Accuracy of Stark Broadening Calculations for Ionic Emitters

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The standard static-ion impact electron theory of line broadening is assessed with a calculation of the He II P_α line over a broad range of plasma conditions. Ion dynamics, an improved electron collision operator, and accurate atomic physics are included in the computation. Simulations also have been performed to validate effects included in the calculation at higher densities. Calculated linewidths are compared with experiment over more than two decades in electron density, and broad agreement is found. This provides the first critical evaluation of the assumptions of Stark broadening theory. The profiles also display the first unambiguous evidence of ion dynamics. [S0031-9007(98)07936-8]

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Stark-broadened line-shape calculations based on the standard static-ion impact-electron theory historically have been used to support the diagnostics of thermal plasmas [1]. In the following, the limits of validity of this theory will be assessed through a line profile computation of the He II Paschen-α ($n = 4$ to 3) transition in a broad range of plasma conditions. The large number of effects involved in the calculation, the wide range of plasma parameters, and the extensive experimental line-shape data available suggest that P_α is the appropriate test bed for these Stark broadening calculations. Moreover, benchmark simulations covering the plasma conditions are also available for comparison. The extensive range of available experimental data spans regions in the plasma parameter space for which almost all of the physical effects that can contribute to the line profile become important. These include the interference terms in the electronic collision operator, ion microfield fluctuations, and fine structure and detailed level splitting. Calculations of the atomic parameters of this transition are accessible, but not trivial, so that errors arising from the atomic physics are minimized, and attention can be focused on the line profile computation itself. All of the effects included in this computation have been studied singly or in combination in previous line shape calculations that were restricted to a smaller range of plasma parameters. The present work derives important new information from the range of plasma conditions covered and from the completeness of effects important for the standard Stark-broadening theory of ionic line profiles. It is for these reasons that the present calculations can be used to assess the accuracy of the standard model.

The results presented here are based on calculations performed with PPP [2], a code that has been shown to produce rapid and accurate profiles of spectral lines emitted by multicharged ions in hot dense plasmas that are in excellent agreement with experimental data [3,4]. It constitutes an important advance in the computation of Stark-broadened line shapes for the diagnostic of high density and temperature plasmas [5] such as those produced by lasers or pinches [6]. The calculated P_α line profiles are compared with recent high density plasma experiments [7] and lower density data from previous measurements [8,9], covering more than a two-decade range of electron density N_e with an associated 2 orders of magnitude change in the transition full width at half maximum (FWHM). The present calculations are seen to be in good overall agreement with experiment, except at the highest densities, where the discrepancy is a measure of the accuracy of the standard model. In order to validate the contribution of the different effects included in the calculations for the high density plasma cases, the computed linewidths are also compared with the results of simulations which include both the ionic and the electronic components of the plasma [10].

The modeling of the Stark broadening of transitions from charged emitters is an extremely complicated problem that involves a complex combination of atomic physics data, statistical mechanics, and detailed plasma physics. In a large number of cases in the recent past, the comparison of calculated profiles with experimental spectra was not very satisfactory, due not only to the theoretical difficulties associated with the calculations but also to experimental uncertainties. An example can be found in experiments using laser produced plasmas, as these are often inhomogeneous and transient in nature, rarely yielding data that derives from independently diagnosed N_e and T_e conditions. In addition, these line profile analyses require a simultaneous study of the radiative and kinetic properties of the plasma [11], so that the experimental observation of ionic lines in these plasmas does not provide a benchmark for the theoretical models of line shapes.

In this paper, experiments from well-defined plasma sources have been relied upon for comparison with the calculations. The experimental data considered in this work are obtained from stable, homogeneous plasma created by various discharges, with measured electron densities from 2×10^{16} to 4×10^{18} cm^{-3}. Computations of the spectral line shape of the P_α line emitted from certain of these plasmas have been performed in the past [12,13], but were not in agreement with the measured profiles over a sufficiently large density domain. Previous attempts to calculate this line, using a simplified impact approximation electron collision operator for the upper and lower emitter levels that ignored the interference term in the electron operator [14], failed to agree with experiment, predicting linewidths 50% larger than the experimental widths at densities above 10^{17} cm^{-3}.

