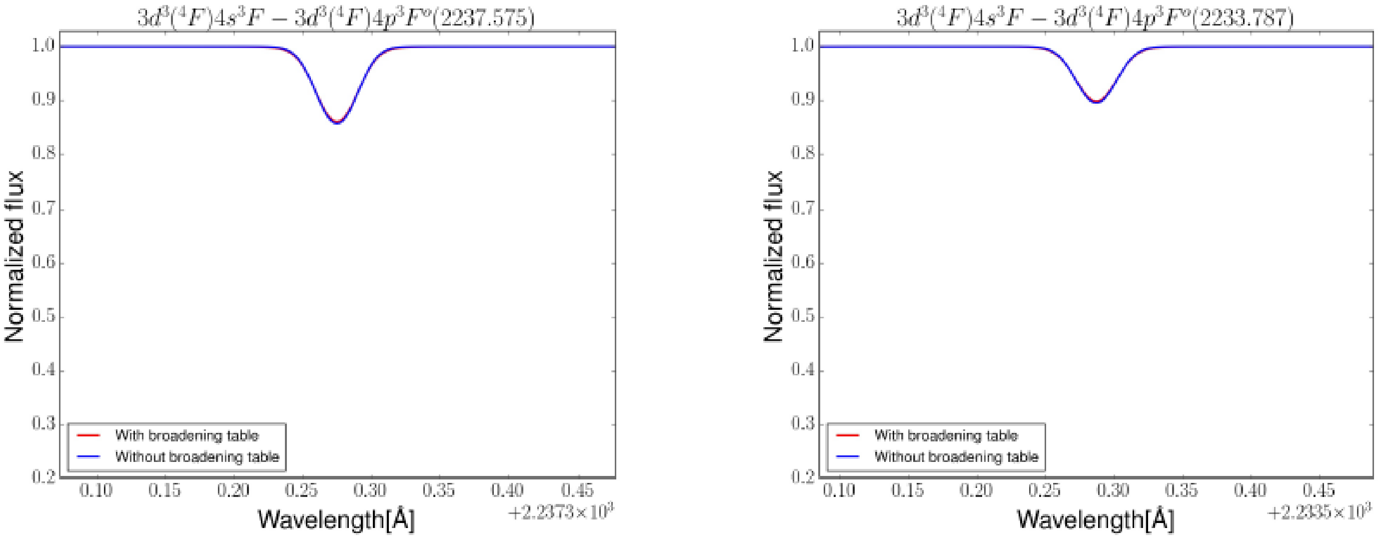
Stark broadening comparison of Cr III lines in CD-24 731



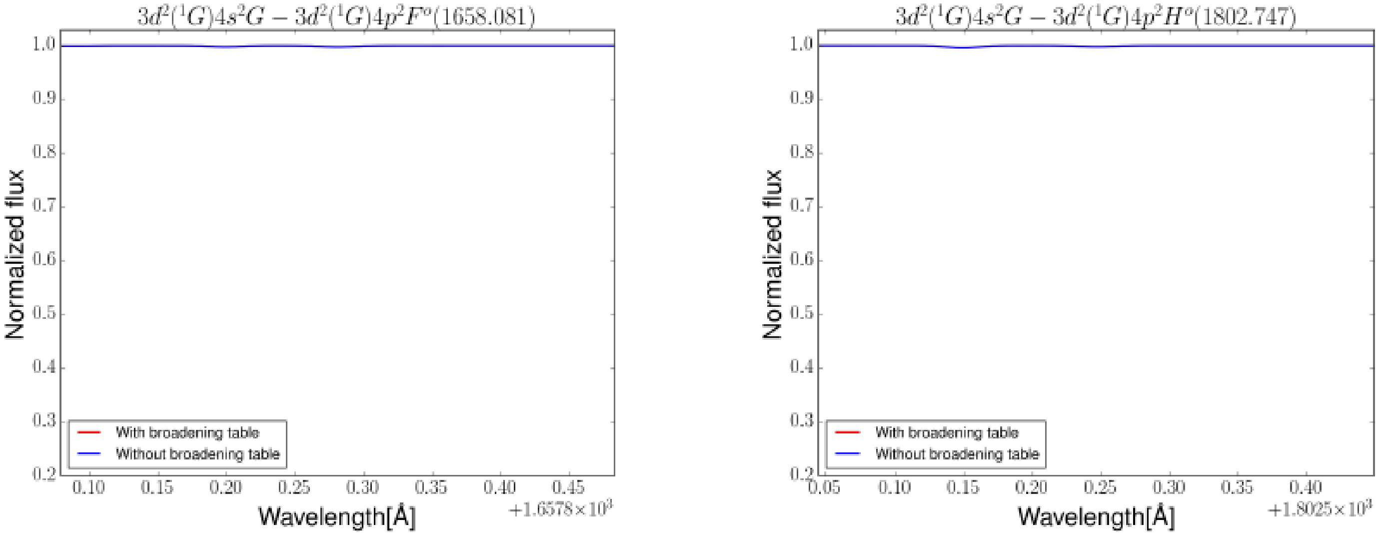
Stark broadening comparison of Cr IV lines in CD-24 731



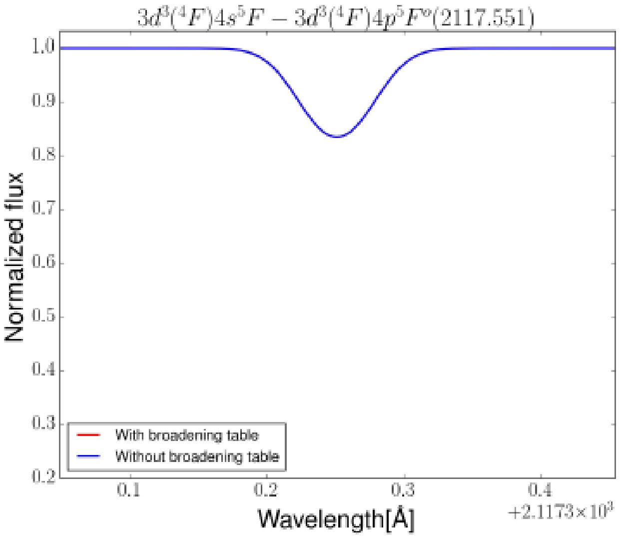
Stark broadening comparison of Cr III lines in HD188112

