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Stark broadening of Fe XXV spectral lines

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ABSTRACT

Stark broadening parameters, full widths at half-maximum of intensity and shifts for 18 spectral lines of Fe XXV, broadened by collisions with electrons, protons, and Fe XXVII ions, have been calculated using the impact semiclassical perturbation formalism for a grid of electron densities and temperatures of interest for neutron star atmospheres and their environment.

Key words: atomic data – atomic processes – line: formation – stars: neutron.

1 INTRODUCTION

Broadening of spectral lines from stellar and laboratory plasmas by interaction with charged particles, called Stark broadening, is often important for hot and dense plasmas. The corresponding Stark widths and shifts of spectral lines are particularly needed and used in astrophysics for different investigations. They are also needed for examination and modelling of neutron star atmospheres and their environment. We notice that up to now, in the case of neutron stars, Stark broadening was taken into account only by using approximate methods, and only for the case of non-magnetic neutron stars.

For example, Paerels (1997) developed a method enabling to measure simultaneously masses and radii of neutron stars on the basis of observations of gravitational redshift and spectral line width, using an approximate method for Stark broadening of hydrogen lines. Madej (1989) and Majczyna et al. (2005), in their models of neutron star atmospheres and iron-rich spectra, used for Stark broadening calculations, approximate formula from Griem (1974, chapter IV, section 6), without magnetic field effects. Suleimanov et al. (2014), in their modelling of carbon neutron star atmospheres, considered the Stark broadening using very approximate formula of Cowley (1971) and magnetic field effects are neglected.

In the case of neutron stars, particularly important are highly ionized iron lines. For example, Cottam, Paerels & Mendez (2002) detected X-ray burst spectra of EXO 0748−676, with a Fe XXV feature ($n = 2$–3 transition). Moreover, Werner et al. (2007) presented detailed spectrum synthesis calculation of neutron star atmospheres, without an analysis of Stark broadening of considered lines, and in the obtained synthetic spectrum are present iron lines from Fe XVII up to Fe XXVI, including Fe XXV. Besides the atmosphere modelling and neutron star spectra analysis and synthesis, Stark broadening of helium-like Fe XXV spectral lines is of interest and for investigations of plasma in environment of neutron stars (see e.g. van Peet et al. 2009) and plasma diagnostics in attempts to create neutron star plasma conditions in laboratory (Moon et al. 2005).

Wishing to provide data for better analysis and synthesis of Fe XXV spectral lines from neutron star spectra, we calculated widths and shifts of 18 Fe XXV spectral lines broadened by electron-, proton-, and Fe XXVII ion-impacts, for temperatures 300 000–20 000 000 K, and perturber densities (10^{17}–10^{24} cm^{-3}), for plasma conditions of particular interest for neutron star atmospheres and their environments.

2 THE IMPACT SEMICLASSICAL PERTURBATION METHOD

For the calculation of helium-like Fe XXV Stark broadening parameters, the semiclassical perturbation formalism (Sahal-Bréchot 1969a,b) has been employed (later innovations may be found in Sahal-Bréchot 1974, 1991; Fleurier, Sahal-Bréchot & Chapelle 1977; Dimitrijević, Sahal-Bréchot & Bommier 1991; Dimitrijević & Sahal-Bréchot 1996; Sahal-Bréchot, Dimitrijević & Ben Nessib 2014; see also various applications in Dimitrijević & Sahal-Bréchot 2014). The method is described many times and only basic formulas will be given here. Full width at half-maximum of intensity (FWHM), W, and the shift (d) of an isolated spectral line of a non-hydrogenic ion are

$$W = N \int \upsilon f(\upsilon)\, \mathrm{d}\upsilon \left(\sum_{i' \neq i} \sigma_{ii'}(\upsilon) + \sum_{f' \neq f} \sigma_{ff'}(\upsilon) + \sigma_{\mathrm{el}} \right),$$

$$d = N \int \upsilon f(\upsilon)\, \mathrm{d}\upsilon \int_{R_3}^{R_D} 2\pi\rho\, \mathrm{d}\rho \sin(2\varphi_{\mathrm{p}}). \quad (1)$$

Here, with i and f are denoted initial and final level of the investigated transition, i' and f' are the energy levels that perturb levels i and f, N is the density of perturbers, υ the perturber velocity, $f(\upsilon)$ the Maxwellian velocity distribution, and ρ the impact parameter of the perturber influencing the emitting ion.

