COWAN CODE AND STARK BROADENING OF SPECTRAL LINES OF S II, S III AND S IV

Nenad Milovanović and Milan S. Dimitrijević

ASTRONOMICAL OBSERVATORY BELGRADE

nmilovanovic@aob.bg.ac.yu, mdimitrijevic@aob.bg.ac.yu

Introduction

Stark broadening of spectral lines is the dominant pressure broadening mechanism in hot, early-type, stars and white dwarf atmospheres.

This type of broadening might also be important in interstellar molecular and ionized hydrogen clouds and in cooler stars such as solar type ones for transitions involving higher principal quantum numbers.

Astrophysical importance

1. Analysis and modeling of stellar spectra
2. Analysis, modeling and diagnostics of stellar plasma
3. Abundances determination
4. Stellar opacity calculations
5. Stellar luminosity calculations

6.Nuclear processes in stellar interiors

etc.

Stark broadening calculation:

1.strong-coupling quantum-mechanical method
2.semi-classical method
3.modified semi-empirical approach (MSE)
…

MSE method

Dimitrijević, M.S., Konjević, N.: 1980, *J. Quant. Spect. Rad. Transfer*, **24**, 451.

Dimitrijević, M.S., Kršljanin, V.: 1986, *Astron. Astrophys*., **165**, 269.

Modified semi-empirical approach includes explicitely only levels with
$\Delta n = 0$ and
$l'_{if} = l_{if} \pm 1$,
- n is the principal quantum number, l is the orbital quantum number and i and f denote initial and final level, respectively.

levels with $\Delta n \neq 0$ are combined and approximately estimated.

Stark broadening parameter calculations needs less atomic data then in the semi-classical method.

The accuracy of the MSE calculations for spectral line widths is around ±50%.

In order to obtain higher accuracy of Stark broadening parameters using MSE calculations we need to have large and reliable amount of atomic data (energy levels, oscillator strengths, etc.).

Atomic data can be experimental and theoretical.

Experimental data are rare and hard to obtain due to complexity and difficulty in experiments.

Theoretical calculations of atomic data are *ab initio* calculations and several of programs packages exist as Cowan code, SUPERSTRUCTURE, ATSP (MCHF atomic structure calculations), etc.

COWAN CODE

Cowan code is a suite of four programs that calculates atomic structures and spectra via the superposition-of-configuration method.

R. D. Cowan, *The Theory of Atomic Structure and Spectra*, UC Press, Berkeley, 1981.

Modified by Yu. Ralchenko and E. Kramida in 1995.

The programs are:

RCN - calculates one-electron radial wavefunctions (bound or free) for each of any number of specified electron configurations, using the Hartree-Fock or any of several more approximate methods.

RCN2 - is an interface program that uses the output wave-functions from RCN to calculate the configuration-interaction Coulomb integrals (R_k) between each pair of interacting configurations, and the electric-dipole (E1) and/or electric quadrupole (E2) radial integrals between each pair of configurations.

RCG - sets up energy matrices for each possible value of the total angular momentum J, diagonalizes each matrix to get eigenvalues (energy levels) and eigenvectors (multi-configuration, intermediate-coupling wavefunctions in various possible angular-momentum-coupling representations), and then computes M1 (magnetic dipole), E2, and/or E1 radiation spectra, with wavelengths, oscillator strengths, radiative transition probabilities, and radiative lifetimes.

When higher accuracy results are desired, **RCE** can be used to vary the various radial energy parameters E_{av}, F_k, G_k, zeta, and R_k to make a least-squares fit of experimental energy levels by an iterative procedure. The resulting least-squares-fit parameters can then be used to repeat the RCG calculation with the improved energy levels and (presumeably) wavefunctions.

Input parameters:

Ion and atomic terms

```
200-90 0 2  01.  0.2    5.E-08    1.E-11-2 00090
0 1.0  0.65  0.0 1.00   -6
    8    30 III  2p2                1S2 2S2 2P2
```

Output parameters:

Energy levels

```
O III      2p2
    -9.838200*    -9.838  -0.000044  0.000  2p2    J= 0.0     100%  2p2   (3P) 3P
    38.465800*    38.466   0.000000  0.000  2p2    J= 0.0     100%  2p2   (1S) 1S
    -9.726000*    -9.726   0.000048  1.501  2p2    J= 1.0     100%  2p2   (3P) 3P
    -9.507100*    -9.507   0.000016  1.501  2p2    J= 2.0     100%  2p2   (3P) 3P
     9.617200*     9.617  -0.000016  1.000  2p2    J= 2.0     100%  2p2   (1D) 1D
O III      2p2
    -9.838200*    -9.838  -0.000044  0.000  2p2    J= 0.0     100%  2p2   (3P 0  ) 0
    38.465800*    38.466   0.000000  0.000  2p2    J= 0.0     100%  2p2   (1S 0  ) 0
    -9.726000*    -9.726   0.000048  1.501  2p2    J= 1.0     100%  2p2   (3P 1  ) 1
    -9.507100*    -9.507   0.000016  1.501  2p2    J= 2.0     100%  2p2   (3P 2  ) 2
     9.617200*     9.617  -0.000016  1.000  2p2    J= 2.0     100%  2p2   (1D 2  ) 2
```

^{16}S V

$1s^2\,2s^2\,2p^6\,3s^2\ \ ^1S_0$ E_i=-394.51368592 a.u.

```
Configuration Term J  Levels
                      cm-1
-------------------------------
3s(2)     1S      0        0.
3s_2S.3p  3P*     0      83094.31
                  1      83468.91
                  2      84234.31
          1P*     1     127424.5
3p(2)1D2  1D      2     193946.4
```

Configuration	Term	J	Level (cm^{-1})
$2p^63s^2$	^1S	0	0.0
$3s3p$	$^3P°$	0	83 024.0
		1	83 393.5
		2	84 155.2
$3s3p$	$^1P°$	1	127 150.7
$3p^2$	^1D	2	193 739.1

RESULTS

S II

$[Ne]3s^2 3p^3\ {}^4S^o_{3/2}$ Ei=188 200 cm^{-1}

S III

$[Ne]3s^2 3p^2\ {}^3P_0$ Ei=280 900 cm^{-1}

Energy levels of S II and multiplets calculated with Cowan code (E_{CC}) and energy levels taken from NIST atomic spectra database (E_{NIST}).

Element	Configuration	Term	E_{CC} (cm^{-1})	E_{NIST} (cm^{-1})
S II	$3p^2$ (^3P) 4s	^4P	110187.36	110004.94
		^2P	113156.63	113286.88
	$3p^2$ (^3P) 3d	^4F	110500.32	110511.56
		^4D	114375.86	114237.38
		^2F	114954.43	115079.36
	$3p^2$ (^3P) 4p	$^4D^o$	128238.30	128287.40
		$^4P^o$	130045.96	129984.44
		$^2D^o$	130865.49	130968.76
S III	3p 4s	$^3P^o$	146823.52	146960.62
	3p 4p	^3D	147856.40	147689.05
		^3S	174196.63	174037.69
	3p 5s	$^3P^o$	210653.26	210339.26

Using complete energy levels of S II and S III calculated using Cowan code combined with experimental energy levels taken from NIST database we have been calculated Stark broadening parameters (FWHM) with MSE method.

Ion	Transition array	Multiplet	λ (nm)	w_{MSE} (nm)	w_{exp} (nm)	T (10^3 K)	Ne (10^{23} m^{-3})
S II	$3p^23d–3p^24p$	$^4F – ^4D^o$	560.615	0.0304	0.038	23.5	1.0
		$^4D – ^4P^o$	630.548	0.0963	0.101	23.5	1.0
		$^2F – ^2D^o$	631.269	0.103	0.084	23.5	1.0
	$3p^24s–3p^24p$	$^4P – ^4D^o$	545.386	0.0301 0.050	0.031 0.046	28.5 32.6	1.0 0.7
		$^2P – ^2D^o$	564.702	0.0424 0.0374	0.0316 0.0396	27.0 34.0	0.67 1.02
S III	3p4s–3p4p	$^3P^o – ^3D$	433.271	0.0401	0.0428	40.0	2.08
	3p4p–3p5s	$^3D – ^3P^o$	250.815	0.0410	0.0402	40.0	2.1
		$^3S – ^3P^o$	278.549	0.0396	0.0380	40.0	2.1

Experimental data were taken from:

N. Konjević, A. Lesage, J. R. Fuhr and W. L. Wiese, *J. Phys. Chem. Ref. Data* **31**, 819 (2002)

D. Hong and C. Fleurier, *Spectral Line Shapes*, edited by R. Stamm and B. Talin, Nova Science, Commack, NY, Vol. 7, pp. 123-124 (1993)