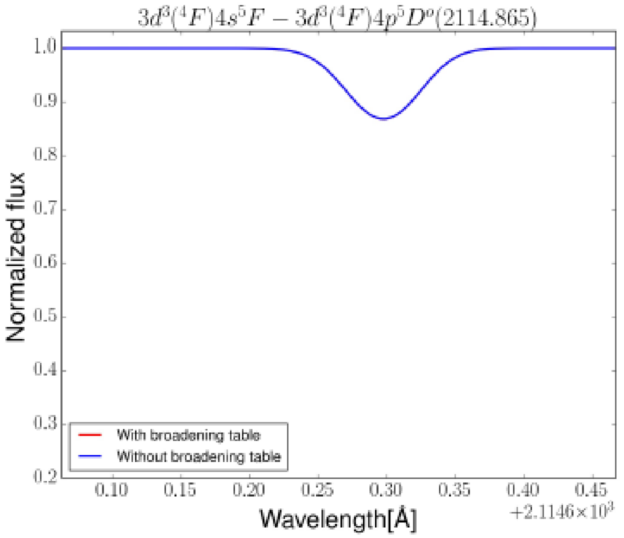


Stark broadening comparison of Cr IV lines in HD188112

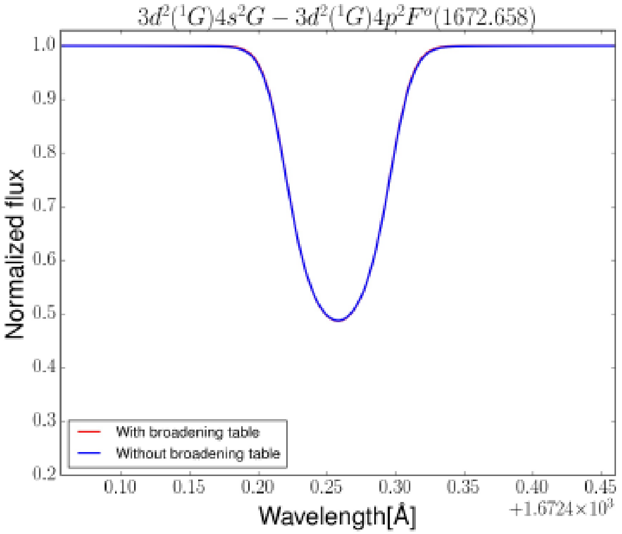


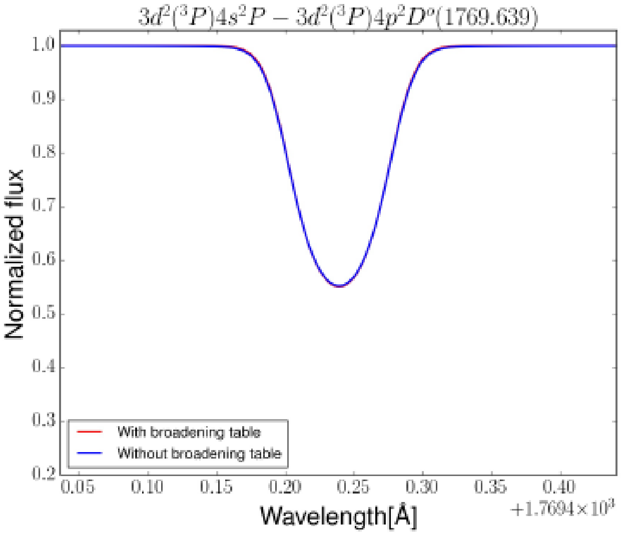
Stark broadening comparison of Cr III lines in Upsilon Orionis