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Table 1. Electron-, proton-, and Fe XXVII ion-impact broadening parameters for Fe XXV lines, calculated using energy levels from NIST data base (Sugar & Corliss 1985; Shirai et al. 2000; Kramida et al. 2021). The wavelengths of the spectral lines (in Å), theoretically determined, and the quantity C are provided as well. If this quantity is divided with Stark width, one obtains maximal perturber density for which one can take that the line is isolated. The notation for transitions is given in an abbreviated form, so that e.g. 2s1-2p0 is for $2s^3S_1$-$2p^3P^o_0$. The Stark broadening parameters for 18 Fe XXV spectral lines are given as Supplementary Material in the online edition of this journal, as Tables S1–S8, for perturber densities 10^{17}–10^{24} cm^{-3}, respectively. Data are provided for temperatures from 300 000 to 20 000 000 K. As in our previous papers the sign of the shift is positive, if the line is shifted in direction of the higher wavelengths. Data for three spectral lines from Table S4, for a perturber density of 10^{20} cm^{-3}, are shown below in order to show the form and content of Tables S1–S16.

Perturber density =	1E+20 cm^{-3}						
		Electrons		Protons		Fe XXVII ions	
Transition	T (K)	Width (Å)	Shift (Å)	Width (Å)	Shift (Å)	Width (Å)	Shift (Å)
Triplets							
Fe XXV 2s1-2p0	300 000	0.442E-01	0.336E-02	0.772E-06	– 0.319E-04	0.515E-08	– 0.186E-06
428.2 Å	500 000	0.295E-01	0.428E-03	0.173E-05	– 0.618E-04	0.101E-05	– 0.447E-04
C = 0.43E+23	1000 000	0.207E-01	– 0.855E-04	0.538E-05	– 0.135E-03	0.189E-04	– 0.102E-02
	5000 000	0.101E-01	– 0.178E-03	0.179E-03	– 0.677E-03	0.112E-02	– 0.164E-01
	10 000 000	0.731E-02	– 0.169E-03	0.718E-03	– 0.116E-02	0.702E-02	– 0.338E-01
	20 000 000	0.533E-02	– 0.149E-03	0.183E-02	– 0.167E-02	0.254E-01	– 0.587E-01
Fe XXV 2s1-2p1	300 000	0.386E-01	0.294E-02	0.677E-06	– 0.273E-04	0.450E-08	– 0.159E-06
400.3 Å	500 000	0.258E-01	0.375E-03	0.152E-05	– 0.529E-04	0.883E-06	– 0.383E-04
C = 0.37E+23	1000 000	0.181E-01	– 0.736E-04	0.470E-05	– 0.116E-03	0.164E-04	– 0.872E-03
	5000 000	0.883E-02	– 0.154E-03	0.152E-03	– 0.581E-03	0.952E-03	– 0.140E-01
	10 000 000	0.639E-02	– 0.147E-03	0.609E-03	– 0.993E-03	0.598E-02	– 0.290E-01
	20 000 000	0.466E-02	– 0.130E-03	0.156E-02	– 0.144E-02	0.216E-01	– 0.504E-01
Fe XXV 2s1-3p0	300 000	0.743E-04	– 0.184E-05	0.155E-07	0.797E-09	0.902E-10	0.465E-11
10.0 Å	500 000	0.579E-04	– 0.388E-06	0.341E-07	0.155E-08	0.183E-07	0.112E-08
C = 0.65E+19	1000 000	0.414E-04	– 0.565E-07	0.978E-07	0.339E-08	0.324E-06	0.255E-07
	5000 000	0.196E-04	0.138E-07	0.139E-05	0.176E-07	0.561E-05	0.411E-06
	10 000 000	0.145E-04	0.180E-07	0.316E-05	0.351E-07	0.141E-04	0.888E-06
	20 000 000	0.108E-04	0.151E-07	0.568E-05	0.664E-07	0.278E-04	0.181E-05