R. Kobilarov and N. Konjević, *Phys. Rev.* A 41, 6023 (1990)

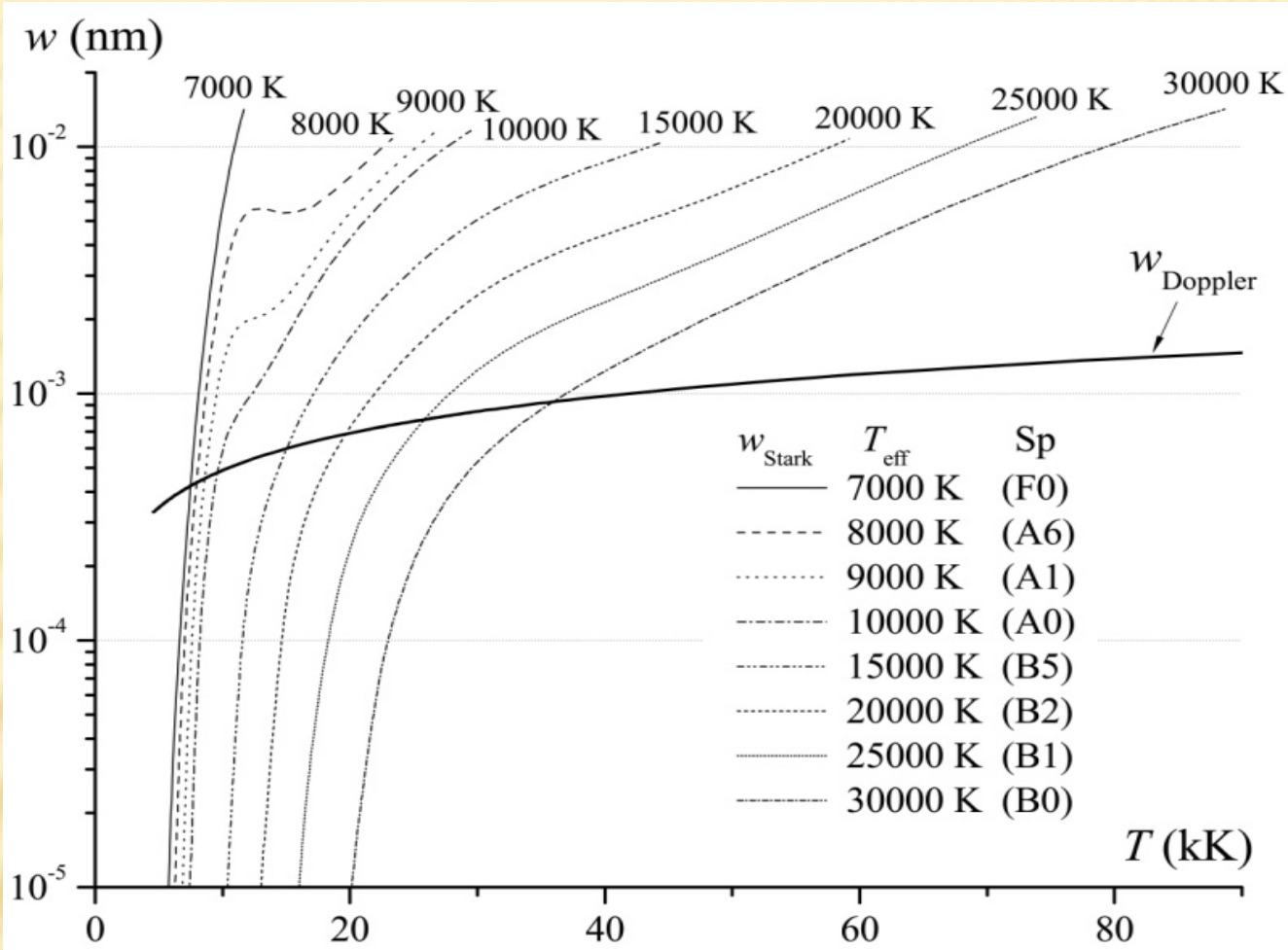
S. Đeniže, A. Srećković, M. Platiša, R. Konjević, J. Labat and J. Purić, *Phys. Rev.* A 42, 2379 (1990)