A number of improvements to the version of PPP that was employed in Ref. [14] have been made for this work. Most importantly, a more accurate description of the electron collisions has been introduced, since electron impact broadening affects the linewidth significantly for the range of plasma conditions considered here. The modification with the most significant effect on the calculated electron impact width is that of retaining the interference terms in the electron collision operator [15]. Including these terms is an important factor in obtaining the agreement with experiment now found over an extremely wide range of N_e. Another modification to the electron impact operator is to include the effect of the energy separation of the perturbing levels [1,16]. Also, the code now utilizes more accurate atomic physics data, retaining the level fine structure and detailed level splitting. This is especially important for the lowest values of N_e that are considered. Finally, it is found that ion microfield fluctuations are important over almost the entire range of plasma conditions, making it necessary to include the ion-dynamics effect in the calculation.

The ion-dynamics effect is accounted for in PPP through a Markovian line mixing algorithm, the frequency fluctuation model (FFM) [17]. This model differs from previous fluctuation models in that, rather than modeling the perturbative effect of ion microfield fluctuations [18] on the line profile, the Stark components of the line are mixed by a random process. In comparison with the rigorous field fluctuation models that are difficult to apply to complex ionic transitions, the FFM is a practical method for rapid calculations. It has been thoroughly tested through simulation and by calculations of ionic spectra in hot dense plasmas, where the use of the FFM in the PPP code was shown to improve the agreement with experiment [3,4]. This improved agreement was an early indication of the importance of ion dynamics in this regime of plasma conditions, but could not be considered as proof of the presence of this effect, because of uncertainties in the data. In this work, including the contribution of ion microfield fluctuations into the calculation of the spectral shape of P_α yields an accord with the data over such a large range of well-defined plasma conditions that it can be considered to constitute the first definite evidence of the ion-dynamics effect on the spectrum emitted by a charged radiator.

The computed FWHM of P_α over the range, $N_e = 2 \times 10^{16}$–4×10^{18} cm^{-3} is compared with experiment in Fig. 1. Broadening caused by levels other than those of the radiative transition is included in PPP through a procedure for retaining all levels which are significantly coupled by the Stark effect to either the upper or lower group of levels belonging to the radiative transition. For the lowest densities calculated, the only levels retained in the calculation were those of the transition itself ($n = 3$ or $n = 4$). However, for higher densities, the additional broadening due to the $n = 5$ level becomes relevant and is included. Experimental results obtained in different plasma conditions are included in this figure. The plasma temperature varies between 34 000 and 87 000 K, and proton or He$^+$ perturbers are involved, depending on the particular experiment. The experiment of Pittman *et al.* [8] was performed in a pure helium plasma with T_e of the order of 4 eV. The data of Stefanovic *et al.* [9] was acquired in a plasma with predominantly proton perturbers at $T_e = 3.27$ eV. For this experiment, N_e was verified with a He-Ne laser interferometric technique. Finally, at higher densities, the precision results recently obtained by Büscher *et al.* [7] were obtained with a gas liner Z pinch of proton perturbers with $T_e = 4$–7.5 eV, which confirm the previous observations of Gawron *et al.* [19]. The plasma parameters in these experiments were determined independently of the spectroscopy through Thompson scattering. These experiments are comparable as only small changes of the width of the P_α line occur for the different temperatures and perturbers.

In Fig. 1, our calculations are seen to be in excellent agreement with the experimental linewidths over the $N_e = 10^{16}$–10^{17} cm^{-3} range. At higher densities, there is good overall agreement with the experimental trend,

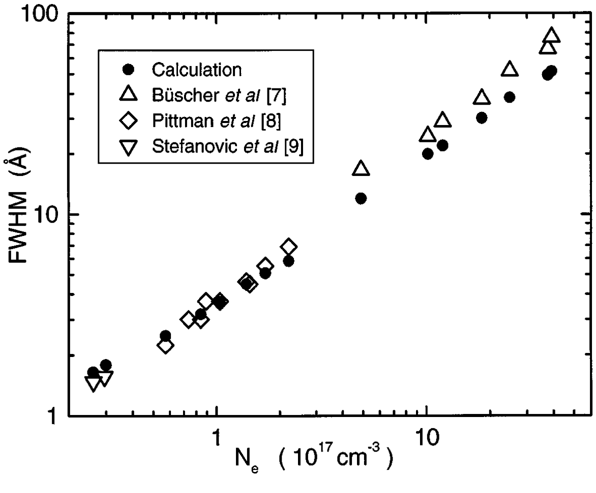

FIG. 1. The FWHM of the He II P_α line versus N_e. Experimental widths obtained by Büscher *et al.* [7] (up triangles), Pittman *et al.* [8] (diamonds), and Stefanovic *et al.* [9] (down triangles) are compared to the calculation (black circles).

but with a tendency for the calculated FWHM to be about 30% below the experimental value. To search for the possible causes of this error, simulations were performed for comparison with the calculations of the high density line shapes. This comparison allows an investigation of the validity of the theoretical assumptions used in the PPP code and gives information on the possible causes of the discrepancy with the high density data.

