Z scaling of the $3P$-$3S$ Li isoelectronic series transition: Quadrupole Stark broadening and resonances

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We here report Stark-broadened widths with error bounds of Li-like ions carbon to neon considered in recent experiments. Good agreement is obtained except for neon, for which the calculated widths, while within the error bounds given, seem too narrow.

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Recently some experimental studies [1–3] have found significant deviations from the Z scaling predicted by the impact theory for isolated ion lines in the Li isoelectronic series. The dipole contribution was recently considered [4] and good agreement was obtained for all species except Ne VIII. The present work includes quadrupole terms (for both electron and ion broadening) and a calculation of the contribution of resonances for Ne VIII.

I. SEMICLASSICAL CALCULATION WITH DIPOLE AND QUADRUPOLE TERMS

We here report semiclassical calculations of the $3P$-$3S$ line including quadrupole broadening and employing self-consistent minimum impact parameter cutoffs (including of course the quadrupole terms), as described in Ref. [4]. (The use of a new analytic expression [5] for the dipole A function—also used in Ref. [4]—has facilitated such calculations.) The dipole channels are as in Ref. [4]. Quadrupole broadening is included in the "hydrogenic" approximation (that is, $\xi = e^2 Z_{\rm em} Z_p \Delta\omega / 4\pi\epsilon_0 \mu_p v^3 = 0$ with $Z_{\rm em}$, Z_p the emitter and perturber charges, respectively, μ_p the reduced perturber mass, v the perturber velocity, and $\Delta\omega$ the frequency separation between the broadened level and the perturbing level) for both the $3P^{3/2}$-$3P^{3/2}$ (for which this is exactly true) and the $3P^{3/2}$-$3P^{1/2}$ channels (for which this is only approximately true). We discuss this point later on.

In Table I we compare experimental and theoretical widths [full width at half maximum (FWHM)] $\mathcal{W}$. For the theoretical widths we list weak collision widths and a strong collision width; this is to mean that the theoretical width lies between the "weak" width and the sum of "weak" and "strong" widths. These "strong" widths have been calculated by taking $\{S_a S_b - 1\} = -1$, where S_a and S_b are the S matrices for the upper and lower level, respectively, and $\{\ \}$ denotes angular average. Since $0 \geq \{S_a S_b - 1\} \geq -2$, the absolutely maximum strong collision contribution is twice what we quote (for more details see Ref. [4]). In parentheses after a total weak collision term we give the electronic and ionic quadrupole contributions, respectively. All theoretical widths are pure Stark widths without contributions from resonances. For Ne VIII where we have the most significant Doppler broadening, the widths listed are increased by at most (i.e., if we neglect the strong collision contribution) 0.1 and 0.13 Å, respectively.

One thing that is rather clear from the calculations is that our strong collision estimate [i.e., replacing $\{S_a S_b - 1\}$ by -1] for strong collisions is clearly an overestimate. (Compared to a pure dipole calculation as

TABLE I. Theory vs experiment (Refs. [2,3]).

Species	kT_e (eV)	n_e (10^{18} e/cm^3)	Expt. (Å)	Weak (Å)	Strong (Å)
C IV	7.0	1.5	6.7±0.4	7.3(0.34–1.046)	3
C IV	8.6	2.4	9.7±0.5	11.6(0.524–2.05)	4.5
N V	14.9	1.2	2.2±0.1	2.2(0.17–0.33)	0.77
N V	18.7	1.6	2.7±0.1	2.87(0.2–0.55)	0.95
N V	21.8	2.0	3.4±0.2	3.57(0.23–0.8)	1.13
N V	23.9	2.3	3.8±0.2	4.1(0.26–1.04)	1.28
O VI	8.3	1.0	1.0±0.1	1.05(0.135–0.05)	0.43
O VI	11.5	1.3	1.4±0.1	1.235(0.15–0.086)	0.5
O VI	15.6	2.1	1.8±0.3	1.83(0.21–0.18)	0.7
O VI	17.5	2.4	2.1±0.2	2.04(0.23–0.23)	0.77
F VII	14.4	1.57	0.87±0.1	0.755(0.12–0.045)	0.33
F VII	16.6	2.1	1.11±0.13	0.97(0.15–0.07)	0.42
F VII	18.5	2.92	1.49±0.18	1.3(0.2–0.1)	0.55
Ne VIII	29.7	2.8	1.2±0.1	0.65(0.11–0.06)	0.29
Ne VIII	42.5	3.2	1.2±0.1	0.684(0.1–0.094)	0.3