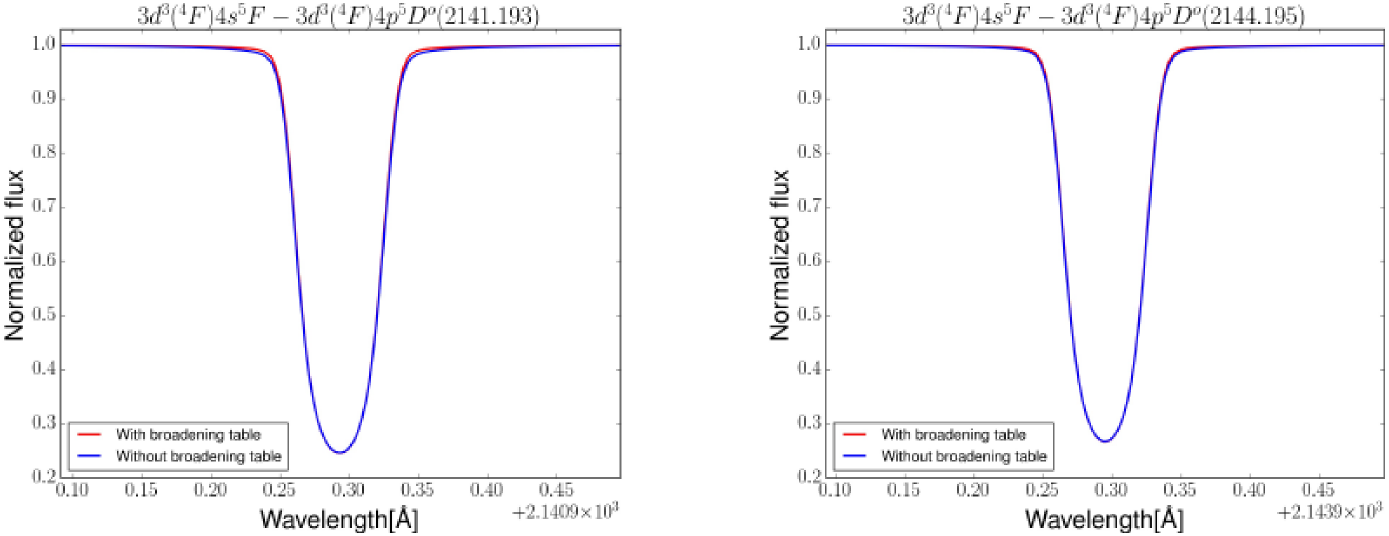


Stark broadening comparison of Cr IV lines in Upsilon Orionis

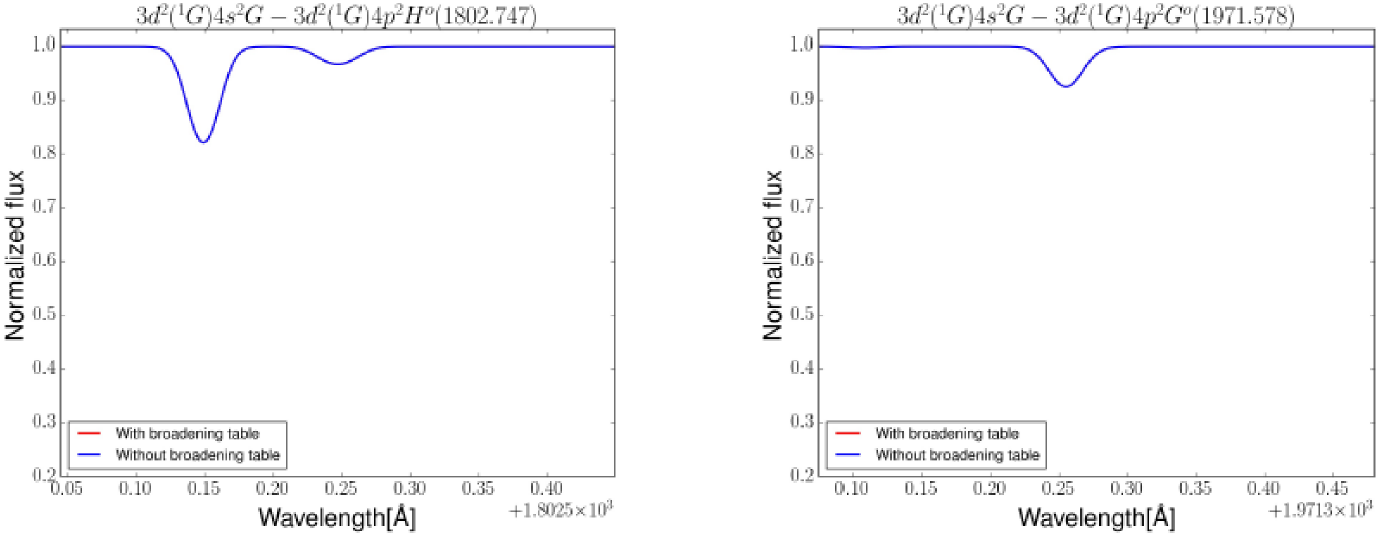




Stark broadening comparison of Cr III lines in Iota Hercules



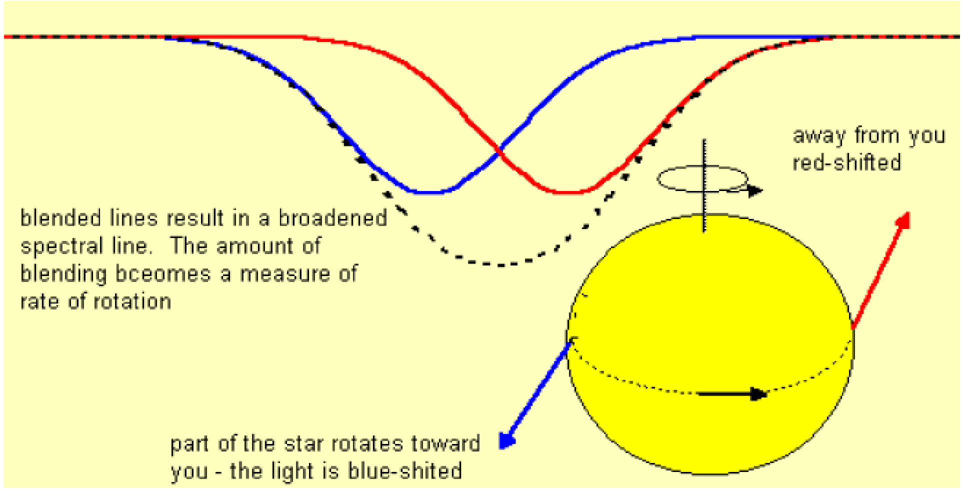
Stark broadening comparison of Cr IV lines in Iota Hercules

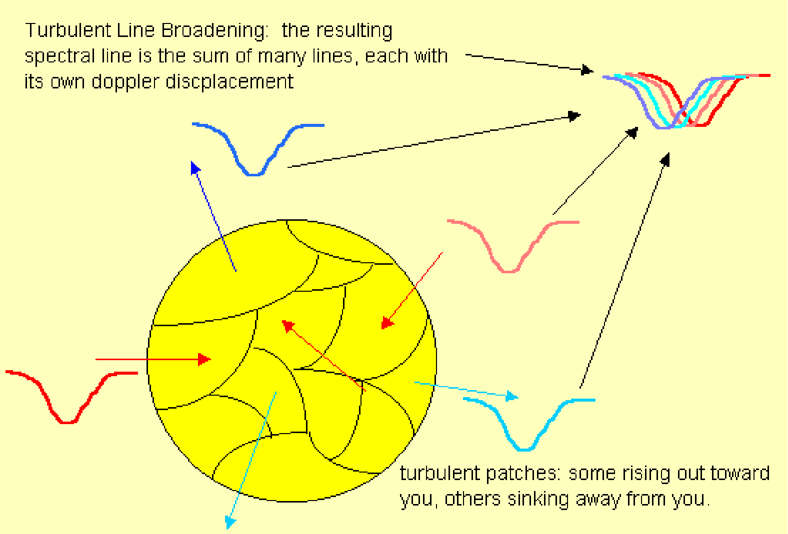


In order to compare with the observations…

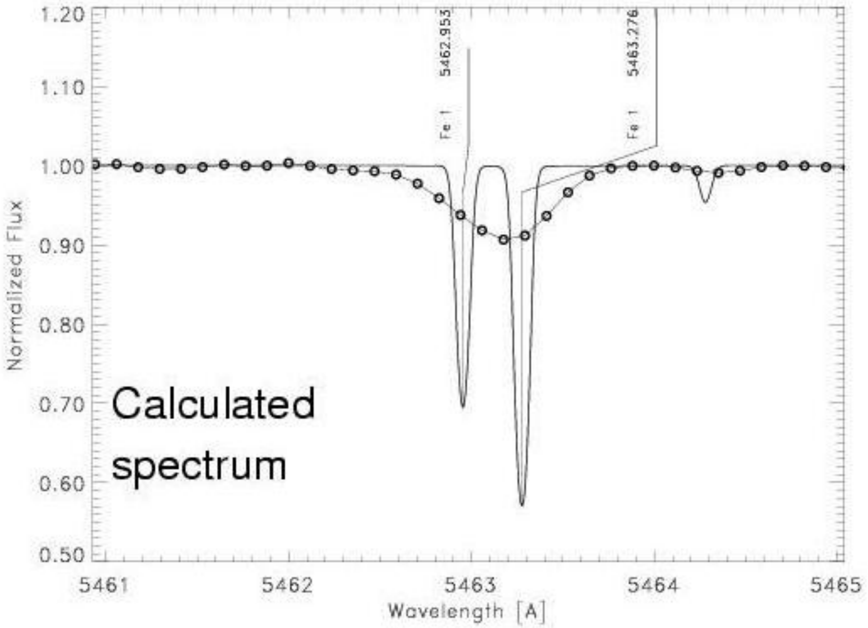
Take other line broadening mechanisms into consideration