Simulations of the evolution of the quantum emitter in the plasma microfield can establish benchmark line profiles without introducing an impact or static approximation as is required in the generalized impact theory computation [20–22]. The simulation does, however, incorporate other important assumptions made in the theoretical calculations such as straight line classical trajectories and the restriction to dipole interaction for the emitter-perturber coupling, in accord with the assumptions [16] used in the calculation of the electron collision operator in PPP. This permits the basic hypotheses of the standard model to be tested.

Using the techniques of Ref. [21] to treat in a unified manner both plasma ions and electrons, two component simulations were performed for comparison with the calculations at high density. In Fig. 2, we compare the high density simulation to the results of the PPP code. The simulations retain only the transition levels and do not include broadening effects arising from other states, so that for purposes of comparison we have not included in the theoretical results the broadening due to levels other than those of the radiative transition. The resulting theoretical widths in this figure are, therefore, about 10% narrower than those reported on Fig. 1 for these densities. It can be seen in Fig. 2 that this restricted PPP calculation and the simulation are in close agreement, indicating that the FFM treatment of ion motion and the assumptions included in the impact electronic operator provide an accurate representation of the plasma-emitter dynamic interactions.

The cause of the disagreement with the experimental values must be sought elsewhere, perhaps in approximations common to the model and the simulations, or problems associated with the experimental data. It is unlikely that the experimental densities or half-width measurements have errors of sufficient magnitude to account for the differences found. On the other hand, in both the simulation and PPP a number of approximations could be in doubt. For instance, the assumption of dipolar interaction neglects higher multipole contributions to the broadening which are known to become more important as N_e increases. In addition, it has been suggested that the use of hyperbolic ion trajectories [23] instead of the classical straight line path assumption [16], used in both the simulations and the calculation of the PPP electron collision operator, might have a large effect on the linewidth. Finally, the treatment of ion dynamics by the FFM or the Markov methods of Ref. [18] assumes abrupt changes in the ion microfield. More gradual changes, such as those associated with microfield rotation, are ignored, so a more detailed calculation of this effect may be required. Other issues could be associated with effects that are not included in the standard line-shape formulation such as quenching collisions or He ion recombination effects. These, of course, also have not been taken into account in the simulations.

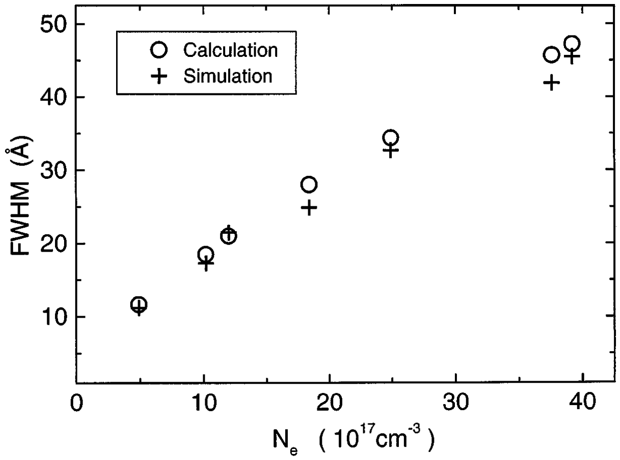

FIG. 2. Comparison of the width (FWHM) of the P_α line versus N_e as calculated by the PPP code (circles) and the simulation (crosses).