in Ref. [4], the strong collision phase space and consequently its maximum strong collision contribution increases, of course.) It is clear that for strong collisions the U matrix will exhibit rather strong oscillations, but in the framework of the impact theory it is not easy to obtain any good and safe estimate for the strong collisions. There seems also to be evidence that including the $4D$-$3P$ dipole channel (for which the energy transfer is of the order of the kinetic energy) overestimates the width somewhat. However, this evidence is by no means clear, particularly in view of the questions about the hydrogenic approximation for the quadrupole functions.

The calculation shows an interesting competition between ion and electron quadrupole broadening. For the lighter species, C IV and N V, ion quadrupole broadening is larger than the electron quadrupole broadening, presumably because small eccentricities

$$\epsilon=\left[1+\left[\frac{4\pi\epsilon_0\mu_p v^2\rho}{e^2 Z_p Z_{\rm em}}\right]^2\right]^{1/2} \tag{1.1}$$

with ρ the impact parameter, where the electron quadrupole broadening is most efficient (since the attractive quadrupole A function blows up for $\epsilon\rightarrow 1$) are not as common as for the more heavily ionized species. For the same reason, the relative contribution of ion quadrupole broadening tends to increase with increasing temperature. This changes for O VI and all heavier species considered. Ion quadrupole broadening always dominates ion dipole broadening, but is always for the cases considered smaller than the dominant electron dipole broadening and, for $Z\geq 6$ is less than or equal to electron quadrupole broadening.

The C IV lines are predicted to be broader than observed. This is probably because the "hydrogenic" ion quadrupole assumption breaks down. In other words, because ϵ of the order of 3 or so are involved and because the quadrupole functions drop rapidly when ϵ is not very close to unity [6] the $3P^{3/2}$-$3P^{1/2}$ channel is no longer hydrogenic and should probably be neglected, in which case we obtain good agreement. Unfortunately, simple and good analytic approximations for the relevant quadrupole functions (analogous to the approximations of Poquerusse [7] for the dipole case) do not exist and we hope to address this question in future work.

As for higher than quadrupole multipoles, it is clear that those with selection rules not allowing $\Delta\omega=0$ will be smaller than the dipole contribution roughly by at least a factor $(9a_0/Z\langle\rho\rangle)^2$ per multipole order with Z the spectroscopic charge number and $\langle\rho\rangle$ the average interionic spacing. This ratio is, for the highest density considered, 0.014, small enough to justify the semiclassical approach. Similarly, for the multipoles for which $\Delta\omega=0$ is allowed, they will be smaller than the quadrupole contribution by roughly the same factor.

II. RESONANCES

In view of the results for Ne VIII we here consider the possibility that resonances may contribute to the width of Ne VIII: By this we mean that the incident electron is captured in some high Rydberg state with an excitation of the upper or lower state $|i\rangle$ to some other state $|i'\rangle$. We refer to i' as specifying a channel. This species will later autoionize and this process contributes to the width. Semiclassically speaking, the perturbing electrons need not come too close to the ion to get captured, because they can be captured into some highly excited level close to the continuum and this can occur at quite large impact parameters. Strictly speaking, there is, of course, a corresponding reduction in dipole and quadrupole Stark broadening, since the velocity phase space contributing to resonances is unavailable for (nonresonant) broadening, but in view of the results obtained this is no cause for concern.

