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Electronic broadening model for high-*n* Balmer line profiles

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A method for line profile computations of Stark broadened high principal quantum number (PQN) Balmer series transitions is presented. Since quasistatic electron effects must be included in these cases, the traditional low density/low quantum number impact approximation for the electron broadening operator cannot describe the entire profile. For the high plasma densities and/or high principal quantum numbers (PQN>12) considered, an improved electron broadening contribution is proposed. Using a frequency dependent electron broadening operator, the line profile of the H Balmer $n=13$ transition is calculated using this electron operator and compared with profiles obtained using very accurate numerical simulations. The good agreement suggests that the procedure is sufficiently accurate to provide a predictive capability. [S1063-651X(98)50312-1]

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INTRODUCTION

Plasma conditions in the edge, divertor, and *X*-point regions of tokamaks strongly affect the conditions in the main plasma [1]. Therefore, a knowledge of the conditions in these region is very important for a better understanding of tokamak performance. Measurements of atomic hydrogen and hydrogen isotope linewidths [2] have been used to infer electron densities in these regions through a comparison of the data with calculated linewidths [3,4]. In Ref. [3], Bengston, Tannich, and Kepple used a fast and reliable computational code, based on the frequency fluctuation model (FFM) [5,6], to calculate the entire spectrum that could be directly compared to the experimental data. The FFM, which uses the usual separation of the plasma emitter interactions into homogeneous broadening effects due to electrons and inhomogeneous broadening arising from ions, works reasonably well in applications to standard cases, e.g., low density or small PQN. Electrons are treated in the impact approximation with a frequency independent electron collision operator in these standard applications, and this results in a Lorentzian shape for the homogeneous components. However, in cases of either high plasma density or large PQN it is necessary to account for quasistatic electron effects and the homogeneous components are not purely Lorentzian. In the following, we develop an improved model for the electron broadening that accounts for quasistatic contributions. Further, we demonstrate through a simulation technique that this leads to improved accuracy of the calculated linewidths and consequently, to improved density diagnostics.

METHOD

At high densities, overlapping strong electron collisions arise and the impact approximation breaks down. Obtaining the effect of the electrons on the line profile then becomes essentially the same as the ion dynamics problem, and equivalent methods can be used whenever the electrons can be described classically [7]. Except for experimental data combined with independent measurements of the plasma conditions, a fundamental insight into the ion dynamics problem is difficult. One method for understanding this problem has been through benchmark numerical simulation [8,9]. This method is based on creating a set of time dependent microfield configurations, generated using a standard molecular dynamics (MD) method, and then calculating the evolution operators, $U_l(t)$, by a stepwise integration of the Schrödinger equation for each configuration. Finally, the mean evolution operator, $U(t)=\langle U_1(t)\rangle$, is obtained by averaging over the configuration set and, the line shape is the Fourier transform of the dipole correlation function, $C(t)=\langle\langle \mathbf{d}|U(t)|\mathbf{d}\rho_0\rangle\rangle$. The number of such integration processes must be large enough to obtain low noise results. Profiles obtained by this procedure can be considered to be benchmarks for theoretical calculations and are used to test the accuracy of different models.

Alternatively, theoretical approximations such as the unified classical path theory [10,11], and semiempirical procedures [12,13], can produce line shape expressions that cover the frequency range from the line center to the static line wing, including the transition region. One semiempirical formulation uses the following prescription for the line profile $I(\omega)$, for $0\leq\Delta\omega\leq\omega_{\mathrm{WF}}$ (where ω_{WF} is the Weisskopf frequency):

$$I(\Delta\omega)\propto\frac{\Phi(\Delta\omega)}{\Delta\omega^2+[\Phi(\Delta\omega)]^2}, \tag{1}$$

with

$$\Phi(\Delta\omega)=\left(\frac{4\pi}{3}\right)\left(\frac{2m}{\pi kT}\right)^{1/2}N_e\left(\frac{\hbar}{m}\right)^2\vec{R}\cdot\vec{R}\times\left(C_n+\frac{1}{2}\int_y^\infty e^{-x}\frac{dx}{x}\right).$$