In order to calculate the inelastic cross-sections $\sigma_{kk'}(\upsilon)$, $k = i, f$, one should integrate the transition probability $P_{kk'}(\rho, \upsilon)$ over ρ:

$$\sum_{k'\neq k} \sigma_{kk'}(\upsilon) = \frac{1}{2}\pi R_1^2 + \int_{R_1}^{R_D} 2\pi\rho \, \mathrm{d}\rho \sum_{k'\neq k} P_{kk'}(\rho, \upsilon). \quad (2)$$

The elastic cross-section σ_{el} is

$$\sigma_{\rm el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi\rho \, \mathrm{d}\rho \sin^2\delta + \sigma_{\rm r},$$

$$\delta = (\varphi_{\rm p}^2 + \varphi_{\rm q}^2)^{\frac{1}{2}}. \quad (3)$$

Here $\varphi_{\rm p}$ (r^{-4}) and $\varphi_{\rm q}$ (r^{-3}) are phase shifts due to the polarization and quadrupolar potential (see section 3 of chapter 2 in Sahal-Bréchot 1969a). The symmetrization procedure and cut-offs R_1, R_2, R_3, and R_D are described in section 1 of chapter 3 in Sahal-Bréchot (1969b). The method for calculation of the contribution of Feshbach resonances σ_r is explained in Fleurier et al. (1977) and Sahal-Bréchot (2021). Since for perturbing ions the Coulomb force is not attractive but repulsive, formulas are analogous but trajectories are different and there is no contribution of Feshbach resonances.

Knowing Stark broadening parameters, line width W and shift d, it is easy to obtain the line profile $F(\omega)$, which has a Lorentzian form

$$F(\omega) = \frac{W/(2\pi)}{(\omega - \omega_{\rm if} - d)^2 + (W/2)^2}. \quad (4)$$

Here

$$\omega_{\rm if} = \frac{E_{\rm i} - E_{\rm f}}{\hbar},$$

where $E_{\rm i}$, $E_{\rm f}$ are the energies of initial and final atomic energy level, respectively.

3 RESULTS AND DISCUSSION

By employing the semiclassical perturbation theory (Sahal-Bréchot 1969a,b), we performed calculations of electron-, proton-, and Fe XXVII ion-impact broadening parameters, FWHM (W) and shift (d) for 18 spectral lines of helium-like Fe XXV. The results are obtained for temperatures of 300 000, 500 000, 1000 000, 5000 000, 10 000 000, and 20 000 000 K for perturber densities from 10^{17} to 10^{24} cm^{-3}.

The set of atomic energy levels needed for computation of Stark line widths and shifts for Fe XXV lines has been taken from Sugar & Corliss (1985), Shirai et al. (2000), and Kramida et al. (2021), while for the calculation of oscillator strengths, the Coulomb approximation of Bates & Damgaard (1949) and tables of Oertel & Shomo (1968) have been used. For transitions involving higher energy levels, when the method of Bates & Damgaard (1949) is not suitable, the approach of van Regemorter, Binh Dy & Prudhomme (1979) has been used.

The results for Stark FWHM and shift for 18 Fe XXV spectral lines broadened by electron-, proton- and Fe XXVII ion-impacts are provided in Supplementary Material, as Tables S1–S8, in online published journal volume. They are presented for perturber densities within the interval between 10^{17} cm^{-3} (Table S1) and 10^{24} cm^{-3} (Table S6). For the sake of demonstration of the form of calculated Stark line widths and shifts, which are provided in Supplementary Material, the results for three lines are given in Table 1, as an example.