The contribution of resonances has been calculated by many authors [8] using Gailitis averaging [9]. The resonance contribution $\mathcal{W}_R^i$ to the width (FWHM) of level i can be written as a sum over channels [10]:

$$\begin{aligned}\mathcal{W}_R^i &= n_e\frac{\hbar^2}{g_i m}\left[\frac{2\pi}{mkT}\right]^{1/2}\sum_{i'}\int_0^{\Delta E_{ii'}/kT}\frac{\Omega_{ii'}^{>2}}{\sum_j \Omega_{i'j}^{>}}e^{-E/kT}d(E/kT)\\ &= n_e\frac{\hbar^2}{g_i m}\left[\frac{2\pi}{m}\right]^{1/2}\sum_{i'}\frac{\Omega_{ii'}^{>2}}{\sum_j\Omega_{i'j}^{>}}\frac{1-\exp(\Delta E_{ii'}/kT)}{(kT)^{1/2}}\end{aligned} \tag{2.1}$$

where we neglected the interference between the resonances. g_i is the statistical weight of level $i[=(2S_i+1)(2L_i+1)]$ and ΔE_{ij} the energy differernce between levels i and j. In (2.1), the collision strengths $\Omega^>$ are calculated above the new threshold and extrapolated (as constants) below this threshold. The i' sum is taken over degenerate closed channels of the new threshold and j runs over all open channels (i.e., levels below i'). For the $3s$-$3p$, $3s$-$3d$, and $3p$-$3d$ channels, collision strengths were taken from Ref. [11]. For the calculation of Ω's for i' with principal quantum number 4 we used the simple formula [12]:

$$\Omega_{ij}=\frac{8\pi g_i f_{ij}\tilde{G}}{\sqrt{3}\Delta E_{ij}} \tag{2.2}$$

with ΔE_{ij} in rydbergs. $\tilde{G}$ is a Gaunt factor, which we take to be 0.6 and 0.16, respectively for $\Delta n=0$ and $\Delta n\neq 0$ dipole-allowed (DA) and 0.2 for dipole-forbidden (DF) transition at the threshold [13]. For DA transitions

TABLE II. Resonant contributions to $\mathcal{W}$ (w_1 refers to the $\mathcal{W}$ contribution for $n_e=2.8\times10^{18}$ e/cm^3, $T=29.7$ eV, and w_2 to the $\mathcal{W}$ contribution for $n_e=3.2\times10^{18}$ e/cm^3, $T=42.5$ eV).

Channel	w_1 (Å)	w_2 (Å)
$3s$-$3p$	0.0177	0.012
$3s$-$3d$	3.2×10^{-4}	2.2×10^{-4}
$3s$-$4s$	0.002 23	0.0018
$3s$-$4p$	$<3.18\times10^{-5}$	$<3.18\times10^{-5}$
$3p$-$3d$	0.001 58	0.001 05
$3p$-$4s$	0.75×10^{-4}	0.6×10^{-4}
$3p$-$4p$	$<3.18\times10^{-5}$	$<3.18\times10^{-5}$

f_{ij} is the true oscillator strength and for DF transitions it is the oscillator strength for the nearest related allowed transition in the sense of Mewe [14]. With this formula, the most important DA collision strengths for Ne VIII agree to within 30% with a close-coupling calculation [11].

The integration limits in (2.1) arise from taking the maximum energy in the Maxwell-Boltzmann distribution to be $\Delta E_{ii'}$ and the minimum to be 0, provided that levels a distance $\Delta E_{ii'}$ below the continuum are high Rydberg levels. This is true in our case, at least for the most important contributions, even if we account for continuum lowering.

In Table II we list calculated resonant contributions from various channels to $\mathcal{W}$ for Ne VIII. It turns out that the dominant resonant contribution comes from the $3S$-$3P$ and after that from the $3P$-$3D$ channels, where (in contrast to usual Stark broadening) only a small part of the Maxwell-Boltzmann distribution can participate to give a resonant contribution. For other channels a larger part of the Maxwell-Boltzmann distribution can participate, but the collision strengths are smaller, since other, more probable decay channels exist (for example, if $3S$ is resonantly excited to $4P$, this is more likely to decay to $4S$, not $3S$).

