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ON THE TEMPERATURE DEPENDENCE OF STARK WIDTHS

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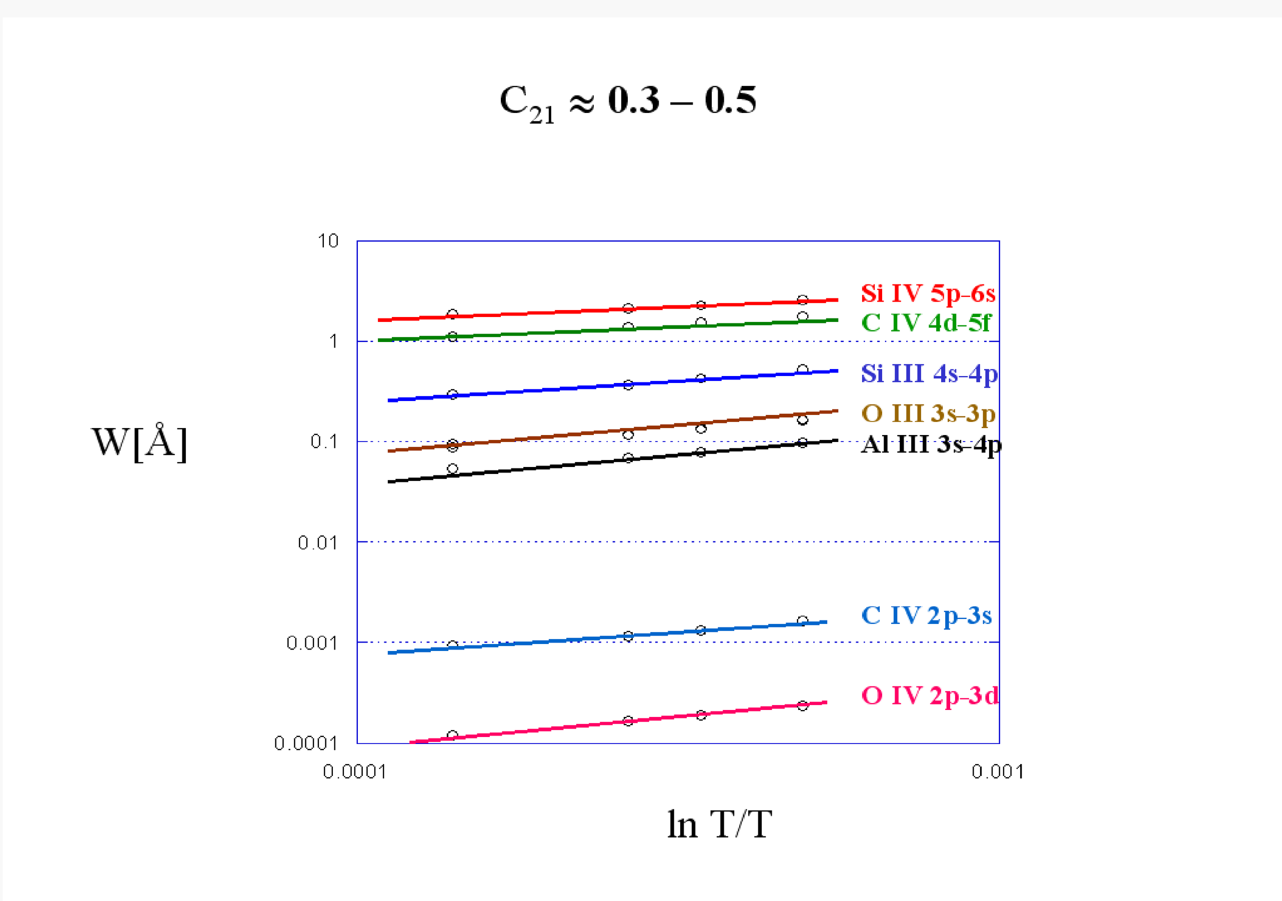
- Several temperature dependence on Stark widths have already been investigated (Elabidi et al 2009, Sahal-Bréchot et al. 2011, Elabidi and Sahal-Bréchot, 2011) on the sample of Stark widths obtained by semiclassical perturbation method (SCF, Sahal-Brechot, 1969a,b) :
- $W_{Stark} \sim 1/\sqrt{T}$ (valid below lower temperature threshold)
- $W_{Stark} \sim \ln T/T$ and $W_{Stark} \sim \ln T/\sqrt{T}$ (valid above upper temperature threshold)
- We wanted to check if the same temperature dependences are valid for the sample of Stark widths obtained by modified semiempirical method (MSE, Dimitrijević and Konjević, 1980)
- We investigated temperature dependences in three different general forms of log-log linear correlations:

- A) $\log W_{MSE} = C_{11} \log T + C_{21}$
- B) $\log W_{MSE} = C_{21} \log (\ln T/T) + C_{22}$
- C) $\log W_{MSE} = C_{31} \log (\ln T/\sqrt{T}) + C_{32}$

- All available Stark widths calculated by MSE approach (STARK-B database, http://stark-b.obspm.fr/, Sahal-Brechot et al. 2014, Sahal-Brechot et al. 2015a,b, Dimitrijević and Konjević, 1981) was analysed (temperature range between 10000 and 80000 K is covered).