One should be taken into account that the values of wavelengths presented in all tables are obtained on the basis of atomic energy levels, so that they may be not the same as the observed or experimental ones. If the correction of this difference is needed,

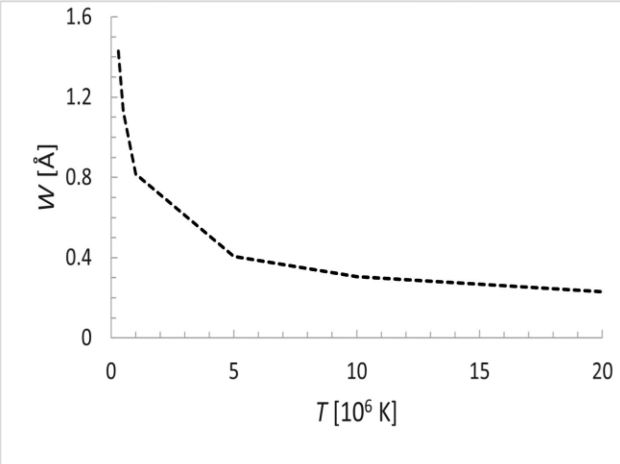

Figure 1. Behaviour of Stark width of Fe XXV $3s^1S$-$3p^1P^o$ spectral line with temperature. Electron density is 10^{20} cm^{-3}.

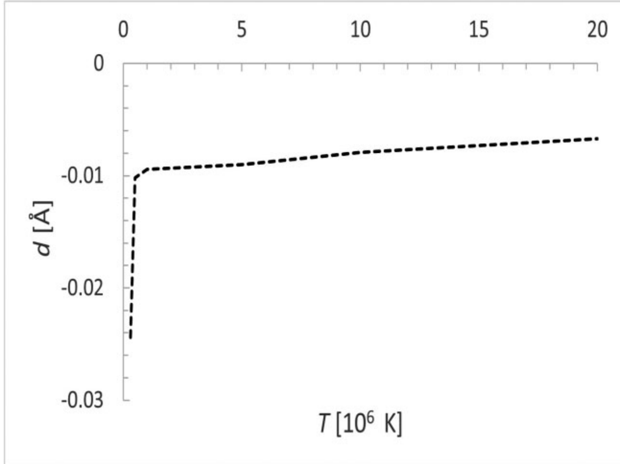

Figure 2. Behaviour of Stark shift of Fe XXV $3s^1S$-$3p^1P^o$ spectral line with temperature. Electron density is 10^{20} cm^{-3}.

it can be done for the width, or in analogous manner for the shift as

$$W_{\rm cor} = \left(\frac{\lambda_{\rm exp}}{\lambda}\right)^2 W. \quad (5)$$

Here, $W_{\rm cor}$ is the corrected width, $\lambda_{\rm exp}$ is the experimental, λ the calculated wavelength, and W the width from tables in this paper.

The provided quantity C (Dimitrijević & Sahal-Bréchot 1984), from Tables S1 to S16, should be divided with the relevant width (W) in order to obtain the highest density of the corresponding perturbing charged particles when the line may be considered as isolated. Concerning the impact approximation, its validity is verified calculating the product of the collision volume V and the perturber density N, namely NV. In the case of $NV < 0.1$, one can take that the impact approximation is valid (Sahal-Bréchot 1969a,b). On the other hand, when $NV > 0.5$, the corresponding results for Stark widths and shifts are not given, and their place is empty in the tables, since the condition for validity of the impact approximation is not satisfied. For $0.1 < NV \leq 0.5$, in front of the relevant Stark widths and shifts an asterisk is put, as a signal that this value is on the limit of validity of impact approximation.

