# Inclusion of ion dynamics in the unified classical path theory of Stark broadening

Ronald L. Greene\*

Department of Physics and Astronomy, University of Florida, Gainesville, Florida 32611 (Received 4 December 1978)

<sup>A</sup> theory of Stark broadening of hydrogenic radiators which adds ion dynamic corrections to the unified theory of Smith, Cooper, and Vidal is presented. The dynamic parts of the ion collisions are treated in an impactlike approximation, which is justified for certain plasma conditions by the static-ion field cutoff in the ion interaction integrals. Approximate results are presented for the Lyman- $\alpha$ , Lyman- $\beta$ , and H- $\alpha$  lines of hydrogen, and comparison is made to experiment and to other theories.

# I. INTRODUCTION

As is well known, the experiment of Grützmacher and Wende<sup>1</sup> on the Stark-broadened Lyman- $\alpha$  line of hydrogen has demonstrated a. large discrepancy in the width of that line between experiment and the theoretical calculations of Smith  $et al.<sup>2</sup>$  and Kepple and Griem.<sup>3</sup> The results of several calculations<sup>4-6</sup> of the Lyman- $\alpha$  line, which include dynamic corrections to the ion broadening, suggest that most of the discrepancy may be removed by including the motion of the perturbing ions in the calculation of the line-shape function. However, there are several disadvantages to the theoretical formulations of Refs. 4-6. The adiabatic method used by Voslamber<sup>5</sup> for the Lyman- $\alpha$ line cannot be easily generalized to other hydrogen lines and relies on an  $ad$  hoc estimation of an important angular average. The second-o'rder calculations of Lee<sup>4</sup> suffer from a lack of a clear theoretical justification for the binary treatment of ion dynamic corrections. Furthermore, the results are very sensitive to the choice of the strong-collision cutoff on the impact parameter of the ion collisions. The model microfield method has been used by Seidel $6$  for a number of different hydrogen lines. However, the physical approximations of the theory are not clear, so it is difficult to see how it might be improved by the removal of approximations.

In view of the above comments it is clear that a truly satisfactory theory including ion dynamics has not been found. In this paper I will present an alternative treatment of ion dynamics. The theory is such that for frequency separations from line center greater than the ion plasma frequency the ion broadening goes over to the familiar quasistatic theory using the microfields of Hooper.<sup>7</sup> The dynamic aspects of ion collisions, which are important inside the ion plasma frequency, are treated with an impactlike approximation. The approximation and its validity are discussed in Sec. II. It will be seen that although

the theory removes some of the shortcomings of previous approaches, it introduces some of its own and thus should be viewed as a different, rather than improved, theory. It is expected, however, that the limitations of the theory are such that it may be consistently improved by further work.

#### II. THEORY

### A. Formalism

As shown by a number of authors (see, for example, Refs. 8 and 9) the line-shape function may be expressed as

$$
I(\omega) = \frac{1}{\pi} \operatorname{Re} \int_0^{\infty} e^{i\omega t} \Phi(t) dt , \qquad (1)
$$

where the dipole autocorrelation function  $\Phi(t)$  is given in the weak-coupling approximation<sup>9</sup> by the trace over atom and perturber subsystems:

$$
\Phi(t) = \mathrm{Tr}_{a} \{ \vec{d} \cdot \mathrm{Tr}_{\rho} [T^{\dagger}(t) \vec{d} T(t) \rho^{(\rho)}] \rho^{(a)} \}.
$$
 (2)

The quantities  $\rho^{(a)}$  and  $\rho^{(b)}$  are density matrices of the free atom and perturbers, respectively, and the time-development operator  $T(t)$  satisfies

$$
i\hbar \frac{\partial T(t)}{\partial t} = [H_a + V(t)]T(t) , \qquad (3)
$$

with

$$
V(t) = \exp(iH_p t/\hbar) V \exp(-iH_p t/\hbar) . \tag{4}
$$

 $H_a$  and  $H_b$  are the Hamiltonians for the atom and perturber subsystems and  $V$  is the interaction between the two.