- Rotation, macrotubulence and instrumental broadening

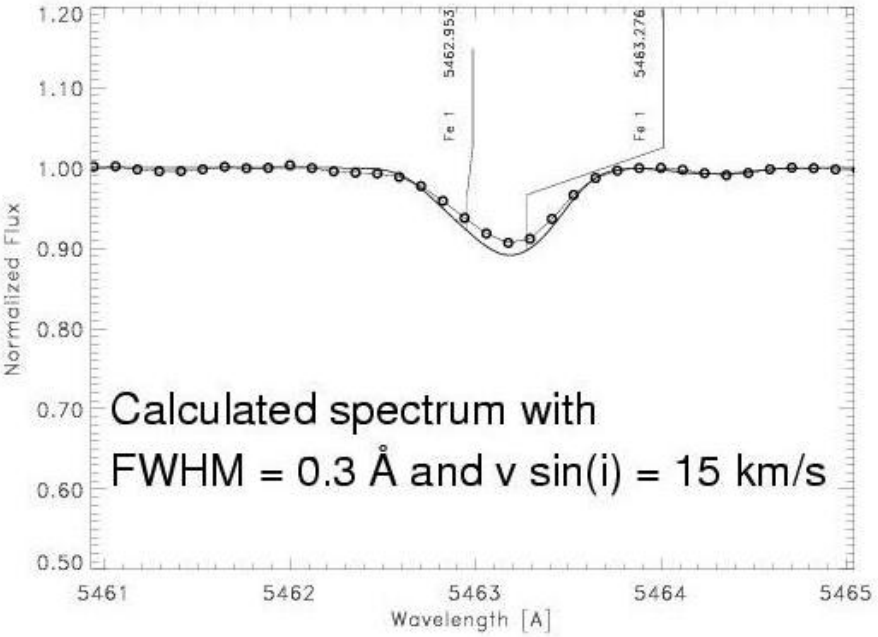




Instrumental broadening: Broadened by the optical systems of the telescope and spectrograph, a Gaussian profile, broadening depends on the spectral resolution



Without instrumental and rotational broadening



With instrumental and rotational broadening

Image credit: Ulrike Heiter

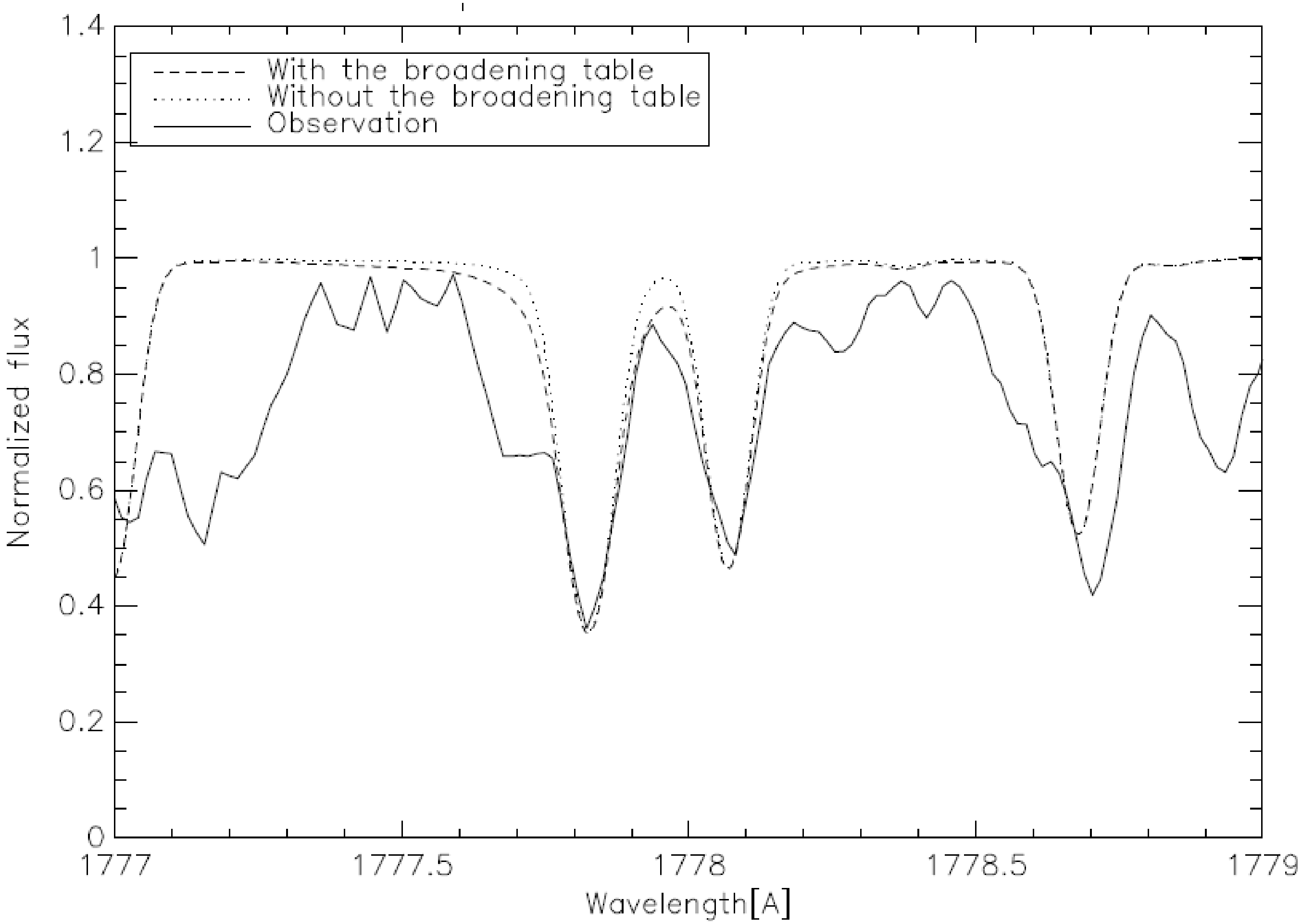
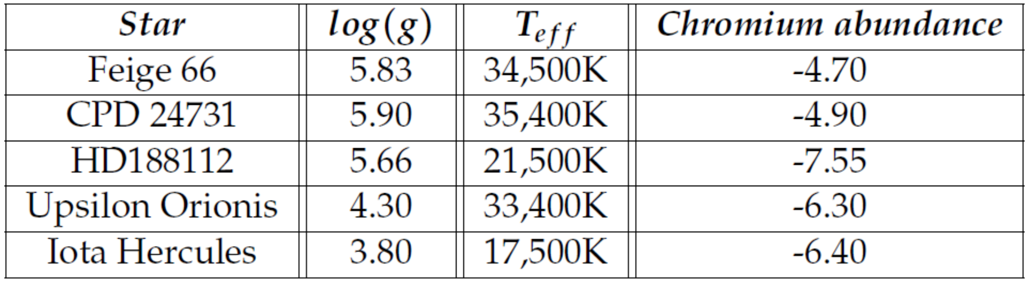


