Collisional broadening of the Balmer-α transition of H and He^+ in plasmas

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We have computed the Stark-broadened width of the H_α transition of neutral hydrogen ($n_e = 10^{15} - 10^{17}$ cm^{-3}) and singly ionized helium ($n_e = 10^{17} - 10^{18}$ cm^{-3}) at several plasma temperatures. Our calculations include dynamical contributions of perturbing ions, which dominated the widths of this important transition, particularly at lower electron densities. We compare our results for neutral hydrogen with experimental results over a span of two decades in electron density (n_e), and excellent agreement is obtained.

I. INTRODUCTION

Some of the most frequently observed transitions in astrophysical and laboratory plasmas are the Balmer ($n_{\text{upper}} \rightarrow 2$) transitions in hydrogen and hydrogenic ions. In neutral hydrogen, the Balmer-α transition is the most prominent feature in the visible spectrum. Also, since the lower level is not the ground state, the self-absorption phenomenon is much less serious than for the Lyman lines. The collisional broadening of the Balmer-α transition in plasmas is quite sensitive to the so-called ion dynamic effect, particularly at lower electron densities. We have performed calculations over a range of temperatures and densities for the Stark-broadened profile of H_α transition of the neutral hydrogen atom and the singly charged helium-ion radiators.

Before the first observation of the "ion dynamic" effect,[1] it was generally assumed that ion perturbers behaved quasistatically. Calculations were performed by averaging over the static electric-microfield distribution[2,3] generated by the perturbing ions. This quasistatic-ion assumption is only valid when the ion collision duration ($\simeq \omega_{pi}^{-1}$, the inverse of ion plasma frequency) is long compared to the "time of interest" or coherence time of the perturbed atomic state (inside the half-width, the time of interest is $\simeq \gamma^{-1}$, the inverse of the collisional width; outside the half-width, it is $\simeq \Delta\omega^{-1}$, the inverse frequency separation from line center). Thus, unless $\gamma \gg \omega_{pi}$, the quasistatic-ion approximation is not valid inside the half-width. Except at quite high electron densities, where the time of interest is short, ion dynamics plays an important role near the center of collision-broadened profiles of hydrogenic transitions. This effect is generally pronounced for hydrogenic radiators, which experience a first-order Stark effect. In this case the perturbing interactions are long range so that important collisions often occur on a time scale long compared to the collisional lifetime of the state. Our calculations show that at low electron densities, ion dynamics increases the half-width of H_α of neutral hydrogen several fold.

We have recently reported[4] our computed widths of the H_α transition for the C^{5+} ion, primarily because of the importance of this transition in x-ray laser schemes. However, precision measurements of H_α Stark broadening have been made extensively only for neutral hydrogen. The present work, using the method of Ref. 4, has been done to provide a comparison of our computed results with the existing measurements over an electron density range of two decades. We have also included our computations for the H_α line of the He^+ ion in the hope of stimulating precision measurements of this transition.

The ion dynamic problem has proven challenging theoretically because it generally involves treating overlapping strong collisions. The "unified" theory[3] treated strong collisions to all orders, but only in the binary limit. To date there is still no analytic solution to this problem. Indeed, any such solution would be tantamount to solving the time-dependent many-body problem. Thus it has proven necessary to resort to numerical methods. So-called model-microfield methods (see, e.g., Ref. 5), not discussed here, have also been applied to this problem.

All of the numerical methods rely on a numerical Monte Carlo–type simulation to generate time-dependent electric fields. This represents what we might call the plasma part of the problem. The atomic problem, i.e., the response of the radiating atom or ion to the plasma fields, has been treated in two different ways. In the fully numerical approaches, the coupled time-dependent Schrödinger equations for the radiator-plasma system are solved numerically.[6,7] Other approaches evaluate the observable plasma effects on the radiator analytically.[8,9] The method adopted here uses a relaxation theory of ion broadening.[9] An approximation to the time-development operator permits the separation of the ion plasma average from the atomic coordinates, with the result that the ion perturber dependence is confined to two functions which depend only on ion field magnitude and time. We have evaluated these functions using a Monte Carlo method similar to that in Ref. 9. Recently, this method has been applied to the broadening of the Balmer-α line of the C^{5+} ion.[4] The fully numerical methods pose more severe computational problems, and until very recently were applied only to Lyman lines. Seidel[7] has recently performed fully numerical calculations for the neutral H_α line and obtained similar results to those we present in this paper.