The important role of ion dynamics as a function of N_e is illustrated in Fig. 3, where the FWHM of P_α calculated for proton perturbers and $T_e = 38\,000$ K with PPP and FFM ion dynamics is compared to a PPP static-ion calculation. As can be seen, ion dynamics results in an increase of the width by 35% for the high density data of Büscher *et al.* [7], and a 50%–70% increase, respectively, for the lower density experimental conditions of Pittman *et al.* [8], and Stefanovic *et al.* [9]. The additional broadening due to ion dynamics affects essentially the central part of the line. These large contributions to the linewidth, necessary for agreement with experiment,

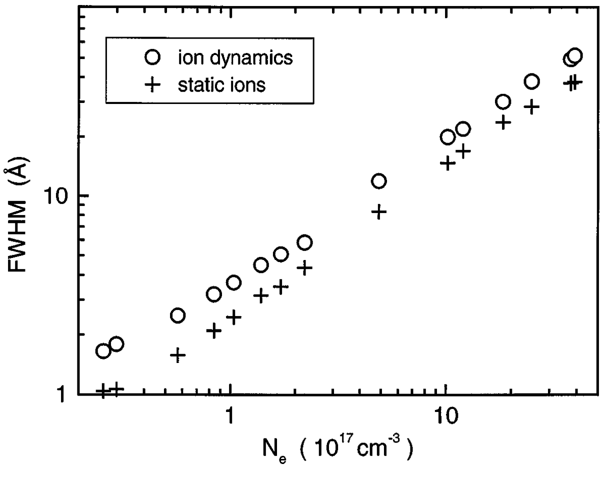

FIG. 3. Calculated FWHM of P_α versus N_e for dynamic ions (circles) compared to the static-ion case (crosses) for the same plasma conditions as in Fig. 1.

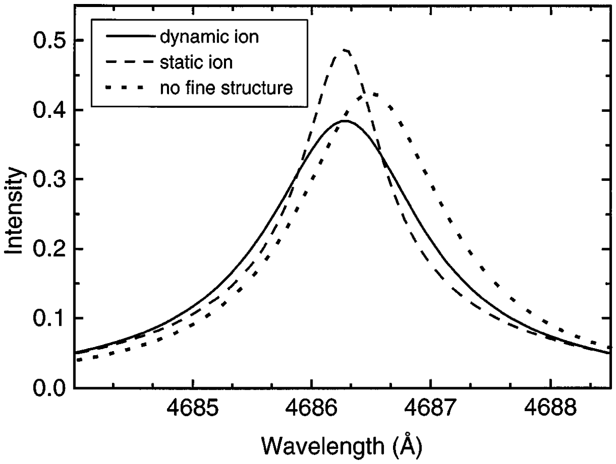

FIG. 4. Calculated P_α profiles for $N_e = 2.61 \times 10^{16}$ cm^{-3} and $T_e = 38\,000$ K. Dynamic-ion (solid line) and static-ion (dashed line) profiles retaining fine structure are compared to a dynamic ion profile without fine structure (dotted line).

constitute the first unambiguous evidence of ion dynamics in lines radiated by ionized emitters.

In Fig. 4, the spectrum calculated with and without fine structure is presented to illustrate the importance of fine structure in the computation of the line profile. This calculation was performed for a plasma composed of 10% He II and 90% protons with an $N_e = 2.61 \times 10^{16}$ cm^{-3} and $T_e = 38\,000$ K. We note that neglecting fine structure results in a profile which is 7% narrower and shifted by 0.2 Å to the red, compared to the full calculation. The asymmetry of this profile is an indication of the underlying effect of the fine structure. In Fig. 4, we have also plotted the profile obtained by retaining the fine structure, but neglected ion dynamics to again illustrate the dramatic effect on the line shape.

In summary, the role of ion dynamics is confirmed for the benchmark case of He$^+$. In addition, we have shown that an impact-electron static-ion calculation of the He II P_α line, including fine structure, ion dynamics, and an electron broadening operator retaining interference terms, is in agreement with experimental observations over more than 2 orders of magnitude in density with a discrepancy only at the highest densities. These results demonstrate that a model with these features will permit accurate plasma density diagnostics to be based on profile calculations of ionized emitters. The calculation presented is also in agreement with simulation calculations at high density, which validates the basic theoretical line-shape assumptions. There remains a 30% discrepancy with the high density data, which we believe can now be stated as the limit of the validity of this theoretical formulation. We note that although line shapes and linewidths of ion lines have been used for the diagnostics of plasmas for many years, the present paper provides the first assessment of the accuracy of the calculations over a very wide range of plasma conditions. Thus, one can now predict plasma density within an accuracy of $\sim$30% using a modified static-ion impact-electron model such as that contained in the PPP code. To improve the accuracy of this model, the electron collision operator may have to be modified in order to include additional effects such as quadrapole interactions, hyperbolic trajectories, and perhaps impact ions. Further work on the observed shift of the line will require, in addition to an accurate model of the ionic shift, a quantum mechanical theory for the emitter-electron perturber interaction [24].

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