At this point the static-ion approximation is usually made. I will not make that assumption, but will assume that the electrons and ions may be treated as independent quasiparticles which interact with the radiator by means of Debyeshielded fields. The approximation of perturber correlations by means of Debye shielding of interactions is common in plasma Stark broadening.<sup>8,9</sup> Its validity requires that the num

19

2002 **2002 2002 2002 2002 2003 2004 2005 2004 2006**

19

ber of particles in a Debye sphere be large, which results in an upper limit to the electron density. This approximation does not consider the possibility of fluctuations in the screening which could be a source of additional broadening.<sup>10</sup> I will not consider fluctuations of this type; this paper will deal with ion dynamic effects only.

With the assumption of statistically independent quasiparticles, the interaction  $V(t)$  may then be written as a sum of ion-atom and electron- atom parts,

$$
V(t) = V_I(t) + V_E(t) \tag{5}
$$

It is convenient to write this in terms of  $V_1(t=0)$ , that is,

$$
V(t) = V_I(0) + W_I(t) + V_E(t) , \qquad (6)
$$

where

$$
W_I(t) = V_I(t) - V_I(0) \tag{7}
$$

Defining a new time-development operator  $U(t)$ by the equation

$$
T(t) = \exp\{-i[H_a + V_I(0)]t/\hbar\}U(t) ,
$$
 (8)

it can be shown that  $U(t)$  satisfies the equation

$$
i\hbar \frac{\partial U}{\partial t}(t) = [\tilde{W}_I(t) + \tilde{V}_E(t)]U(t) , \qquad (9)
$$

with

$$
\tilde{W}_I(t) = \exp\left\{i[H_a + V_I(0)]t/\hbar\right\}W_I(t)
$$
\n
$$
\times \exp\left\{-i[H_a + V_I(0)]t/\hbar\right\}
$$
\n(10)

and

$$
\begin{aligned} \tilde{V}_E(t) &= \exp\left\{i[H_a + V_I(0)]t/\hbar\right\} V_E(t) \\ &\times \exp\left\{-i[H_a + V_I(0)]t/\hbar\right\}. \end{aligned} \tag{11}
$$

For convenience I will henceforth use

$$
H_0 = H_a + V_I(0) \tag{12}
$$

 $H_0$  is thus the Hamiltonian of an atom in the (static) initial field of the iona. Note that the interactions  $W_I(t)$  and  $V_E(t)$  may be written as a sum of single-particle interactions over all ions or electrons, respectively; that is,

$$
\widetilde{W}_I(t) = \sum_j \widetilde{W}_j(t) \tag{13}
$$

and

$$
\tilde{V}_E(t) = \sum_j \tilde{V}_j(t) \tag{14}
$$

For the sake of simplicity I will consider lines for which the broadening of the lower state is negligible for the remainder of this discussion. The more general case will follow the same

analysis if tetradic operators are used. For the case of no lower-state broadening, the trace over perturber states becomes

$$
\mathrm{Tr}_{\mathbf{p}}[T^{\dagger}(t)\bar{\mathbf{d}}T(t)\rho^{(\mathbf{p})}] - \mathrm{Tr}_{\mathbf{p}}[e^{iH_{0}t/\hbar}\bar{\mathbf{d}}]
$$

$$
\times e^{-iH_{0}t/\hbar}U(t)\rho^{(\mathbf{p})}].
$$
 (15)

Since I am assuming that the electrons and ions act as statistically independent quasiparticles, the trace over perturbers may be broken into separate traces over ion and electron states; hence

$$
\mathrm{Tr}_{\rho}[e^{iH_0t/\hbar}\tilde{\mathbf{d}}e^{-iH_0t/\hbar}U(t)\rho^{(\rho)}]
$$
  
\n
$$
=\mathrm{Tr}_{I}[e^{iH_0t/\hbar}\tilde{\mathbf{d}}e^{-iH_0t/\hbar}\hat{U}_I(t)\rho^{(I)}]
$$
  
\n
$$
\times\mathrm{Tr}_{E}[U_E(t)\rho^{(E)}].
$$
\n(16)

The ion and electron time-development operators satisfy

$$
i\hbar \frac{\partial \hat{U}_I(t)}{\partial t} = \tilde{W}_I(t) \hat{U}_I(t)
$$
\n(17)

and

$$
i\hbar \frac{\partial U_{R}(t)}{\partial t} = \tilde{V}_{R}(t) U_{R}(t) . \qquad (18)
$$

The average over electron states will be treated with the impact approximation so that it may be  $written<sup>11</sup>$ 

$$
Tr_E[U_E(t)\rho^{(E)}] = \exp[N_E\langle U_e(t)-1\rangle], \qquad (19)
$$

where  $N_E$  is the number of electrons present and  $\langle U_{\mathbf{e}}(t) - 1 \rangle$  is an average over single electron-radiator collisions.