II. PLASMA CONDITIONS FOR COMPARISON WITH EXPERIMENTAL RESULTS

The comparison of the experimental line profile for the Balmer-α transition at a single plasma density showed good agreement with the computed one in Ref. 9. In the present work, we have extended the calculation to an extensive range of electron densities where experimental results are available (see Table I and discussion below). Since the measured line profiles and our computed line profiles are Lorentzian in shape,[10(a)] it is convenient to make a comparison of the half-width parameter compactly in a single figure (Fig. 1) over an extensive range of plasma conditions. The electron contribution is computed with the effects of time ordering included. The profiles depart from Lorentzian shape in the wings where ion dynamics is not important for plasma conditions considered here. We remark here that we are examining the effect due to dynamic ions which dominates the electron contribution to the half-width quite significantly.

In the present calculations we followed the method described in Ref. 9. However, the computer codes used were modified to treat the numerically difficult case of near-impact ion calculations with dynamic ions. The radius of the sphere used in the numerical simulations was set to two or more times the Debye radius. At lower densities, where there is significant deviation from the condition of static ions, the Debye radius has an extensive range. In common with nearly all other approaches

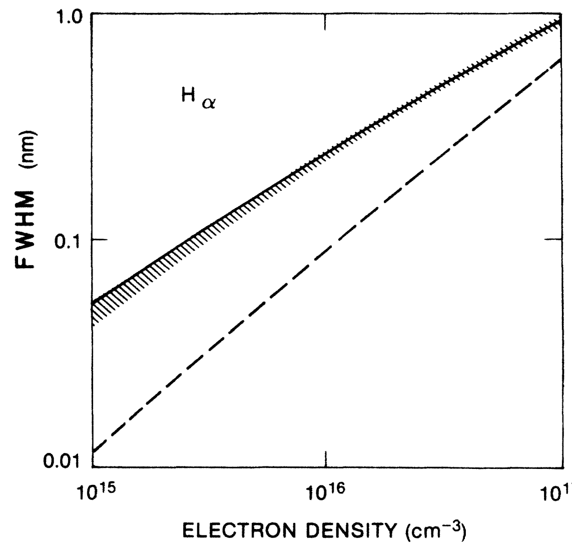

FIG. 1. Full width at half maximum (FWHM) for Balmer-α line of a neutral hydrogen radiator with collisional-broadening effects only. Solid curve, present calculations with dynamic-ion effects (see Table I for perturbers and temperatures used); dashed curve, static-ion approximation (Ref. 3); hatched area, experimental results without Doppler and instrumental broadening (Refs. 10 and 13).

to dynamic ion broadening, we assume a simple model of fixed radiator perturbed by fictitious particles of reduced mass μ. The actual problem is more complicated in a plasma since the reduced mass arises naturally only in the two-body problem. Nevertheless, the reduced mass has proven to be a useful scaling parameter in predicting ion-radiator dynamic effects.

In Fig. 1 we compare our computed results performed using the method of Ref. 9 for the H_α line with the experimental values. In making the comparison with the experiment, there is a considerable amount of uncertainty in the appropriate ion temperature to be used in the calculations, particularly at low electron density. The lower-density measurements we compare with were performed in a helium plasma with a small admixture of hydrogen.[10(b)] Such a plasma is very far from thermal equilibrium. In particular, the temperatures of the heavy particles are considerably lower than the electrons; the electrons take up most of the energy from the

TABLE I. Plasma parameters corresponding to the experimental conditions (Refs. 10 and 13) for which the calculations (shown in Fig. 1) are performed. At lower densities the effective temperature was estimated to be between the electron and the gas temperature, closer to the gas temperature. At higher densities, it was chosen to be the electron temperature (see discussion in text).

