Mem. S.A.It. Suppl. Vol. 15, 148

Memorie della
Supplementi

Ab initio calculations of Ca V Stark broadening parameters

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Abstract. We have determined Stark broadening parameters for 8 Ca V multiplets by using the semiclassical perturbation approach. The calculations have been performed ab initio, since energy levels and oscillator strengths are calculated using SUPERSTRUCTURE code. The obtained results are presented as a function of temperature, for perturber density of 10^{17} cm^{-3}. In order to provide Stark broadening data for the most important charged perturbers in stellar atmospheres, electron-, proton-, and ionized helium-impact full halfwidths and shifts have been calculated. There is no other theoretical or experimental Stark broadening data for Ca V for comparison and new Stark broadening parameters calculations and measurements will be of interest for comparison with our calculations.

Key words. atomic processes – line: profiles – atomic data

1. Introduction

Stark broadening mechanism is important for the investigation, analysis, and modelling of B-type, and particularly A-type stellar atmospheres as well as for white dwarf atmospheres. In Popović et al. (2001), the influence of Stark broadening on Nd II lines in A-type stellar atmospheres was investigated. It was demonstrated that neglecting this mechanism introduces an error between 10% and 45% in the equivalent width determination and influences on abundance values. Hamdi et al. (2008) investigated the influence of Stark broadening on Si VI lines in DO white dwarf spectra. It was found that this mechanism is dominant in broad regions of the atmospheres considered.

Spectral analysis by means of NLTE model atmospheres has presently arrived at a high level of sophistication, which is now hampered largely by the lack of reliable atomic data and accurate line-broadening tables. Strong efforts should be made to improve upon this situation (Rauch et al. 2007).

Ca V belongs to the sulfure-like sequence, its ground state configuration is [Ne]3s^{2}3p^4

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with the term ^{3}P. The cosmic abundance of calcium is 2×10^{-6} by number relative to hydrogen (Allen 1973), and lines emitted by neutral and ionized calcium are visible in astrophysical spectra. In particular, Calcium lines are detected in the atmospheres of white dwarfs (see Zuckerman et al. (2003), for example). Recently, calcium in higher ionization stage (Ca X) is observed in photosphere of the hot white dwarf KPD 0005+5106 (Werner, Rauch, & Kruk 2008). Ca V lines are introduced in atmospheric model used by Rauch et al. (2007) to study the white dwarf central star of Sh 2-216 planetary nebula.

The aim of this work is to provide ab initio calculations of Stark broadening parameters of Ca V lines. In addition to electron-impact full halfwidths and shifts, Stark broadening parameters due to proton- and ionized helium-impacts have been calculated. Thus, we have provided Stark broadening data for all the important charged perturbers in stellar atmospheres. In previous papers (Ben Nessib, Dimitrijević, & Sahal-Bréchot 2004; Hamdi et al. 2007), we have calculated Stark broadening parameters of Si V and Ne V using SUPERSTRUCTURE and Bates & Damgaard (1949) method for oscillator strengths. It was found that the difference is tolerable.

2. The method

The energy levels and oscillator strengths were carried out with the general purpose atomic structure program SUPERSTRUCTURE (Eissner, Jones, & Nussbaumer 1974), as modified by Nussbaumer & Storey (1978). The adopted atomic model for Ca V includes 12 configurations $3s^23p^4$, $3s3p^5$, $3s^23p^33d$, $3s^23p^34\ell$, $3s^23p^35\ell$ ($\ell \leq n-1$). The wave functions are of configuration mixing type, and each configuration is expanded in terms of Slater States. The radial functions are calculated in scaled Thomas-Fermi statistical model potential, which depends on parameters λ_{nl} determined variationally by optimizing the weighted sum of energy terms. Scaling parameters used in this work are λ_{1s}=1.4368, λ_{2s}=1.1125, λ_{2p}=1.0540, λ_{3s}=1.1460, λ_{3p}=1.1346, λ_{3d}=1.1080, λ_{4s}=1.1491, λ_{4p}=1.1144, λ_{4d}=1.1249, λ_{4f}=1.2739, λ_{5s}=1.1581, λ_{5p}=1.1285, λ_{4d}=1.14699, λ_{4f}=1.9600, λ_{5g}=1.800. Relativistic corrections are introduced by means of Breit-Pauli approximation in intermediate coupling.

We have calculated mean radii and mean square radii within the hydrogenic approximation with a quantum defect, using the effective quantum numbers n_i^* obtained from the Ritz formula.

Stark broadening parameter calculations have been performed within the semiclassical perturbation method (Sahal-Bréchot 1969a,b). This formalism has been reviewed briefly .e.g. in (Hamdi et al. 2008).