- Although all of three linear correlations A, B and C fit very well to our investigated sample, in the case of B slope coefficient is almost constant for all considered Stark widths, $C_{21} \approx 0.4$, so the new temperature dependence is found:

$$W_{Stark}(T) \propto \left(\frac{\ln T}{T}\right)^{2/5}$$



- We tried to prove the validity of new temperature function on simplified modified semiempirical formula (SMSE, Dimitrijević and Konjević, 1987) as a special case of MSE formula when condition of lower temperature threshold is satisfied, e. g. when adiabatic and elastic collisions of radiators and perturbers in high temperature plasma overcome.

Simplified modified semiempirical (SMSE) formula for Stark width calculation

$$W_{SMSE} = 2.2155\cdot10^{-24}\cdot\lambda^2 N\left(0.9-\frac{1.1}{Z}\right) f_{OLD}(T)\sum_{j=i,f}\left(\frac{3n_j^*}{2Z}\right)^2 (n_j^{*2}-l_j^2-l_j-1)$$

$$f_{OLD}(T)=\frac{1}{\sqrt{T}} \qquad x=\frac{E}{\Delta E_\pm} \qquad E=\frac{3kT}{2}$$

$$\Delta E_\pm = \left|E_j - E(l_j \pm 1)\right| \qquad n_j^{*2}=\frac{Z^2 E_H}{E_{ion}-E_j} \qquad j=i,f$$

W_{SMSE} is Stark width in Å, λ wavelength in Å, N – perturber density in cm^{-3}, E – average perturber energy, T – temperature in K, Z-1 is ionic charge, n_j^* - effective principal quantum number for level j, and l_j – orbital quantum number for level j, $j \in \{i, f\}$. Letters i and f stand for initial and final state respectively, E_H – hydrogen atom energy, E_{ion} – ionization energy, and E_j – energy of jth level. $E(l_j \pm 1)$ the energies of perturbed levels with orbital number l_j+1 e.g. l_j-1 are signed, and k is Boltzmann's constant

- We determined the constant of proportionality C for the new temperature function:

$$f_{NEW}(T)=C\left(\frac{\ln T}{T}\right)^{2/5}$$

from the condition

$$f_{OLD}(T_X)=f_{NEW}(T_X)$$

where T_X is temperature for $x = 2$ (lower temperature threshold condition is satisfied for $x \leq 2$)

- T_X is found from least square error function

$$LSE(T_X)=\min_C \sum_i \left(f_{NEW}(T_i)-f_{OLD}(T_i)\right)^2$$

resulting with critical temperature T_X = 7500 K and corresponding C_X = 0.17072 obtaining a new formula (NF) for Stark width estimate:

$$W_{NF} = 3.7823\cdot10^{-25}\cdot\lambda^2 N\left(\frac{\ln T}{T}\right)^{2/5}\left(0.9-\frac{1.1}{Z}\right)\sum_{j=i,f}\left(\frac{3n_j^*}{2Z}\right)^2 (n_j^{*2}-l_j^2-l_j-1)$$

Some of the best results of comparison of NF values with theoretical values

	T/kK	W_{NF}[Å]	W_{SMSE}[Å]	W_{NF}/W_{MSE}
Zr IV, λ=760.16 Å, 5s $^2S_{1/2}$ – 6p $^2P_{1/2}$	10	0.0104	0.0099	1.05
	20	0.0081	0.0070	1.15
	50	0.0058	-	1.2
	100	0.0045	-	1.24
	200	0.0035	-	1.15
	300	0.0029	-	0.97
	500	0.0024	-	0.81

	T/kK	W_{NF}[Å]	W_{SMSE}[Å]	W_{NF}/W_{MSE}
Zr IV, λ=754.39 Å, 5s $^2S_{1/2}$ – 6p $^2P_{3/2}$	10	0.0104	0.0099	1.01
	20	0.0081	0.0070	1.1
	50	0.0058	-	1.24
	100	0.0045	-	1.24
	200	0.0035	-	1.08
	300	0.0029	-	0.95
	500	0.0024	-	0.81