Electron density (cm^{-3})	Electron temperature (K)	Gas temperature (K)	Effective temperature (K)	Perturber
10^{15}	17 000	3 500	7 500	He^+
5×10^{15}	18 000	11 000	14 000	He^+
10^{16}	19 000	12 000	15 000	He^+
6.4×10^{16}	12 000		12 000	Ar^+
10^{17}	13 000		13 000	Ar^+

electrodes and the heavy particles are in turn heated by collisions with the electrons. At low densities the heavy-particle temperature lags behind that of the electrons, due to the inefficient energy transfer between the particles of very different mass. In the experiment, only the neutral gas and the excitation temperatures were measured. The excitation temperature is presumed to reflect the electron temperature rather closely. However, the ion temperature is not measured explicitly. At low densities, where ion dynamics is very important, the linewidth will depend most sensitively on the ion temperature. For lack of a better estimate, we have chosen the ion temperature to be slightly larger than the gas temperature. We make the further approximation of using a net effective temperature between the electron and estimated ion temperatures. The temperature used was closer to the gas temperature at lower densities where ion dynamics dominates, and equal to the electron temperature at near-quasistatic-ion conditions (high density), where only the electrons exhibit a temperature dependence. The actual conditions used for Fig. 1 are indicated in Table I. No attempt was made to adjust the estimated effective temperature to optimize agreement with experiment. In fact, as seen in Fig. 2, the half width at half maximum (HWHM) of the H_α transition is quite insensitive to the temperature, so that the large difference between electron and gas temperature at low densities corresponds to less than 10% difference in the width. No Doppler convolutions were performed. Rather, comparisons were made with experimental data in which the Doppler broadening was deconvolved using the gas temperature (shown as hatched area in Fig. 1).

A further uncertainty in comparing with the lower density experimental widths is the "effective" reduced mass. The lower density measurements[10(b)] were made in a helium plasma with 1–2% of hydrogen added. In our calculations, we assumed the perturbers to be He^+ ions,[10(b)] but it is possible that a significant fraction of the perturbers were actually protons. The ionization potential of hydrogen is so much lower than that of helium that a significant portion of the perturbing ions could be stripped hydrogen nuclei, even if hydrogen is only a 2% admixture. However, in the lower density range of Fig. 1, the width of the H_α line is relatively insensitive to the reduced mass. The difference in the reduced mass for hydrogen perturbers ($\mu=0.5$) and helium perturbers ($\mu=0.8$) corresponds to a difference in the H_α width of a few percent.

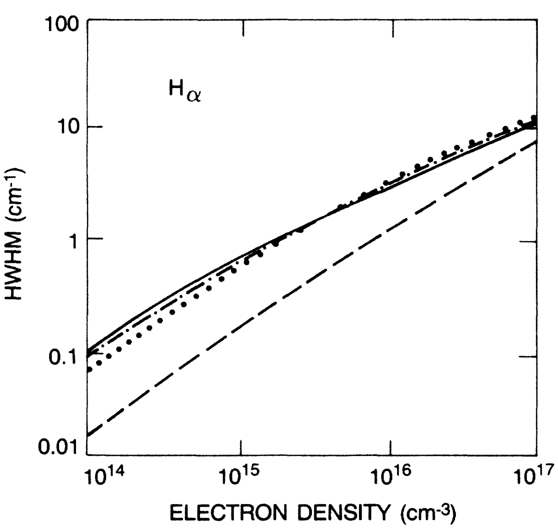

FIG. 2. Calculated half width at half maximum (HWHM) for Balmer-α line of neutral hydrogen with protons as perturbers. Solid curve, dynamic ions at $T=10\,000$ K; dash-dot curve, dynamic ions at $T=20\,000$ K; dotted curve, dynamic ions at $T=40\,000$ K; dashed curve, static ions at $T=40\,000$ K.