FIGURE 4.13: Comparison of theoretically calculated $3d^2(^1G)4s^2G^o$ – $3d^2(^1G)4p^2H^o$ (1777.825 Å) and $3d^2(^1D)4s^2D$ – $3d^2(^1D)4p^2D^o$ (1778.069 Å) transition line profiles with the observations in case of Feige 66. The theoretical line profiles were convoluted with the instrumental, the rotational, and the macroturbulence profiles. The spectral line calculated using MSE is broader than that calculated using approximate Stark broadening. The theoretical spectra were calculated with the Cr abundance of -4.40.

Conclusion



Star	*log(g)*	T_{eff}	*Chromium abundance*
Feige 66	5.83	34,500K	-4.70
CPD 24731	5.90	35,400K	-4.90
HD188112	5.66	21,500K	-7.55
Upsilon Orionis	4.30	33,400K	-6.30
Iota Hercules	3.80	17,500K	-6.40

TABLE 4.1: Properties of the stars under consideration.

Stark broadening is expected to be prominent in the wings of strong lines.

- appropriate abundance and temperatures are required for their formation.

But... The effect strongly depends on surface gravity

Subdwarfs CD 24731 and Feige 66 have higher values of g, T and A → show signatures of SB or any change of it

Hence, in appropriate cases, Stark broadening calculated using MSE affects the line profiles and hence chemical abundance determination.

Abundance value changed from -4.70 to -4.40 : a good fit to the observations was obtained. However, a detailed abundance analysis should be done.

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Thank you !

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Bonus slides!

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Failing of isolated line approximation: At high densities or for lines arising from high levels

- The electron impact width becomes comparable to the separation ΔE(nl, nl+1) between the perturbing energy levels and the initial or final level .

- The corresponding levels become degenerate and the isolated line approximation is invalid (Griem 1974).

- Then it is not obvious that the profile is Lorentzian.

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Why quadratic Stark effect?

Our calculations are for Quadratic Stark effect. Linear is for Hydrogen and Hydrogen-like ions.

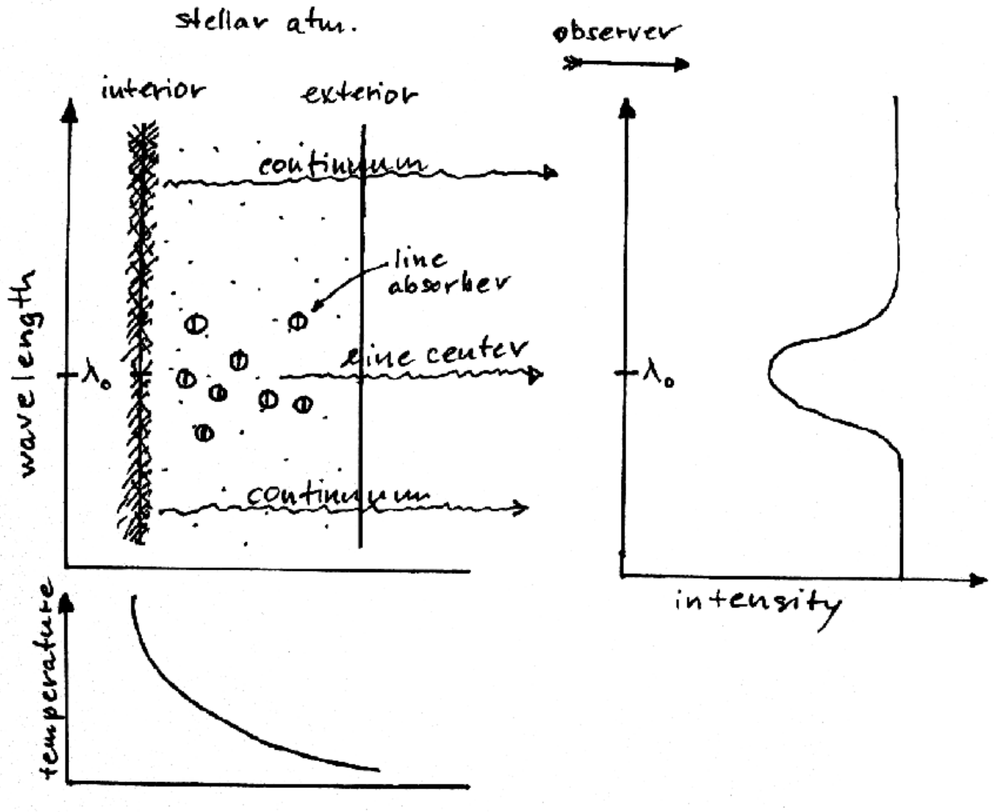
For non-hydrogenic ions
it is Quadratic except for very excited states where transition to the linear occurs.