When the impact approximation is not valid, which is more frequently for the case of ion perturbers, Stark broadening parameters can be calculated using the quasi-static approach (Griem 1974; Sahal-Bréchot 1991). If neither impact nor quasi-static approximation is valid, a unified-type theory, as for example the theoretical approach from the paper of Barnard, Cooper & Smith (1974), may be employed.

In Figs 1 and 2, the behaviour of Stark width and shift of Fe XXV $3s^1S$-$3p^1P^o$ spectral line with temperature is shown. One can see that in the case of the Stark width, it decreases sharply at low temperatures, where elastic collisions dominate, while for higher temperatures, where the contribution of inelastic collisions is dominant, the change of width values with temperature is weak. The behaviour of shift with temperature is similar. For lowest temperatures the change is fast and after, for higher, slow.

In Fig. 3, we present behaviour of electron-, proton-, and Fe XXVII-impact width of Fe XXV $3s^1S$-$3p^1P^o$ spectral line with temperature. One can see that for lower temperatures, broadening by collisions with protons and Fe XXVII ions is negligible in comparison

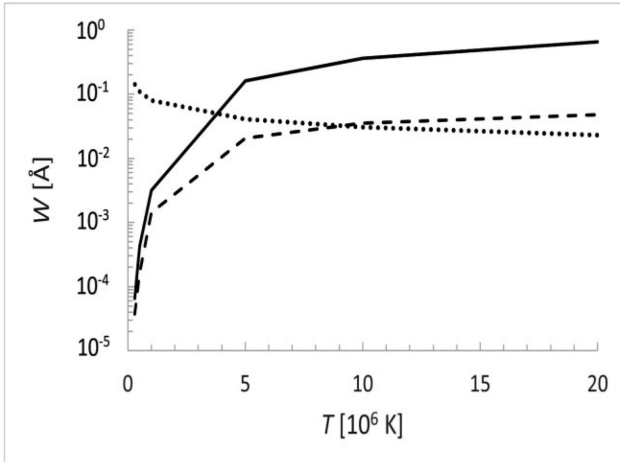

Figure 3. Behaviour of electron-impact (dotted line), proton-impact (dashed line), and Fe XXVII-impact (solid line) width of Fe XXV $3s^1S$-$3p^1P^o$ spectral line with temperature. Perturber density is 10^{19} cm^{-3}.

with electron-impact broadening. On the other hand, for higher temperatures, the broadening by collisions with Fe XXVII ions becomes dominant and its influence increases with temperature. For temperatures higher than 5000 000 K even proton broadening becomes comparable with electron broadening and with the increase of temperature becomes more important. We can conclude that for conditions in neutron star atmospheres ion broadening is very important.

4 CONCLUSIONS

We calculated Stark broadening parameters, FWHM W and shift d for 18 spectral lines of Fe XXV, by employing the semiclassical perturbation formalism. For these lines there are no other theoretical or experimental results. The results obtained in this work are of interest for investigation and modelling of neutron star atmospheres and their environment, as well as the analysis and synthesis of their spectra. These results may also be useful for analysis of iron impurities and additions in inertial fusion plasma. The calculated Stark widths and shifts for Fe XXV spectral lines will be also implemented in the STARK-B data base (Sahal-Bréchot 2010; Sahal-Bréchot, Dimitrijević & Moreau 2012, 2022; Sahal-Bréchot et al. 2015), a part of Virtual Atomic and Molecular Data Center (VAMDC; Dubernet et al. 2010, 2016; Albert et al. 2020).

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DATA AVAILABILITY

The data underlying this paper are available in the paper and in its online Supplementary Material.

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SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

Table 1 S1_FeXXV-17
Table 2 S2_FeXXV-18
Table 3 S3_FeXXV-19
Table 4 S4_FeXXV-20
Table 5 S5_FeXXV-21
Table 6 S6_FeXXV-22
Table 7 S7_FeXXV-23
Table 8 S8_FeXXV-24