Here $\Phi(\Delta\omega)$ is the frequency dependent collision operator, m is the perturber mass, and $\vec{R}$ is the position operator of the emitter electron. The C_n is a strong collision term dependent on the PQN, n, with $C_2=1.5$, $C_3=1.0$, $C_4=0.75$, $C_5=0.5$, and $C_n=0.4$ for $n>5$. Finally, y is a frequency dependent parameter, given by

$$y\approx\left(\frac{\hbar n^2}{2}\right)^2\frac{\omega_{\mathrm{PE}}^2+\Delta\omega^2}{E_{\mathrm{H}}kT}, \tag{2}$$

with ω_{PE} the electronic plasma frequency and E_{H} the hydrogen ionization energy. For $\omega_{\mathrm{WF}}\leqslant\Delta\omega$, the line profile is taken to be

$$I(\Delta\omega)\propto\Delta\omega^{-5/2}, \tag{3}$$

corresponding to the well-known Holtsmark [14] asymptotic quasistatic limit. The three different regimes described by this empirical expression for the electron contribution can be considered as related to three parts of the line profile. From the center of the line to ω_{PE}, the collision operator Φ is essentially frequency independent. Then from ω_{PE} to ω_{WF}, the profile is obtained using the impact theory corrected for a frequency dependent impact parameter cutoff (the Lewis cutoff [15]). Finally, for frequency separations from line center greater than ω_{WF}, the electrons are assumed to be static, and the corresponding profile in this region is well described by the quasistatic Holtsmark theory.

The various theories, valid in the regions defined above, are based on one or more of the following set of approximations. First, the collective properties are assumed to occur through the electron plasma frequency. Second, the impact approximation, which relies on the following hypotheses: (i) strong collisions do not overlap in time, (ii) a weak collision overlapping a strong one is negligible in comparison, and (iii) the average collision is weak, allowing treatment by second-order perturbation theory. Finally, the quasistatic approximation assumes that the time of interest (essentially the inverse of the frequency separation from line center) for the calculation of the corresponding region of the profile is sufficiently short so that the perturber collision process can be considered to be effectively static, i.e., time independent.

If, as in the present case, the regions, as defined above, for the impact and quasistatic regimes overlap significantly, the influence of the perturbation (or the corresponding field fluctuations) on a profile should not be described by a purely collisional point of view. In fact, due to the long-range nature of the Coulomb interaction, even with Debye screening the field at the emitter can be considered to result from a number of electrons. The electron configuration creating this field changes when the electrons move, and it is usual to assume that the correlation is lost when the configuration changes. That is, when the average displacement in a configuration is approximately the mean distance between the plasma electrons, the correlation can be considered to be lost. Hence, in place of the electron plasma frequency limiting the impact regime, we shall use the inverse time corresponding to a configuration change, r/v, as the characteristic time of the interaction, with the average distance, $r=(N_e4\pi/3)^{1/3}$, and the average thermal velocity $v=(kT/m)^{1/2}$. This cutoff is suitable whenever both this inverse correlation time and the linewidth are larger than the plasma frequency. It is thus appropriate for the present problem with high PQN states of the emitter or for high density.

RESULTS

We report here pure electron profile calculations of a high PQN hydrogen Balmer transition ($n=13\rightarrow n=2$) using the line shape formulation and electron operator described above. Further, comparisons with accurate simulations for tokamak plasma conditions are presented. The ion contribution is neglected to focus on our revised electron broadening mechanism. In addition, in order to perform efficient simulations for comparison with the calculated line profiles, a simplified atomic system will be considered in the following. That is, in the spherical basis set used to write the coupling terms between the MD stochastic electric fields and the emitter dipole, only the *s*, *p*, and *d* levels in the $n=13$ to $n=2$ level system of the Balmer α line are retained. That is, the levels $|13,0,0\rangle$, $|13,1,m_l\rangle$, $|13,2,m_l\rangle$, and $|2,0,0\rangle$, $|2,1,m_l\rangle$ are extracted from the set of levels of the atomic system belonging to the transition. In addition, for comparison, model computations and simulations that include the *f* states, the next most relevant states for Stark broadening of the Balmer α lines in the upper manifold for PQN>3, have been carried out. This is useful to understand the essential behavior of the profiles that would result from atomic systems with the complete H_{13} transition set. The comparisons will be illustrated for the case $N_e=10^{15}$ cm^{-3}, the mid-density of the investigated density domain. The other calculations are performed without the *f* level. Although the profiles, as approximated, are not a good representation of the H_{13} line, the results of the model calculations and the simulations are in excellent agreement when the same reduced system is used for the two methods. These comparisons are useful to confirm the accuracy of the model for the electron density range studied. As a result, it can be assumed that the model calculation will produce accurate profiles when the whole quantum system of the H_{13} transition is used, even though it is no longer possible to compare with simulations in this case.