Our calculations do not presently include effects due to fine structure; the states of a given n level are assumed to be degenerate. The fine-structure splitting between different fine-structure components of H_α is on the order of 0.015 nm (0.33 cm^{-1}).[10(b)]. This is small enough to be unimportant for electron densities (n_e) greater than 10^{15} cm^{-3}, the lowest density included in Fig. 1. We have recently performed calculations of the H_α profile for the experimental plasma conditions of Sanchez, Fulton, and Griem,[11] $n_e=6.7\times10^{14}$ cm^{-3} and $T=2.8$ eV with He^+-ion perturbers. Our calculations yielded Lorentzian profiles of HWHM of 0.51 cm^{-1} for hydrogen radiators and 0.54 cm^{-1} for deuterium radiators. Sanchez *et al.* superimposed the different Stark- and Doppler-broadened fine-structure components having our computed widths and obtained a net width in $\sim$10% agreement with their measured width. Such a superposition is an approximate method to compensate for the fact that fine structure has not been incorporated into the Stark-broadening calculations. Thus the 10% agreement may be somewhat fortuitous because the fine-structure splitting is of comparable magnitude to the collisional broadening. In Fig. 1 we have limited the range of densities to those for which fine structure can be ignored. Fine structure for the H_α transition has been included by Stehle and Feautrier[12] in the impact-ion limit at electron densities at least an order of magnitude lower than considered here.

III. RESULTS AND DISCUSSION

We compared our computed half-widths of the H_α line of neutral hydrogen atoms with the experimental results over a range of densities $n_e=10^{15}-10^{17}$ cm^{-3}. The temperatures and reduced masses are discussed in the previous section. Good agreement is obtained with experimental values[10,13] over the full range of densities. Both the experimental and the computed profiles of the H_α transitions are observed to be Lorentzian in shape out to more than two half-widths. For comparison, the widths obtained by treating the perturbing ions as static[3] are included in Fig. 1. At the lower densities, the static-ion results are too low by a factor of 3 to 4; the agreement is better at higher densities because the static-ion approximation becomes more valid at these densities. Making quantitative estimates of the uncertainty of our theoretical values is difficult, but we estimate the uncertainty of our computed results, including the effect of uncertainty in plasma parameters discussed above, to be larger than

TABLE II. Half width at half maximum (HWHM) in cm^{-1} calculated for the Balmer-α transition ($\lambda = 656.3$ nm) of a neutral hydrogen radiator in plasmas consisting of different perturber ions. These values include collisional broadening due to dynamic ions and electrons but not due to the Doppler effect.

Plasma temperature (K)	Perturber	Electron density (cm^{-3}) 10^{14}	10^{15}	10^{16}	10^{17}
10 000	Proton	0.0962	0.640	2.81	11.5
	He^+	0.113	0.650	2.73	10.9
	Ar^+	0.119	0.646	2.67	10.6
	Static ions	0.028	0.223	1.49	8.83
	Doppler	0.544			
20 000	Proton	0.0804	0.597	3.10	11.9
	He^+	0.0954	0.634	2.88	11.2
	Ar^+	0.103	0.641	2.76	10.9
	Static ions	0.0209	0.181	1.31	8.29
	Doppler	0.770			
40 000	Proton	0.0604	0.515	3.24	12.5
	He^+	0.0741	0.589	3.04	11.5
	Ar^+	0.0803	0.617	2.92	11.1
	Static ions	0.0156	0.145	1.15	7.63
	Doppler	1.09			

the difference between computed and measured results in Fig. 1, so that the extent of the agreement may be partly fortuitous. However, the good agreement over such a wide range in electron density is encouraging. Similar good agreement has been obtained in the fully numerical results of Seidel.[7]

In Fig. 2 and Table II we have indicated our theoretical results for the H_α line of neutral hydrogen at three different temperatures. The static-ion results are also included for comparison. The three curves in Fig. 2 exhibit an interesting crossing at $n_e \simeq 5\times10^{15}$ cm^{-3}. Such a crossing can be expected roughly in the density region where the ion collisions start to become "impact", i.e., where $\gamma \simeq \omega_{pi}$. At sufficiently low densities, the duration of an ion collision ($\sim\omega_{pi}^{-1}$) becomes shorter than the coherence time for the transition ($\sim\gamma^{-1}$). In this limit the collisions are completed in the time of interest and become fully dynamical, at least near the line center. In this impact limit, the width decreases with increasing temperature. The situation is quite the opposite at higher densities in the ion dynamic region near the quasistatic region. Here the width increases with increasing temperature because dynamical contributions give rise to more broadening than quasistatic ones. These two opposing trends result in the crossover of the different temperature curves in Fig. 2. Compared to the higher temperature curve, the low temperature curve gives rise to larger widths at lower densities and smaller widths at higher densities. In Ref. 14 we identify four regions of different dependence of the width on reduced mass, temperature, and density, and discuss their physical origins.