	T/kK	W_{NF}[Å]	W_{SMSE}[Å]	W_{NF}/W_{MSE}
Lu III, λ=2801.7 Å, 6d $^2D_{3/2}$ – 6f $^2F^o_{5/2}$	10	0.2910	0.2792	1.08
	20	0.2270	0.1974	1.19
	50	0.1630	0.1249	1.16
	100	0.1267	-	0.88

	T/kK	W_{NF}[Å]	W_{SMSE}[Å]	W_{NF}/W_{MSE}
Lu III, λ=2782.0 Å, 6d $^2D_{5/2}$ – 6f $^2F^o_{5/2}$	10	0.2914	0.2796	1.1
	20	0.2274	0.1977	1.21
	50	0.1633	0.1250	1.17
	100	0.1269	-	0.89

	T/kK	W_{NF}[Å]	W_{SMSE}[Å]	W_{NF}/W_{MSE}
Lu III, λ=2722.5 Å, 6d $^2D_{5/2}$ – 6f $^2F^o_{7/2}$	10	0.2771	0.2659	1.1
	20	0.2162	0.1880	1.21
	50	0.1553	0.1189	1.17
	100	0.1206	-	0.88

Comparison of NF values with experimental values:

Ion		Transition	λ[A]	T[K]	N[cm^{-3}]	W_{EXP}[A]	W_{NF}[A]	W_{NF}/W_{EXP}
C	IV	$3s^2S-3p^2P^o$	5812	15700	1.45	0.964	0.91122	0.94525
C	IV	$3s^2S-3p^2P^o$	5812	17000	1.87	1.154	1.1421	0.98968
C	IV	$3s^2S-3p^2P^o$	5812	17800	1.96	1.084	1.1775	1.0862
C	IV	$3s^2S-3p^2P^o$	5812	18300	1.82	1.074	1.0825	1.0079
C	IV	$3s^2S-3p^2P^o$	5812	19000	1.66	1.042	0.97413	0.93487
C	IV	$3s^2S-3p^2P^o$	5812	19500	1.44	0.762	0.83718	1.0987
C	IV	$3s^2S-3p^2P^o$	5812	19800	1.37	0.735	0.79212	1.0777
C	IV	$3s^2S-3p^2P^o$	5812	20300	1.25	0.694	0.71629	1.0321
C	IV	$3s^2S-3p^2P^o$	5812	72400	0.58	0.229	0.20973	0.91586
C	IV	$3s^2S-3p^2P^o$	5812	78300	0.76	0.304	0.26709	0.87857
Al	III	$3d^2D-4p^2P^o$	3605.2	50000	64	8.5	16.185	1.9042
Al	III	$3d^2D-4p^2P^o$	3605.2	50000	97	25	24.531	0.98125
Al	III	$3d^2D-4p^2P^o$	3605.2	50000	104	26.5	26.301	0.99251
Al	III	$3d^2D-4p^2P^o$	3605.2	50000	119	29	30.095	1.0378
Al	III	$3d^2D-4p^2P^o$	3605.2	50000	133	32	33.635	1.0511
Mg	II	$3s^2S-3p^2P^o$	2795.5	13000	1.18	0.12	0.077886	0.64905
Mg	II	$3s^2S-3p^2P^o$	2795.5	12970	1.1	0.048	0.072666	1.5139
Mg	II	$3s^2S-3p^2P^o$	2795.5	14260	1.64	0.077	0.10472	1.36
Ca	II	$4s^2S-4p^2P^o$	3933.7	13000	1.08	0.235	0.25322	1.0775
Ca	II	$4s^2S-4p^2P^o$	3933.7	43000	1.76	0.286	0.26818	0.9377
Pb	II	$6d^2D-5f^2F^o$	4386.5	24000	11	7.7	3.358	0.4361
Pb	II	$6d^2D-5f^2F^o$	4386.5	27000	1.62	0.51	0.47397	0.92936

Conclusion

- Our NF can approximate MSE results in the reasonable tolerance of accuracy when x is in range from 0.2 to 10, where best accuracy is expected for x from 0.2 to 0.35, from 5.5 to 7 and around 10, while in other subranges of x we can expect less accuracy, but mostly not lesser than 50%.
- Concerning about transitions, our NF could be acceptable approximation in the cases of ns-np and np-(n+1)s types of transtions, and particularly when np-nd and (n-1)d-np are considered, if n = 4, which is confirmed with comparison of results calculated with NF and experimental results.
- Our suggested new temperature function is found to follow original MSE results in the range from 10000 K to 80000 K mostly with acceptable accuracy, even when higher temperatures are used.

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