In the simulations, the following equation is solved by stepwise integration on a time dependent electron field configuration:

$$\frac{dU_1(t)}{dt}=-i[L_0+\vec{d}\cdot\vec{E}_1(t)]U_1(t)\qquad U_1(0)=1, \tag{4}$$

where L_0 is the Liouville operator corresponding to the unperturbed emitter transition energies. The time dependent electron field configurations are obtained by MD simulation where atomic deuterium is considered to be perturbed by an electron thermal bath. The interactions between electrons are included and the exclusion volume around neutrals, neces-

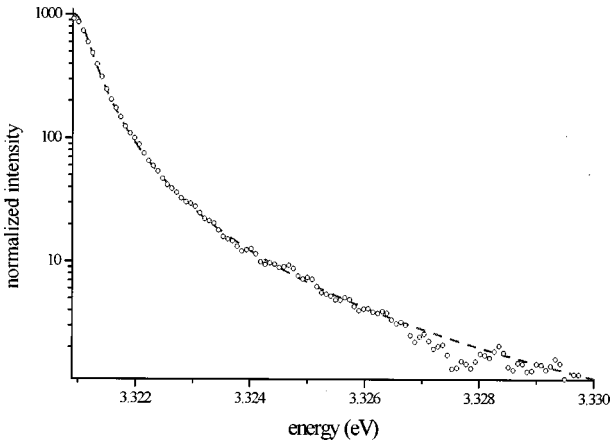

FIG. 1. Comparison between the simulation (circles), and the semiempirical model (dashed line) calculated with the $13spdf$-$2sp$ atomic system. The calculations were performed with plasma conditions $N_e=10^{14}$ cm^{-3} and $T=4$ eV.

sary to avoid divergence, has been chosen so as to account for strong collisions. Due to the occurrence of strong, short events, the integration time step must be chosen carefully. To obtain the reference simulations, profiles for various densities ($10^{14}\leqslant N_e\leqslant 10^{17}$ cm^{-3}) and one temperature ($T_e=4$ eV) have been calculated.

In Figs. 1 and 2, we have plotted the simulation and the model results for two different densities, $N_e=10^{14}$ cm^{-3} and $N_e=10^{16}$ cm^{-3}, respectively. We choose a logarithmic intensity scale to illustrate the frequency extent of the overall agreement for profiles calculated in the two different ways. Results obtained for $N_e=10^{15}$ cm^{-3} show similar agreement. However, the $N_e=10^{17}$ cm^{-3} results exhibit a larger discrepancy, since the electrons become more static and the impact description is no longer applicable. Figure 3 illustrates the same results as Fig. 2 but with a linear intensity scale to more clearly show the relative location of the characteristic cutoff frequencies. The results for the full width at half maximum have been summarized in Table I. The small discrepancies result from the effect of both the semiempirical model itself and remaining noise in the simulation calculations. It should be kept in mind that in these comparisons, relaxation effects due to ions are not considered, and that, since this further damping mechanism would smooth the line shape,

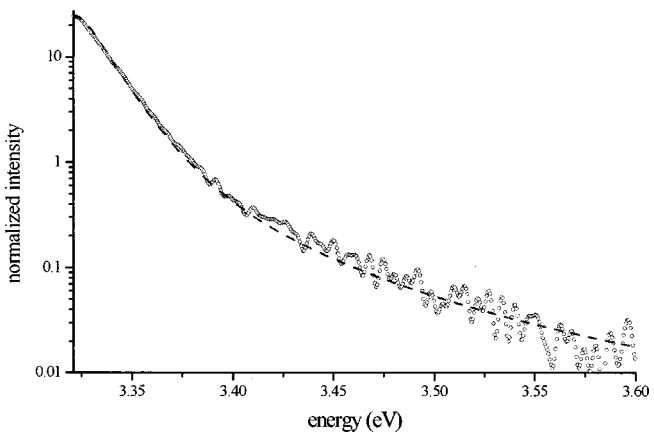

FIG. 2. Same as Fig. 1 but with $N_e=10^{16}$ cm^{-3}.

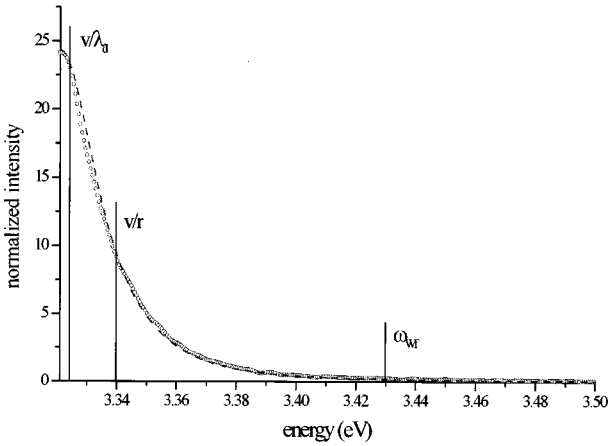

FIG. 3. Comparison between the semiempirical model (dashed line) and the simulation (circles). The present results were obtained for $N_e=10^{16}$ cm^{-3} and $T=4$ eV. Vertical lines indicate the positions of the electronic plasma frequency, the new cutoff frequency, and the Weisskopf frequency.

the line profiles would become less sensitive to these effects. Consequently, a model giving reasonable agreement without considering ions will certainly appear more accurate when the perturbing ions are taken into account.