In Fig. 3 we compare our theoretical computation with the "impact limit" expression of Stehle.[15] In Fig. 3 the two theoretical results have only a single electron density in common because the impact approximation is not valid at higher densities, and our computational method experiences numerical problems at low densities. At lower densities, more and more particles are contained within the Debye shielding radius, and it becomes difficult to include them all in the numerical simulation of the time-dependent microfields. At $n_e = 10^{14}$ cm^{-3},

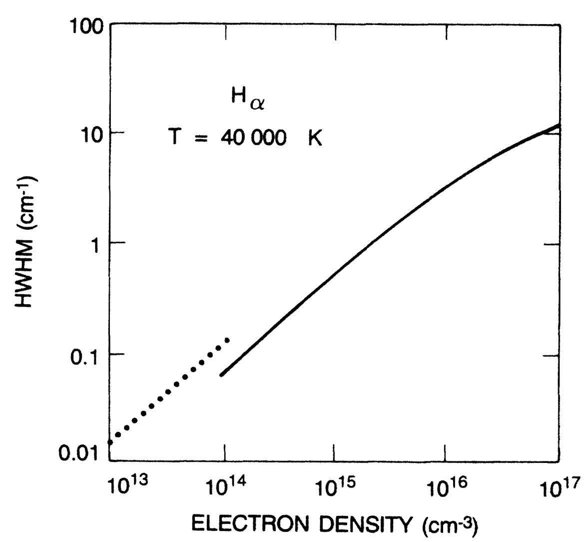

FIG. 3. Calculated half width at half maximum (HWHM) for Balmer-α line of neutral hydrogen with protons as perturbers. Solid curve, dynamic-ion approximation; dotted curve, impact-ion approximation (Ref. 15).

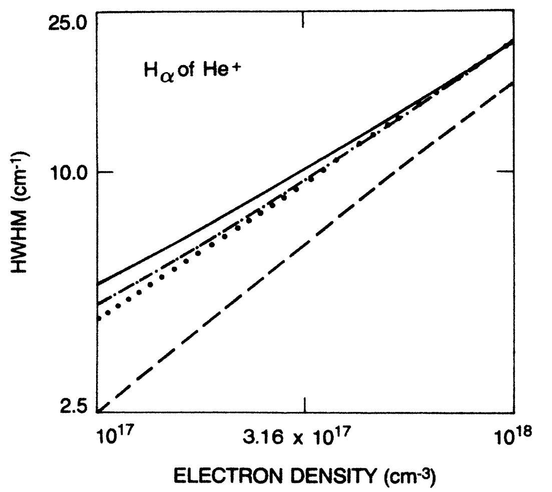

FIG. 4. Calculated half width at half maximum (HWHM) for Balmer-α line of singly charged helium ion with singly charged helium ions as perturbers. Solid curve, dynamic ions at $T=4$ eV; dash-dot curve, dynamic ions at $T=2$ eV; dotted curve, dynamic ion at $T=1$ eV; dashed curve, static ions at $T=4$ eV.