In most Stark-broadening theories the average over ion perturbers has been transformed to an<br>average over static-ion fields.<sup>12</sup> This static-io average over static-ion fields. $^{12}$  This static-io: approximation is excellent over most of the line profile, but breaks down near the line center where the time of interest  $t \sim 1/\Delta \omega$  becomes large. Because of the ability of the static method to treat simultaneous multiple interactions (via the ion microfield<sup>7, 12</sup>), it is advantageous to retain the static field average and treat the dynamics as a correction. For this reason I shall assume a dipole approximation for  $V_1(0)$ ,

$$
V_I(0) = -\,\overline{\dot{\mathbf{d}}}\cdot\overline{\dot{\boldsymbol{\xi}}}_I(0)\,,\tag{20}
$$

and write the trace as

$$
\operatorname{Tr}_{I}[e^{iH_{0}t/\hbar}\tilde{\mathbf{d}}e^{-iH_{0}t/\hbar}\hat{U}_{I}(t)\rho^{(I)}]
$$
\n
$$
=\int_{0}^{\infty}d\epsilon e^{iH_{0}t/\hbar}\tilde{\mathbf{d}}e^{-iH_{0}t/\hbar}\operatorname{Tr}_{I}[\hat{U}_{I}(t)\rho^{(I)}]
$$
\n
$$
\times \delta(\epsilon-\epsilon_{I}(0))]
$$
\n
$$
=\int_{0}^{\infty}d\epsilon e^{iH_{0}t/\hbar}\tilde{\mathbf{d}}e^{-iH_{0}t/\hbar}P(\epsilon)\langle \hat{U}_{I}(t)\rangle_{\epsilon}. (21)
$$

The average  $\langle \hat{U}_{I}(t) \rangle_{\epsilon}$  is a conditional average over ions such that  $|\Sigma_i \xi_i(0)| = \epsilon$ , and  $P(\epsilon)$  is the ion field probability distribution function.<sup>7</sup> Note that

 $\langle \hat{U}_r(t-0) \rangle_{\epsilon} = 1$ , so that the quasistatic limit of the trace is maintained. Since the ion interaction  $W_r(t)$  may be written as a sum of single-particle interactions, the operator  $\hat{U}_I(t)$  may be written as an ordered product of overlapping single- particle time-de-

$$
\hat{U}_I(t) = O_N \prod_j \hat{U}_j(t) . \tag{22}
$$

Each  $\hat{U}_i(t)$  may be formally written as a timeorde red exponential,

velopment operators, $<sup>11</sup>$ </sup>

$$
\hat{U}_j(t) = O \exp[(i/\hbar) \int_0^t \tilde{W}_j(t') dt'] \,. \tag{23}
$$

Because of the initial ion field exponentials of  $\tilde{W}_i(t)$ , the upper limit of the integral is effectively bound by a time

$$
\tau \sim \hbar / \Delta_{\epsilon} , \qquad (24)
$$

where  $\Delta_{\epsilon}$  is the ion field splitting of the atomic states. This cutoff is also present for electron collisions, $8$  but is usually ignored because it is a small effect. Since for times less than  $\tau$  given in (24) the exponentials are approximately one, the argument of the exponential may be approximated by dropping the exponential and using an upper cutoff of  $\tau$ .