In Fig. 4, we present the results of the model calculation and the numerical simulation for the larger atomic system, e.g., $n=13s$, p, d, and f to $n=2s$ and p. Here again, the agreement is excellent, which suggests that the validity of the model is independent of the number of states retained in the calculation. Although, of course, the profile is only correctly described if all the states are included. This comparison provides justification for the use of the model in the calculation of the high-n Balmer lines. Figure 5 emphasizes the strong discrepancy between the results of Fig. 4 and the H_{13} line profile calculated as a pure Lorentzian profile using Eq. (1) with $\Delta\omega=0$.

CONCLUSION

In conclusion, we have shown through detailed calculation of the H_{13} line that a semiempirical model of electron broadening taking into account a quasistatic electron effect can be justified. The model is limited here to a quantum system representative of the H_{13} line and a plasma density domain of over three orders of magnitude. Comparisons with accurate MD simulations provided a clear estimate of the validity domain. For densities smaller than a critical density, $N_e=10^{16}$ cm^{-3}, excellent agreement is obtained. Above this

TABLE I. Summary of the comparisons between the results of the simulation and the model for the reduced ($13spd$-$2sp$) atomic system, in terms of the full width at half maximum.

Density (cm^{-3})	$\Delta\omega_{1/2}$ (eV) simulation	$\Delta\omega_{1/2}$ (eV) model	Relative error
10^{14}	7.01×10^{-4}	6.13×10^{-4}	13%
10^{15}	4.81×10^{-3}	4.64×10^{-3}	3.5%
10^{16}	2.93×10^{-2}	3.04×10^{-2}	4%

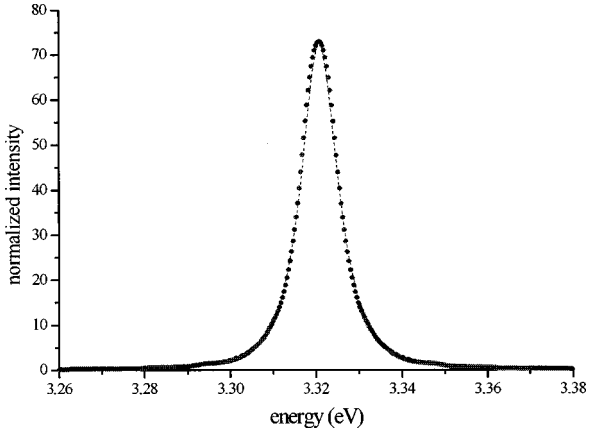

FIG. 4. Comparisons between the simulation results (circles) and the model results (dashed line) for the line calculated with the $13spdf$-$2sp$ atomic system. The calculations were performed with the plasma conditions $N_e = 10^{15}$ cm^{-3} and $T = 4$ eV.

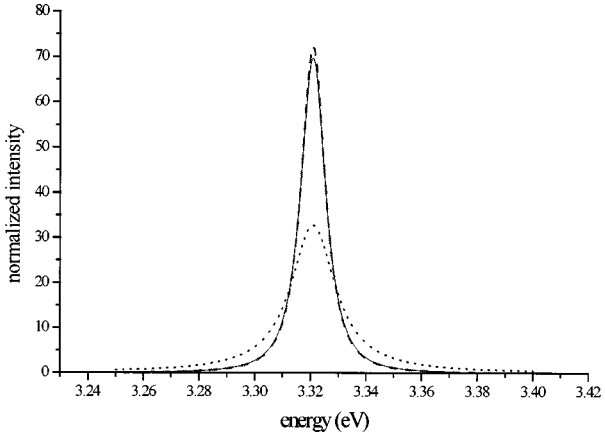

FIG. 5. Neutral deuterium H_{13} line profile (solid line) compared with the line calculated with the reduced atomic system $13spdf$-$2sp$ (dashed line) and with a pure Lorentzian profile (dots). The calculations were performed with plasma conditions $N_e = 10^{15}$ cm^{-3} and $T = 4$ eV.

density, the model fails due to the occurrence of simultaneous strong collisions, and another description of the electron effect on the line profile must be used. These cases, where the impact approximation breaks down, are similar to the ion dynamics effects that have been addressed previously. Therefore, it is likely that the same methods can be used. One possibility for the calculation of profiles in such conditions would be to use the frequency fluctuation model for the electrons. This would permit one to obtain a dynamical profile for the electrons. The convolution of the profile thus obtained with the ion quasistatic profile should give a good approximation for the total profile in cases where the proposed model is invalid. A detailed investigation of the limits of validity of the model and a thorough description of the alternative possibilities for calculations outside the region of validity will be given in a future publication.

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