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THE COMPLETE CALCULATION OF STARK BROADENING PARAMETERS FOR THE NEUTRAL COPPER ATOMS SPECTRAL LINES OF 4s ^{2}S-4p ^{2}P^0 AND 4s^2 ^{2}D-4p ^{2}P^0 MULTIPLETS IN THE DIPOLE APPROXIMATION

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Abstract. The complete calculation of Stark broadening parameters for the neutral copper atoms spectral lines of 4s ^{2}S-4p ^{2}P^0 and 4s^2 ^{2}D-4p ^{2}P^0 multiplets in the dipole approximation according to Cooper and Oertel (1969) is carried out in which the necessary coordinate operator matrix elements have been found through the known experimental absorption oscillator strengths. The importance of taking into account such aspects as the ''back reaction'' of copper atom on perturbers (electrons) in inelastic collisions and corrections to the broadening function in the classical-path approximation ($\hat{\lambda}$ cutoff) is discussed.

The knowledge of the Stark broadening parameters of the copper atoms spectral lines is of great interest for the diagnostics of the laboratory and astrophysical plasmas. However for the row of the important spectral lines to which the spectral lines of 4s ^{2}S-4p ^{2}P^0 multiplet (Cu I 324.754 nm and Cu I 327.396 nm resonance spectral lines) and 4s^2 ^{2}D-4p ^{2}P^0 multiplet (Cu I 510.554 nm, Cu I 570.024 nm and Cu I 578.213 nm spectral lines) we do not have yet enough reliable experimental data and the theoretical data obtained on the basis of the quantum-mechanical calculations. In this paper the new theoretical values of the parameters for the mentioned lines are presented.

The theoretical values of the Stark broadening parameters of the copper atoms spectral lines of 4s ^{2}S-4p ^{2}P^0 and 4p ^{2}P^0 multiplets have been presented by Konjević and Konjević (1986), Dimitrijević *et al.* (1996), Grishina *et al.* (1998a, 1988b, 1999) and Sibgatullin *et al.* (2000). In Konjević and Konjević (1986) the quantum-mechanical calculations have been carried out for the first time in the dipole approximation for the lines of 4s^2 ^{2}D-4p ^{2}P^0 multiplet by using simplified semiclassical formulae given by Dimitrijević and Konjević (1986) in which the necessary coordinate operator matrix elements taking account of the interaction of the different energetic levels have been found in the Coulomb approximation. In Dimitrijević *et al.* (1996), Grishina *et al.* (1998a, 1998b, 1999) and Sibgatullin *et al.* (2000) the quantum-mechanical calculations in the dipole approximation have been carried out with more rigorous representation of the coordinate operator matrix elements through the known experimental absorption oscillator strength that has allowed for the first time to carry out the calculations also for the resonance spectral lines of 4s ^{2}S-4p ^{2}P^0 multiplet for which the Coulomb approximation is customary unacceptable in the case of heavy atoms. Thereby favourable circumstances have contributed that for the spectral lines of 4s ^{2}S-4p ^{2}P^0 and 4s^2 ^{2}D-4p ^{2}P^0 multiplets of the neutral copper atoms the perturbing levels are

sufficiently widely spaced from the disturbed levels and between the levels the convenient transitions for the experimental investigations are possible which fall in UV- and visible region of the spectrum.

Table 1. The Stark widths of the Cu I spectral lines for $n_e=10^{17}$ см$^{-3}$.

λ, nm	T, K	$2\omega_e$, nm (2)/(1)	$2\omega_e$, nm (3)	A (2)/(1)	A (3)	ω_{tot}, nm (2)/(1)	ω_{tot}, nm (3)
	5000	0.0117 (0.0103)	0.00846	0.0450 (0.0498)	0.0575	0.0120 (0.0105)	0.0088
	10000	0.0122 (0.0126)	0.0099	0.0436 (0.0427)	0.0512	0.0127 (0.0131)	0.0139
510.554	20000	0.0139 (0.0156)	0.0123	0.0396 (0.0362)	0.0435	0.0146 (0.0163)	0.0129
	30000	0.0161 (0.0177)	0.0142	0.0364 (0.0311)	0.0390	0.0163 (0.0184)	0.0149
324.754	17000	0.00473 (0.00567)	0.00401	0.0350 (0.0301)	0.0396	0.00520 (0.00627)	0.00419*
	5000	0.00403 (0.00332)	0.00267	0.0357 (0.0413)	0.0485	0.00412 (0.00339)	0.00276
	10000	0.00400 (0.00433)	0.00304	0.0359 (0.0338)	0.0440	0.00414 (0.00447)	0.00317
327.396	20000	0.00475 (0.00581)	0.00408	0.0315 (0.0271)	0.0354	0.00493 (0.00600)	0.00425
	30000	0.00563 (0.00687)	0.00508	0.0278 (0.0239)	0.0300	0.00583 (0.00708)	0.00527