3. Results and discussion

By combining the SUPERSTRUCTURE code for calculating energy levels and oscillator strengths and the code for the Stark broadening calculations, we calculated ab initio Stark broadening parameters. Calculated Stark broadening widths [full width at half-maximum (FWHM)] and shifts for a perturber density of 10^{17}cm^{-3} and temperature from 50 000 K to 500 000 K are shown in Table 1 for electron-, proton-and singly ionized helium-impact broadening. Such temperatures are of interest for modelling of some hot star atmospheres. Higher temperatures are of interest for fusion plasma as well as for stellar interiors. We also specify a parameter C (Dimitrijević & Sahal-Bréchot 1984), which gives an estimate for the maximal perturber density for which the line may be treated as isolated, when it is divided by the corresponding full width at half maximum. For each value given in Table 1 the collision volume V multiplied by the perturber density N is much less than one and the impact approximation is valid (Sahal-Bréchot 1969a,b). When the impact approximation is not valid, the ion broadening contribution may be estimated by using the quasi-static approach (Sahal-Bréchot 1991). In the region where neither approximation is valid, a unified-type theory should be used. For example, in Barnard, Cooper, & Smith (1974)

Table 1. This table gives electron-, proton and singly-charged helium-impact broadening parameters for Ca V lines calculated using SUPERSTRUCTURE oscillator strength, for a perturber density of 10^{17} cm^{-3} and temperatures from 50000 to 500000 K. Transitions, averaged wavelength for the multiplet (in Å) and parameter C are also given. This parameter when divided with the corresponding Stark width gives an estimate for the maximal pertuber density for which the line may be treated as isolated. w_e: electron-impact full Stark width at half maximum, d_e: electron-impact Stark shift, w_{H^+}: proton-impact full Stark width at half maximum, d_{H^+}: proton-impact Stark shift, w_{He^+}: singly charged helium-impact full Stark width at half maximum, d_{He^+}: singly charged helium-impact Stark shift.

Transition	T(kK)	w_e	d_e	w_{H^+}	d_{H^+}	w_{He^+}	d_{He^+}
$3p^4\ ^3P$-$3s3p^5\ ^3P^\circ$	50.	0.19E-2	-0.28E-3	0.76E-5	-0.95E-5	0.14E-4	-0.94E-5
694.6 Å	100.	0.14E-2	-0.17E-3	0.20E-4	-0.18E-4	0.30E-4	-0.18E-4
C= 0.69E+20	150.	0.11E-2	-0.14E-3	0.30E-4	-0.26E-4	0.42E-4	-0.24E-4
	200.	0.95E-3	-0.14E-3	0.40E-4	-0.31E-4	0.49E-4	-0.28E-4
	300.	0.78E-3	-0.12E-3	0.51E-4	-0.39E-4	0.61E-4	-0.34E-4
	500.	0.62E-3	-0.11E-3	0.70E-4	-0.50E-4	0.72E-4	-0.42E-4
$3p^4\ ^1D$-$3s3p^5\ ^1P^\circ$	50.	0.12E-2	-0.82E-4	0.70E-5	-0.51E-5	0.13E-4	-0.51E-5
591.6 Å	100.	0.87E-3	-0.52E-4	0.17E-4	-0.10E-4	0.26E-4	-0.97E-5
C= 0.48E+20	150.	0.71E-3	-0.47E-4	0.25E-4	-0.14E-4	0.35E-4	-0.13E-4
	200.	0.62E-3	-0.49E-4	0.33E-4	-0.17E-4	0.41E-4	-0.16E-4
	300.	0.51E-3	-0.47E-4	0.41E-4	-0.23E-4	0.50E-4	-0.19E-4
	500.	0.41E-3	-0.46E-4	0.54E-4	-0.29E-4	0.57E-4	-0.25E-4
$3p^4\ ^1D$-$3p^3(^2D)3d\ ^1D^\circ$	50.	0.63E-3	-0.30E-4	0.16E-5	-0.19E-5	0.29E-5	-0.19E-5
433.7 Å	100.	0.43E-3	-0.18E-4	0.42E-5	-0.38E-5	0.67E-5	-0.37E-5
C= 0.30E+20	150.	0.35E-3	-0.16E-4	0.68E-5	-0.55E-5	0.98E-5	-0.52E-5
	200.	0.30E-3	-0.18E-4	0.90E-5	-0.69E-5	0.12E-4	-0.64E-5
	300.	0.25E-3	-0.18E-4	0.13E-4	-0.91E-5	0.15E-4	-0.79E-5
	500.	0.20E-3	-0.18E-4	0.17E-4	-0.12E-4	0.19E-4	-0.10E-4
$3p^4\ ^3P$-$3p^3(^2P)3d\ ^3D^\circ$	50.	0.59E-3	-0.39E-4	0.12E-5	-0.21E-5	0.23E-5	-0.21E-5
376.5 Å	100.	0.39E-3	-0.24E-4	0.34E-5	-0.40E-5	0.54E-5	-0.39E-5
C= 0.20E+20	150.	0.32E-3	-0.22E-4	0.56E-5	-0.57E-5	0.79E-5	-0.53E-5
	200.	0.27E-3	-0.22E-4	0.74E-5	-0.70E-5	0.97E-5	-0.65E-5
	300.	0.22E-3	-0.21E-4	0.10E-4	-0.91E-5	0.12E-4	-0.78E-5
	500.	0.18E-3	-0.20E-4	0.14E-4	-0.12E-4	0.16E-4	-0.99E-5
$3p^4\ ^3P$-$3p^3(^2P)3d\ ^3P^\circ$	50.	0.58E-3	-0.37E-4	0.12E-5	-0.20E-5	0.23E-5	-0.20E-5
375.6 Å	100.	0.39E-3	-0.23E-4	0.38E-5	-0.40E-5	0.54E-5	-0.38E-5
C= 0.20E+20	150.	0.32E-3	-0.21E-4	0.56E-5	-0.56E-5	0.78E-5	-0.52E-5
	200.	0.27E-3	-0.21E-4	0.74E-5	-0.69E-5	0.97E-5	-0.64E-5
	300.	0.22E-3	-0.20E-4	0.10E-4	-0.90E-5	0.12E-4	-0.77E-5
	500.	0.18E-3	-0.20E-4	0.14E-4	-0.11E-4	0.15E-4	-0.98E-5
$3p^4\ ^3P$-$3p^3(^2D)3d\ ^3S^\circ$	50.	0.53E-3	-0.56E-4	0.12E-5	-0.18E-5	0.23E-5	-0.18E-5
343.6 Å	100.	0.38E-3	-0.33E-4	0.33E-5	-0.35E-5	0.52E-5	-0.33E-5
C= 0.12E+20	150.	0.31E-3	-0.28E-4	0.53E-5	-0.49E-5	0.75E-5	-0.45E-5
	200.	0.27E-3	-0.28E-4	0.70E-5	-0.60E-5	0.91E-5	-0.55E-5
	300.	0.22E-3	-0.25E-4	0.96E-5	-0.78E-5	0.11E-4	-0.67E-5
	500.	0.18E-3	-0.22E-4	0.13E-4	-0.98E-5	0.14E-4	-0.85E-5