the value of the H_α half-width estimated by Stehle's impact-limit expression is a factor 2 larger than our result. Part of this difference may be due to the fact that the validity criterion for the impact limit is only satisfied by a narrow margin. At $n_e=10^{14}$ cm^{-3}, $T=40\,000$ K, the ratio of the duration of a collision (with impact parameter at the Debye radius) to the time between phase-interrupting collisions (the inverse width) is equal to 0.6, i.e., only slightly less than 1. However, we believe it unlikely that this marginal satisfaction of the validity criterion could account for a factor as large as 2. When the validity criteria are clearly violated, i.e., when the above ratio is a factor of 2 to 3, the slope of the impact-limit curve starts to dip down drastically. But in Fig. 3, the slope of the impact-limit curve is virtually the same as it is at lower densities (not shown). Also, the slope is almost exactly the same as that of our computed results over the next higher decade in density, as seen in Fig. 3. We infer from this that, in the region $n_e \sim 10^{15}$ cm^{-3}, the impact-limit results of Stehle for H_α are roughly a factor of 2 larger than our results and the experimental results in Fig. 1. However, it is worthwhile to note that Stehle's result is contained in a simple analytical expression.[15] It is therefore useful for making estimates within its validity region. The impact limit of Ref. 15 provides effectively an upper limit to the computed collisional width for α lines at low density, a considerably more accurate result in this region than the static-ion approximation, which is the opposite extreme of the impact limit.

In Fig. 4 and Table III we present our theoretical results for the collisional broadening of the H_α line of the He^+ ion. The method of computation is the same as discussed earlier for the H_α line of neutral hydrogen atoms. In this case, the nuclear charge and the reduced mass are, of course, larger. Also, the static-ion microfield distribution[16] against which we normalize our simulated microfields (yielding small corrections) are for a charged point rather than a neutral one. In the numerical simulation of the time-dependent microfield, the perturbers are assumed to move along straight-line paths. According to Greene,[17] the fact that the perturbers actually move in hyperbolic paths around a charged radiator can be safely ignored when $Z_r Z_p^{2/3} a^{2/9} \ll 1$, where the plasma parameter a is equal to ρ_{0_e}/ρ_D.[4] This criterion is satisfied for the conditions of this paper. Also, we note that the fine-structure splitting (not included in our computations) of the two dominant components of the H_α line for the He^+ ion are 5.28 and 4.81 cm^{-1}, respectively. We have not included any experimental results in Fig. 4 because we are not aware of any precise measurements in optically thin uniform plasma conditions. We hope that the challenge of making such measurements will be met in the near future.

In conclusion, our theoretical computations for the

TABLE III. Half width at half maximum (HWHM) in cm^{-1} calculated for the Balmer-α transition ($\lambda=164.0$ nm) of He^+ radiators in plasmas consisting of He^+ perturbers and electrons. Effects due to Doppler mechanism are not folded in.

Plasma temperature (eV)	Approximation	Electron density (cm^{-3}) 10^{17}	3.16×10^{17}	10^{18}
1.0	Dynamic ions	4.28	9.30	21.3
	Static ions	3.15	7.83	20.1
	Doppler	1.17		
2.0	Dynamic ions	4.64	9.53	20.9
	Static ions	2.90	7.24	18.1
	Doppler	1.66		
4.0	Dynamic ions	5.23	10.11	21.2
	Static ions	2.50	6.62	16.6
	Doppler	2.34		

collisional width of the H_α transition of neutral hydrogen are in good agreement with measured values over a wide range of electron densities. The temperature dependences we find are weak, with higher temperature decreasing the width at low densities and increasing the width at higher densities near the quasistatic region. We also present our computed results for the H_α line of the He^+ ion, for which precise experimental results are still not available.

Note added in proof. It has recently been noted by C. Stehle (J. Quant. Spectrosc. Radiat. Transfer) that if one uses the more appropriate "spherical" Debye cutoff for impact approximation for the perturber ions rather than the "cylindrical" one used earlier,[15] one obtains widths that are approximately 15% smaller. This would decrease the difference between the results of impact-ion approximation and dynamic ion calculations shown in Fig. 3.

Vitel [J. Phys. B **20**, 2327 (1987)] has recently reported measurements of line profiles of H_α line in a plasma density near 10^{18} cm^{-3}. We have extended our calculations to the densities between 10^{17} and 10^{18} cm^{-3} [D. H. Oza and R. L. Greene, J. Phys. B (to be published)] and find them in agreement with the experimental results.

ACKNOWLEDGMENTS

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