(1) - in the brackets (...) the calculation results of the works (Grishina, Il'in *et al.* 1998a, 1998b) are presented without the accounting for the ''back reaction'' and $\hat{\lambda}$ cutoff;
(2 - the calculation results of the work (Grishina, Il'in *et al.* 1999) with the accounting for the ''back reaction'';
(3) - the new calculation results with the accounting for the ''back reaction'' and $\hat{\lambda}$ cutoff.
* - in (Sculjan, Bucovic *et al.* 1995) for the Cu I 324.754 nm spectral line the experimental width ω_{tot}=0.0097 nm has been obtained at T=17000 K and $n_e=0.66\cdot10^{17}$ см$^{-3}$ that gives the width $\omega_{tot}\approx$0.015 nm at $n_e=10^{17}$ см$^{-3}$ in the proportion to an increase of n_e. This value of ω_{tot} is greater by 3.6 fold than the theoretical value of ω_{tot} in Table 1.

In Dimitrijević *et al.* (1996) the calculations have been carried out according to the scheme in Dimitrijević and Konjević (1986) and Konjević and Konjević (1986) by using the known values of the absorption oscillator strengths presented in Radzig and Smirnov

(1986). In Grishina *et al.* (1998a, 1998b) the calculations have been carried out by using more rigorous the quantum-mechanical formulae in Griem (1974), Griem *et al.* (1962) according to the scheme described in Griem (1962) and the results have been obtained which differ noticeably from the results of the work Dimitrijevic *et al.* (1996).

Table 2. The Stark shifts of the Cu I spectral lines for $n_e=10^{17}$ см$^{-3}$

(in the wave-length scale all the shifts and η are positive).

λ, nm	T, K	d_e, nm (2)/(1)	d_{tot}, nm (2)/(1)	d_{tot}, nm (3)	$\eta=d_e/\omega_e$. (2)/(1)	$\eta=d_e/\omega_e$ (3)
	5000	0.00783	0.00802	0.00800	1.33	1.85
		(0.00799)	(0.00816)		(1.56)	
	10000	0.00889	0.00917	0.00916	1.45	1.79
		(0.00883)	(0.00912)		(1.40)	
510 554	20000	0.00947	0.00984	0.00983	1.36	1.54
		(0.00929)	(0.00967)		(1.19)	
	30000	0.00945	0.00986	0.00985	1.21	1.33
		(0.00925)	(0.00968)		(1.05)	
	5000	0.00230	0.00234	0.00234	1.14	1.71
		(0.00237)	(0.00242)		(1.43)	
	10000	0.00254	0.00262	0.00262	1.27	1.67
		(0.00251)	(0.00259)		(1.16)	
327.396	20000	0.00250	0.00260	0.00260	1.05	1.23
		(0.00243)	(0.0254)		(0.84)	
	30000	0.00234	0.00245	0.00245	0.83	0.92
		(0.00227)	(0.00239)		(0.66)	

(1), (2), (3) - see the comments to Table 1.

In Grishina *et al.* (1999) the calculations have been carried out according to the scheme of the work Cooper and Oertel (1969) in which in contrast to the scheme of the work Griem (1962) the inelastic collisions of electrons with the atoms are taken into account more strictly by way of accounting for an effect of the atoms (''back reaction'') on the perturbing electrons flying by the atoms. In Sibgatullin *et al.* (2000) the calculations have been carried out also according to the scheme of the work Cooper and Oertel (1969) however apart from the accounting for ''back reaction'' the estimation of the role of the $\lambda\!\!\!^{-}$ cutoff, as it is called, has been carried out at the specifying the cross section of the impact broadening by the electrons with the strong collisions in the limits of the Weisskopf radius. The $\lambda\!\!\!^{-}$ cutoff in point of fact consists in the cutting out in the broadening cross-section of the central part with the radius equaling the value of the de Broglie wave-length (divided by 2π) and in the elimination from the consideration of the broadening of the close electron transits because of the uncertainty in the trajectory of electrons according to the

Heisenberg's uncertainty relation for the coordinate and impulse of the electron and correspondingly of the small probability of very close transits.