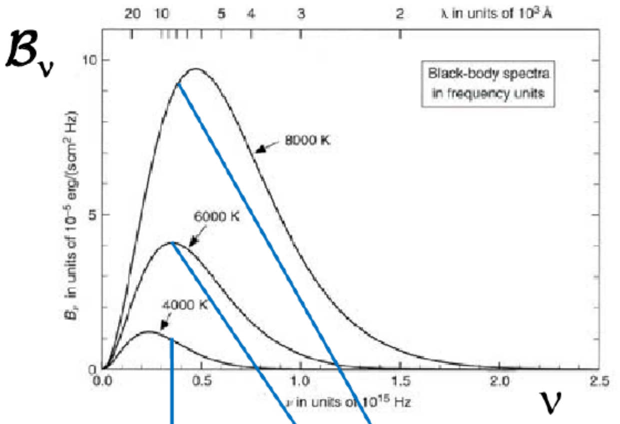
On using Bates and Damgraad…

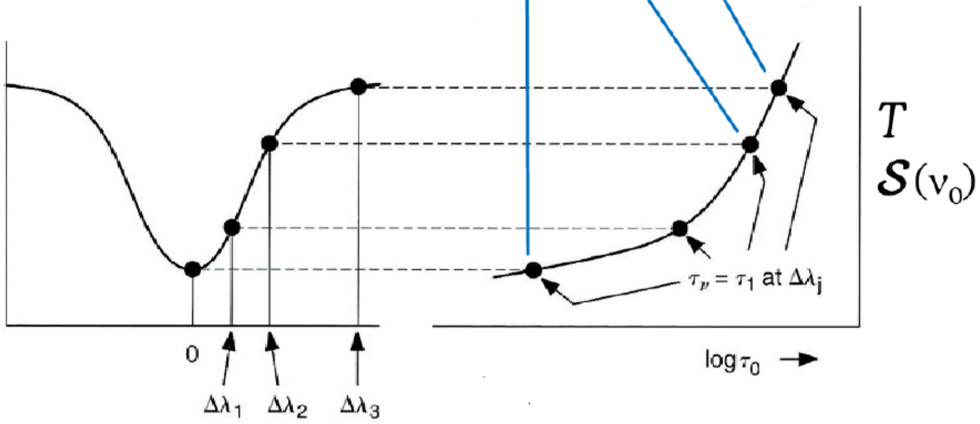
The needed oscillator strengths have been determined by using the method of Bates & Damgaard (1949) and the tables of Oertel & Shomo (1968) while for higher levels, the calculations have been performed as in van Regemorter, Hoang Binh & Prud’homme (1979).
Within the method of Bates and Damgaard, only oscillator strengths for transitions allowed in the LS coupling are different from zero.

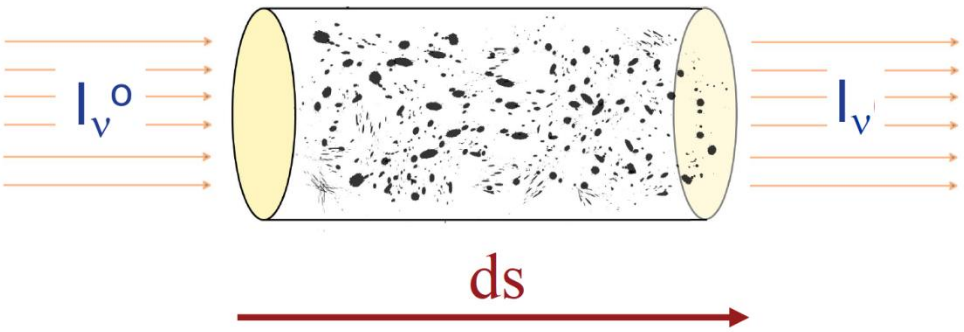
Concerning the use of a set of Bates and Damgaard’s oscillator strengths, which is complete according to the corresponding sum rules, Ben Nessib, Dimitrijevi´c & Sahal-Br´echot (2004) and Hamdi et al. (2007), who calculated line widths and shifts of Si V and Ne V ions, compared SCP ab initio Stark widths obtained with Bates and Damgaard oscillator strengths and with SUPERSTRUCTURE (Thomas–Fermi–Dirac interaction potential model with relativistic corrections; Eissner, Jones & Nussbaumer 1974) oscillator strengths.
They obtained that the difference between the two sets of calculations did not exceed 30 per cent.

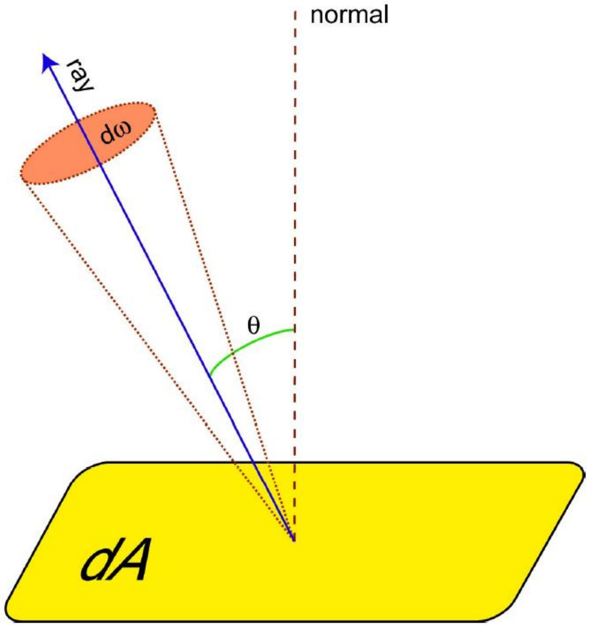
Since the accuracy of the SCP method is about 20 per cent, such a difference, due to different sets of oscillator strengths used in Stark broadening calculation, is not crucial.


stellar atm.
observer
interior
exterior
continuum
line absorber
line center
continuum
wavelength
λ_0
λ_0
intensity
temperature


$\mathcal{B}_\nu$
20 10 5 4 3 2 λ in units of 10^3 Å
Black-body spectra in frequency units
8000 K
6000 K
4000 K
B_ν in units of 10^{-5} erg/(scm² Hz)
10
5
0
0.0 0.5 1.0 1.5 2.0 2.5
ν in units of 10^{15} Hz
ν


0
$\Delta\lambda_1$
$\Delta\lambda_2$
$\Delta\lambda_3$
T
$\mathcal{S}(\nu_0)$
$\tau_\nu = \tau_1$ at $\Delta\lambda_j$
$\log \tau_0$ →