To continue, I shall define a "weakly dynamic"

collision as one for which  
\n
$$
\frac{1}{\hbar} \int_0^t \tilde{W}_j(t') dt' \simeq \frac{1}{\hbar} \int_0^{\tau} W_j(t) dt \ll 1,
$$
\n(25)

and a "strongly dynamic" collision as one for which

$$
\frac{1}{\hbar} \int_0^t \tilde{W}_j(t') dt' \simeq \frac{1}{\hbar} \int_0^{\tau} W_j(t) dt \ge 1.
$$
 (26)

Since the two or more particle overlap terms are of fourth order or higher in the interaction inteof fourth order or higher in the interaction inte-<br>gral,<sup>11</sup> if strongly dynamic collisions do not overlap in time, the ordering operator  $O<sub>N</sub>$  may be dropped from Eq. (22). In this case

$$
\widehat{U}_I(t) = \prod_j \widehat{U}_j(t) \tag{27}
$$

I will examine the validity of this approximation later in this section.

Using the statistically independent quasiparticle assumption, the average over ions may now be written

$$
\langle \hat{U}_{I}(t) \rangle_{\epsilon} = \left\langle \prod_{j} \hat{U}_{j}(t) \right\rangle_{\epsilon} = \langle \hat{U}_{I}(t) \rangle^{N_{I}}. \tag{28}
$$

Equation (28) is not strictly correct since the

ions are related through the condition  $|\sum_i \vec{\xi}_i(0)|$  $=\epsilon$ ; however, if  $N_I$  is sufficiently large this requirement should have only a small effect on the average. It is difficult to assess the effect of this approximation at this time. A study of its validity is planned for future work. Using Eq. (28), the ion average may now be written in terms of a one-particle average using the same terms of a one-particle average usi<br>approach as for electrons,<sup>11</sup> that is,

$$
\langle \hat{U}_{I}(t) \rangle_{\epsilon} = \exp[N_{I} \langle \hat{U}_{I}(t) - 1 \rangle]. \tag{29}
$$

[Compare with Eq. (19).] Thus the autocorrelation function  $\Phi(t)$  has been simplified to

$$
\hat{\Phi}(t) = \int_0^\infty d\epsilon \, P(\epsilon) \, \mathrm{Tr}_a \{ \vec{d} \cdot e^{iH_0 t/\hbar} \vec{d} \, e^{-iH_0 t/\hbar} \}
$$
\n
$$
\hat{U}_j(t) = O \exp\left[ \left( i/\hbar \right) \int_0^t \tilde{W}_j(t') \, dt' \right].
$$
\n(23)\n
$$
\times \exp\left[ N_E \langle U_e(t) - 1 \rangle + N_f \langle \hat{U}_i(t) - 1 \rangle \right] \rho^{(a)} \}.
$$
\n(30)

The Fourier transform of Eq. (30) may be obtained in the manner of Smith  ${et}$   ${al.}, ^{11}$  which leads to an expression for the line shape  $I(\omega)$  identical to the unified theory result<sup>2,11</sup> except that the broadening operator  $\mathfrak{L}(\Delta\omega)$  includes both electron and dynamic-ion contributions:

$$
\mathcal{L}(\Delta \omega) = -i \int_0^\infty dt \, e^{i\Delta \omega t} \left[ N_E \langle U_e(t) - 1 \rangle \right. \\
\left. + N_I \langle \hat{U}_i(t) - 1 \rangle \right], \tag{31}
$$

where  $\Delta\omega$  is the frequency separation from line center. The operator  $\hat{U}_i(t)$  depends on the initial ion field  $\epsilon$  through the cutoff  $\tau$ . Although the average could be calculated for each value of  $\epsilon$ , for the calculations presented in this paper I have used a representative field strength.

#### B. Validity conditions

The major limitation to the theory comes in the assumption that strongly dynamic collisions do not overlap during the effective time  $\tau \sim \Delta_c^{-1}$ . To determine the validity condition for this assumption, it is first necessary to estimate the interaction integral

$$
\frac{1}{\hbar}\int_0^\tau W_{\pmb{i}}(t)dt\;.
$$

This is done as follows:

$$
W_{i}(t) = V_{i}(t) - V_{i}(0) \sim \left(\frac{dV_{i}}{dr}\frac{dr}{dt}\right)_{t=0} t.
$$
 (32)