Table 1. continued

Transition	T(kK)	w_e	d_e	w_{H^+}	d_{H^+}	w_{He^+}	d_{He^+}
$3p^4\ ^3P$-$3p^3(^2D)3d\ ^3P^\circ$	50.	0.48E-3	-0.84E-4	0.13E-5	-0.19E-5	0.24E-5	-0.19E-5
322.1 A	100.	0.35E-3	-0.47E-4	0.34E-5	-0.37E-5	0.53E-5	-0.35E-5
C= 0.11E+20	150.	0.29E-3	-0.40E-4	0.54E-5	-0.51E-5	0.75E-5	-0.47E-5
	200.	0.25E-3	-0.38E-4	0.72E-5	-0.63E-5	0.90E-5	-0.57E-5
	300.	0.21E-3	-0.34E-4	0.96E-5	-0.79E-5	0.11E-4	-0.69E-5
	500.	0.17E-3	-0.28E-4	0.13E-4	-0.10E-4	0.14E-4	-0.86E-5
$3p^4\ ^3P$-$3p^3(^4S)3d\ ^3D^\circ$	50.	0.47E-3	-0.70E-4	0.13E-5	-0.15E-5	0.24E-5	-0.15E-5
316.2 A	100.	0.34E-3	-0.38E-4	0.33E-5	-0.30E-5	0.52E-5	-0.29E-5
C= 0.75E+19	150.	0.28E-3	-0.33E-4	0.53E-5	-0.42E-5	0.74E-5	-0.39E-5
	200.	0.24E-3	-0.32E-4	0.69E-5	-0.52E-5	0.87E-5	-0.48E-5
	300.	0.20E-3	-0.28E-4	0.91E-5	-0.67E-5	0.11E-4	-0.58E-5
	500.	0.16E-3	-0.24E-4	0.12E-4	-0.85E-5	0.13E-4	-0.73E-5

a simple analytical formula for such a case is given.

We see that using the SUPERSTRUCTURE code one obtains a set of energy levels and oscillator strengths, enabling an ab initio calculation of Stark broadening parameters. This is suitable especially for multicharged ions when other theoretical and experimental atomic data are scare. The Stark broadening parameters obtained here, contribute to the creation of a set of such data for as large as possible number of spectral lines, of significance for a number of problems in astrophysics. As for example, spectral analysis by means of NLTE model atmospheres, that need a large set of atomic data and accurate line-broadening tables.

There is no other theoretical or experimental Stark broadening data for Ca V for comparison and new Stark broadening parameters calculations and measurements will be of interest for comparison with our calculations.

Acknowledgements. This work is a part of the Project 146 001 Influence of collisional processes on astrophysical plasma lineshapes, supported by the Ministry of Science and Technological Development of Serbia.

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