This paper continues the work of Sibgatullin *et al.* (2000) in which only estimation results have been presented for the Cu I 327.396 nm resonance spectral line. The calculation program used by us in Grishina *et al.* (1998a, 1998b, 1999) and Sibgatullin *et al.* (2000) has been extended by the accounting of the $\hat{\lambda}$ cutoff whereby some errors of the program have been eliminated that results in the small correction of the calculation data of works Grishina *et al.* (1998a, 1998b, 1999). Some new results with the accounting for the $\hat{\lambda}$ cutoff obtained by us are presented in Tables 1 and 2 for some copper atoms spectral lines of 4s ^{2}S-4p ^{2}P^0 and 4s^2 ^{2}D-4p ^{2}P^0 multiplets. In Tables 1 and 2 ω_e and d_e are correspondingly the electron impact half-width and shift in the wave-length scale, A is the ionic broadening parameter, $\omega_{tot}=2\omega_e[1+1.75A(1-0.75R]$ and $d_{tot}=d_e+2A(1-0.75R)\omega_e$ are correspondingly the full width and shift when the ionic broadening is taken into account also (R is the Debay schielding parameter) (Griem 1974). Table 1 and 2 allow to present on the example of the copper atoms spectral lines the full picture of the effect of the accounting for the ''back reaction'' and $\hat{\lambda}$ cutoff on the results of calculations carried out in the dipole approximation. As it is seen from Table 1 and 2 the accounting for the ''back reaction'' and $\hat{\lambda}$ cutoff effect on the results of calculations and these circumstances must be taken into consideration at the comparison of the experimental and theoretical profiles of the spectral lines. However as a whole the effect for the accounting of the ''back reaction'' and $\hat{\lambda}$ cutoff is comparatively moderate and substantially does not change the results of calculations obtained by using the scheme described Griem (1962) in which the ''back reaction'' and $\hat{\lambda}$ cutoff are not taken into account.

References

Cooper, J., Oertel, G.K.: 1969, *Phys. Rev.*, **180**, 286.

Dimitrijević, M.S., Il'in, G.G., Salakhov, M.Kh., Sarandaev, E.V.: 1996, *18th SPIG Contributed papers*, 283.

Dimitrijević, M.S., Konjević, N.: 1986, *Astron. Astrophys.* **163**, 297.

Grishina, N.A., Il'in, G.G., Salakhov, M.Kh., Sarandaev, E.V.: 1998a, *19th SPIG Contributed papers*, 361.

Grishina, N.A., Il'in, G.G., Salakhov, M.Kh., Sarandaev, E.V.: 1998b, *Coherent Optics and Optical Spectroscopy*, Kazan, Russia, 43.

Grishina, N.A., Il'in, G.G., Salakhov, M.Kh., Sarandaev, E.V.: 1999, *Coherent Optics and Optical Spectroscopy*, Kazan, Russia, 23.

Konjević, R., Konjević, N.: 1986, *Fizika*, **18,** 327.

Radzig, A.A, Smirnov, B.M.: 1986, *Atomic and Ionic Parameters*, Energoizdat, Moscow.

Griem, H.R.: 1962, *Phys. Rev.*, **128**, 515.

Griem, H.R., Baranger, M., Kolb, A.C., Oertel, G.: 1962, *Phys. Rev.*, **125**, 177.

Griem, H.R.: 1974, *Spectral Line Broadeninig by Plasmas*, Academic Press, New York.

Skuljan, Lj., Bucović, S., Djeniže, S.: 1995, *Publ. Obs. Belgrade*, **50**, 127.

Sibgatullin, M.E., Il'in, G.G., Salakhov, M.Kh., Sarandaev, E.V.: 2000, *Coherent Optics and Optical Spectroscopy*, Kazan, Russia, 123.