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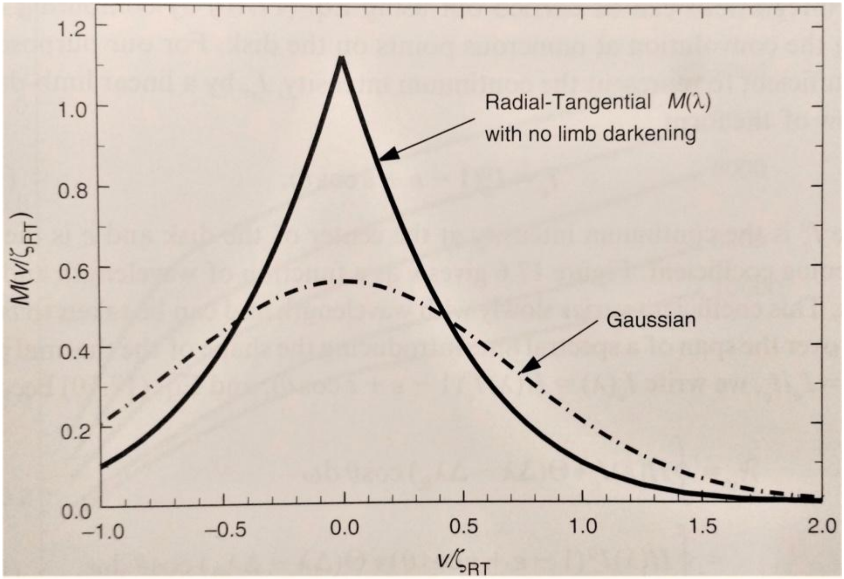
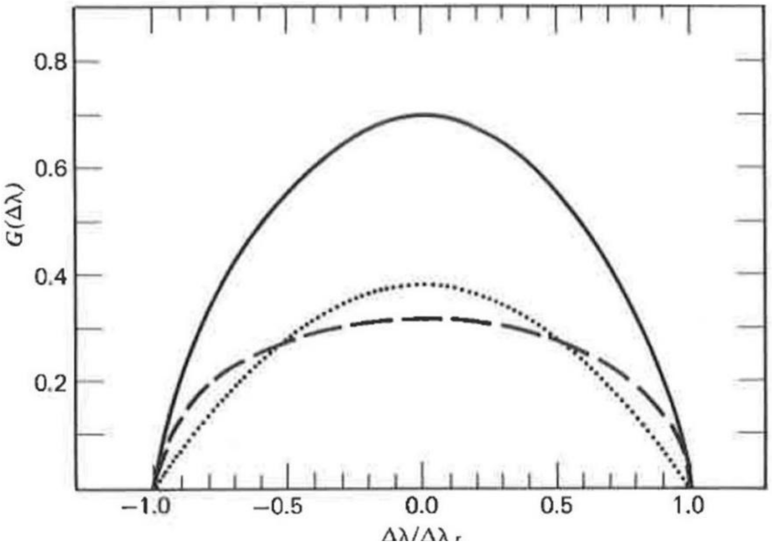
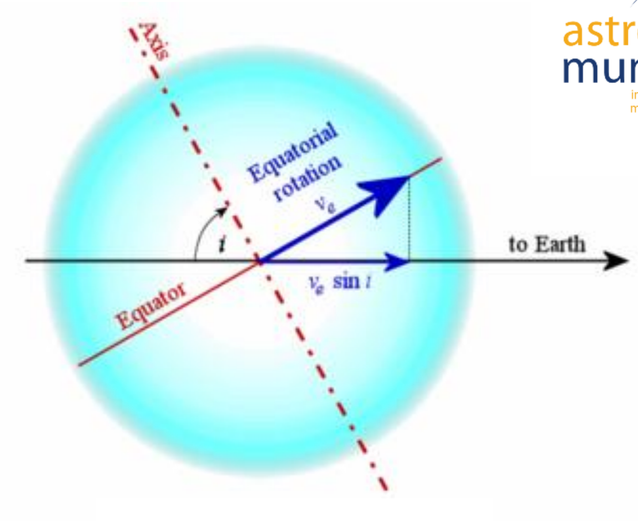


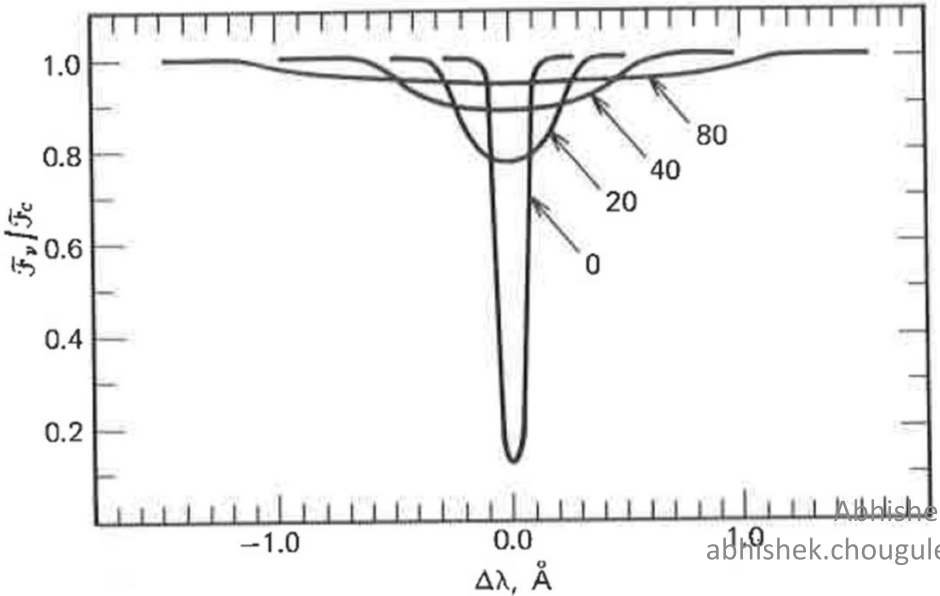
$$M(\Delta\lambda) = \frac{2A_R\Delta\lambda}{\pi^{1/2}\zeta_R^2}\int_0^{\frac{\zeta_R}{\Delta\lambda}} \exp\left(\frac{-1}{u^2}\right) du + \frac{2A_T\Delta\lambda}{\pi^{1/2}\zeta_T^2}\int_0^{\frac{\zeta_T}{\Delta\lambda}} \exp\left(\frac{-1}{v^2}\right) dv$$

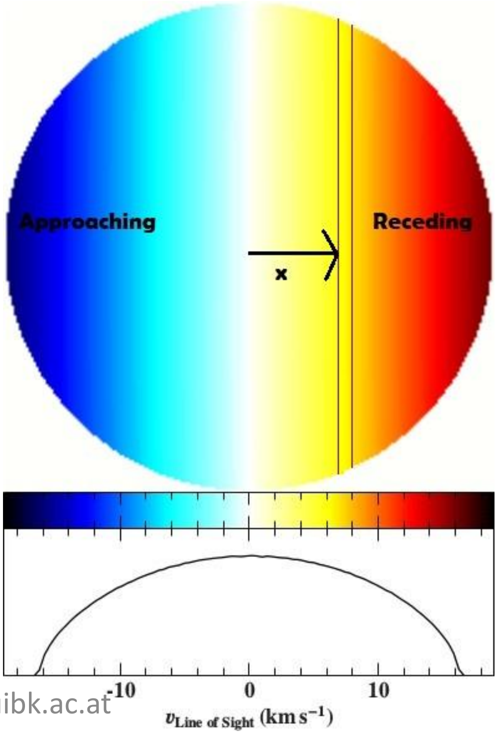




$$\Delta\lambda_L = v_{eq}\sin i$$

$$G(\Delta\lambda) = c_1\left[1-\left(\frac{\Delta\lambda}{\Delta\lambda_L}\right)^2\right]^{\frac{1}{2}} + c_2\left[1-\left(\frac{\Delta\lambda}{\Delta\lambda_L}\right)^2\right]$$