The total contribution from resonances to $\mathcal{W}$ is thus estimated to be 0.022 ($n=2.8\times10^{18}$ e/cm^3, $T=29.7$ eV) and 0.016 ($n=3.2\times10^{18}$ e/cm^3, $T=42.5$ eV) Å, respectively. This increases the widths listed in Table I for Ne VIII by about 0.12 and 0.146 Å, respectively if in addition to the above contributions we include Doppler broadening.

In conclusion, resonances are found to be unimportant, at least within our approximations because, to put it simply, the temperature is too high.

III. CONCLUSIONS

N V, O VI, and F VII are in good agreement with the experimental results, while Ne VIII continues to show significant discrepancies. While the theory-experiment difference is easily within the maximum [i.e., replacing $\{S_aS_b-1\}$ by -2] and almost within the quoted strong collision contribution, it is hard to see why this should be constant over the effective interaction time so as to produce this maximum contribution. Unless the root of these discrepancies lies in the atomic structure, it is hard to think of other mechanisms that could play a significant role: Even though the not completely hydrogenic $3P^{3/2}\rightarrow3P^{1/2}$ quadrupole channel could conceivably give a larger contribution than our hydrogenic treatment, such a contribution is unlikely to be too large because of unitarity constraints. Nevertheless, developing simple and accurate approximations for the quadrupole broadening functions beyond the hydrogenic limit would seem useful.

Further experiments with even higher ionization stages could be of great help in deciding whether we really have something new here or not.

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[1] F. Böttcher *et al.*, Phys. Rev. A **38**, 2690 (1988).
[2] S. Glenzer, N. I. Uzelac, and H. J. Kunze, Phys. Rev. A **45**, 8795 (1992).
[3] S. Glenzer, N. I. Uzelac, and H. J. Kunze, in *Spectral Line Shapes,* edited by R. Stamm and B. Talin (Nova Science, Commack, NY, 1993), Vol. 7.
[4] S. Alexiou, Phys. Rev. A **49**, 106 (1994).
[5] S. Alexiou, J. Quant. Spectrosc. Radiat. Transfer (to be published).
[6] S. Klarsfeld, Inst. Phys. Nucl. Orsay, Report No. IPNO/TH 71-42, 1971 (unpublished).
[7] A. Poquerusse, Phys. Lett. **59A**, 438 (1977).
[8] M. J. Seaton, J. Phys. B **2**, 5 (1969); K. S. Barnes and G. Peach, *ibid.* **3**, 350 (1970); M. D. Hershkowitz and M. J. Seaton, *ibid.* **6**, 1176 (1973); C. Fleurier, S. Sahal-Brechot, and J. Chapelle, J. Quant. Spectrosc. Radiat. Transfer **17**, 595 (1977); M. J. Seaton, J. Phys. B **21**, 3033 (1988).
[9] M. Gailitis, Zh. Eksp. Teor. Fiz. **44**, 1974 (1963) [Sov. Phys. JETP **17**, 1328 (1963)].
[10] M. J. Seaton, J. Phys. B **20**, 6363 (1987); since we use a different definition of the collision strength as in Ref. [11], we have divided in Seaton's formula in Eq. (2.1) by the statistical weight.
[11] K. Bhadra and R. W. Henry, Phys. Rev. A **26**, 1848 (1982).
[12] A. Burgess, Mem. Soc. R. Sci. Liege **4**, 299 (1961); M. J. Seaton, in *Atomic and Molecular Processes,* edited by D. R. Bates (Academic, San Diego, 1962); H. Van Regemorter, Astrophys. J. **136**, 906 (1962).
[13] V. Fisher (private communication).
[14] R. Mewe, Astron. Astrophys. **20**, 215 (1972).