M. S. Dimitrijević, S. Đeniže, A. Srećković and M. Platiša, *Phys. Scr.* 53, 545 (1996)

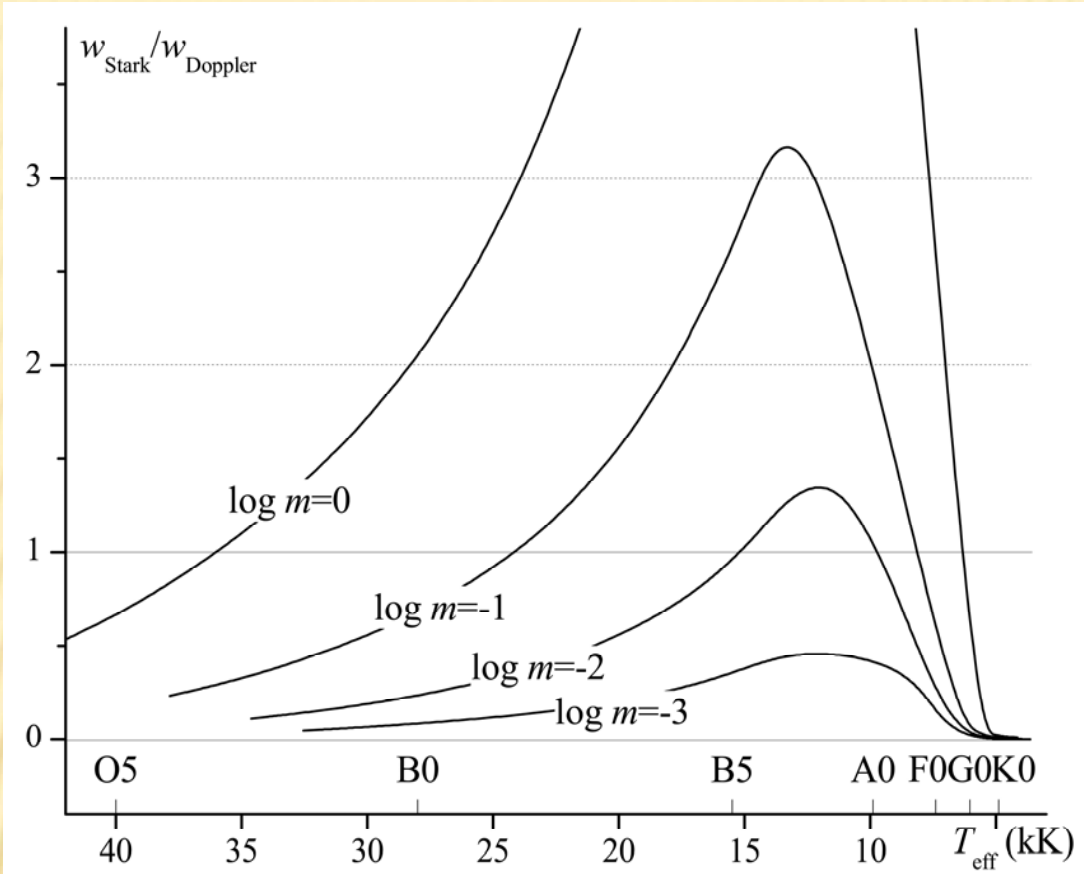
DISCUSSION

Behavior of Stark and Doppler spectral line widths in stellar atmospheres were calculated for **S III λ=250.815 nm**, a strong spectral line, in various atmospheric models. These calculations were performed for solar element abundance atmospheric models given in Kurucz (1979) and Kurucz's web site (http://kurucz.harvard.edu).

Each model is characterized by the effective temperature T_{eff}, logarithm of gravity log g and turbulent velocity vt and each atmospheric layer within the model is characterized by electron density N and temperature T.



Stark widths (FWHM) (thinner lines) and Doppler width (thicker line) for S III spectral line as a function of atmospheric layer temperatures. Stark widths are shown for 8 atmospheric models with effective temperatures T_{eff} =7 – 30 kK, corresponding to spectral classes (Sp) from F0 to B0, log g=4 and turbulent velocity v_t =0 km/s.



Ratio of Stark and Doppler widths $w_{Stark}/w_{Doppler}$ as a function of the model effective temperature T_{eff} (upper part of horizontal axis is spectral class). Dependence is shown for 4 values of logarithm of the column mass at temperature minimum log m from 0 to -3, log g=4 and velocity v_t=0 m/s.

CONCLUSION

This method of Stark width calculation can be widely used in getting more accurate results were extensive set of data are needed.

Thank you