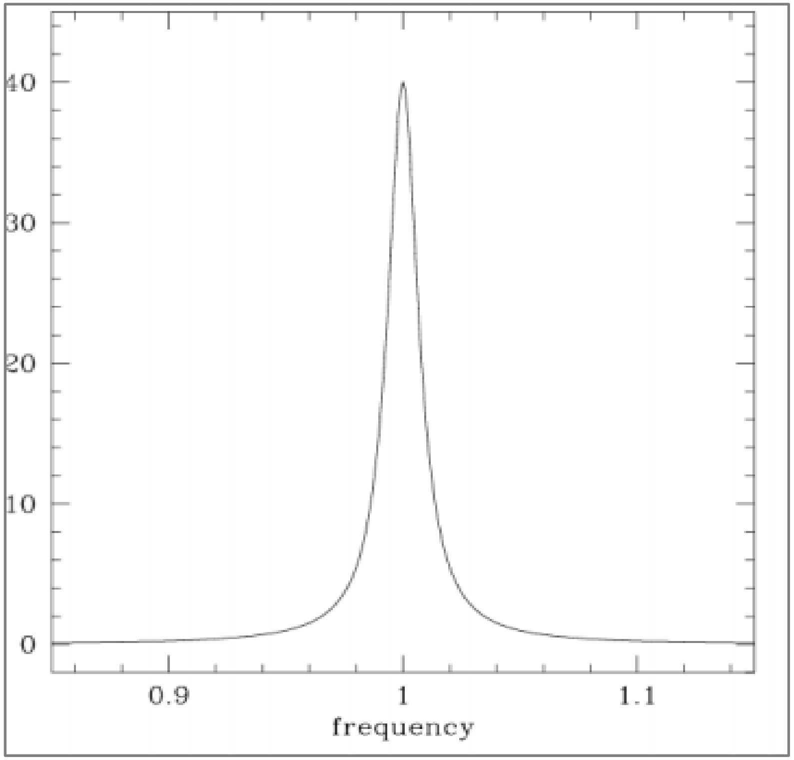


Bates and Damgraad in our case

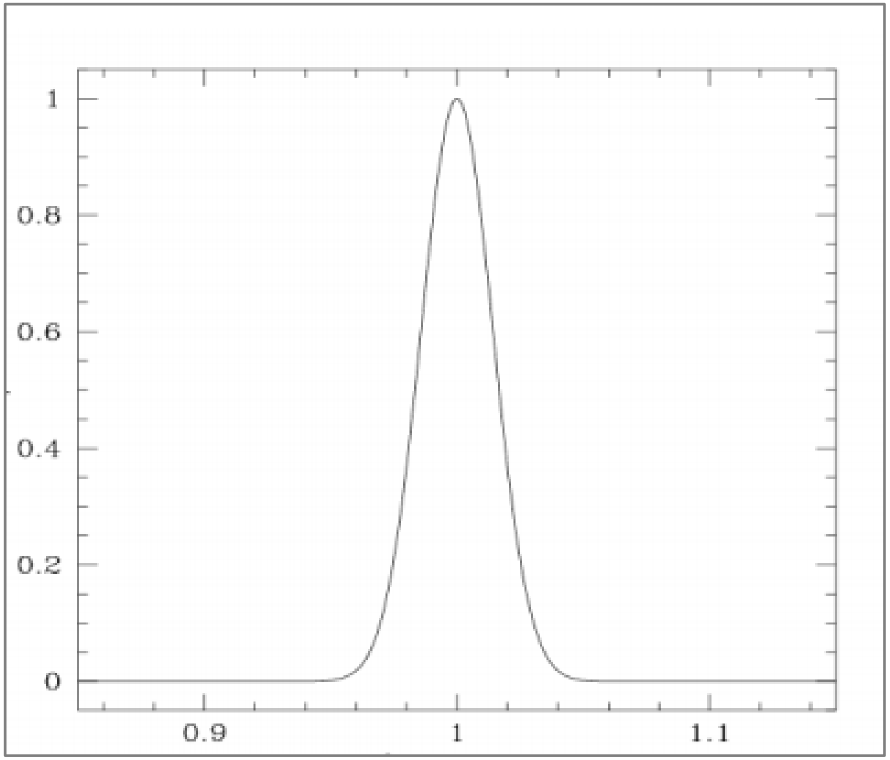
- Of course the error is higher for Cr III. But in Stark broadening calculations we work not with a single value but with an ensemble of values for all transitions from a particular level forming the line. This diminish the total error since a more sophisticated method will result in the redistribution of the values but the total sums should be close. If you want to improve calculations you have two methods. One to use existing energy levels and to calculate needed oscillator strengths with for example a Hartree-Fock method. But my experience is that this will not always give a better result since the sum in the formula is obtained within Coulomb approximation and if you calculate two parts in different way this is not consistent. The other method is to use for example COWAN code or SUPERSTRUCTURE code and to calculate the energy levels and oscillator strengths together. This is difficult and maybe you can do this for PhD thesis but such a task is out of the scope of a master thesis. Another problem is that a crucial part of COWAN code is the adjustment to the system of measured energy levels which for Cr III are scarce. So, our results are relatively good, better than approximate formulae of Cowley and Kurucz and useful since there are no others. Also I doubt that someone will do the better calculations in the near future. Also you may find many examples where this one or other similar semiempirical theories have been used for very complex elements.

Line broadening

Lorentz profile



Gaussian profile



$$\phi(\lambda) = \frac{constant\ \lambda^2}{c} \frac{\gamma\lambda^2/4\pi c}{\Delta\lambda^2 + (\frac{\gamma\lambda^2}{4\pi c})^2}$$

$$\phi(\lambda) = \frac{constant\ \lambda^2}{c\Delta\lambda_D} \exp\left(-\frac{\Delta\lambda^2}{\Delta\lambda_D^2}\right)$$

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