Approximating  $V_i$  by a dipole interaction

$$
V_i \sim \chi_i e^2 R / r^2 \,, \tag{33}
$$

where  $\chi_i$  is the charge on the perturbing ion,  $r$  its distance from the atom, and R the atomic electron's coordinate, yields

$$
W_{i}(t) \sim [2\chi_{i}e^{2}R/r(0)^{3}]v_{r}t \sim [2eR\epsilon/r(0)]v_{r}t. \qquad (34)
$$

The quantity  $v_r = dr/dt$  is the radial component of the perturbing ion's velocity. The interaction integral is then estimated by

$$
\frac{1}{\hbar}\int_0^\tau W_i(t)\,dt \sim \frac{eR\,\epsilon}{\hbar r(0)}\,v_\tau\tau^2 \sim \frac{v_\tau\tau}{r(0)}\,,\tag{35}
$$

where I have used

$$
\tau \sim \hbar/\Delta_{\epsilon} \sim \hbar/eR\epsilon \ . \tag{36}
$$

From (35) and (26) it can be seen that a collision will be strongly dynamic if  $r(0)$  satisfies

$$
r(0) \le v_r \tau \tag{37}
$$

The assumption that strongly dynamic collisions do not overlap in time requires

$$
\frac{4}{3}\pi n_i (v_\tau \tau)^3 \ll 1\,. \tag{38}
$$

Using  $v_r \leq (2kT/M_t)^{1/2}$ ,  $R \sim \frac{3}{2}n(n-1)a_0/Z$ , and  $\epsilon \sim 2.6 \chi_i en_i^{2/3}$  results in the following condition on temperature and density in order for the theory to hold:

$$
n_i (M_i/T)^{3/2} \gg 10^{17} \left[ Z/n(n-1) \chi_i \right]^3, \tag{39}
$$

where  $n_i$  is in units of cm<sup>-3</sup>, T is in eV, and the mass  $M_{\star}$  of the perturber is in units of the proton mass. In this relation  $n$  is the principal quantum number and  $Z$  is the atomic number of the radiator. For the case of hydrogen  $(Z=1, \chi_i=1)$  at moderate temperatures  $(T<sup>1</sup> eV)$ , it can be seen that the theory should be applicable (within 10-20%) to Lyman  $\alpha$  for proton densities  $n_i$  $\approx 10^{17}$  cm<sup>-3</sup>. The theory should be valid for much smaller densities for the higher members of the Lyman series. In Sec. III I present the results of calculations on hydrogen.

# III. RESULTS FOR HYDROGEN A. Additional approximations

In order to obtain a good estimate of the effect of ion dynamics upon the line profile using the theory described above, it is first necessary to obtain an expression for the cutoff time  $\tau$ that is more accurate than that in Eq. (24). This can be done in the impact limit by calculating the average correctly (with static field exponentials and a representative field  $\bar{\epsilon}$ ) for a second-order expansion of the long-time limit of  $\hat{U}_i(t)$ :

$$
\langle \hat{S}_i - 1 \rangle
$$
  
=  $\hbar^{-2} \Biggl( \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt' e^{iH_0 t / \hbar} W_i(t) e^{-iH_0 t / \hbar}$   
 $\times e^{iH_0 t'/\hbar} W_i(t') e^{-iH_0 t'/\hbar} \Biggr)_{\text{av}}$ , (40)

and then searching for  $\tau$  such that the righthand side of (40) is equal to

$$
\langle \hat{S}_i - 1 \rangle = -\hbar^{-2} \left( \int_{-\tau}^{\tau} dt \int_{-\tau}^{t} dt' W_i(t) W_i(t') \right)_{\text{av}} . \tag{41}
$$

The matrix elements of Eq. (40) are obtained by first choosing the z axis along the direction of  $\zeta$ . With this choice,  $H_0$  is diagonal in parabolic states (for field splittings small compared to the level differences).  $W_i(t)$  may then be approximately diagonalized using rotation operators which rotate to a frame with the  $x$  axis moving with the ion, in the manner of Lisitsa and Sholin.<sup>13</sup> The average over angles can be performed using identities involving the rotation matrices from Edmonds.<sup>14</sup> In terms of the rotation operators Eq. (40) becomes

$$
\langle \hat{S}_i - 1 \rangle = -\hbar^{-2} \Biggl( \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt' \exp(iH_0 t/\hbar) D^{-1}(\Omega) D^{-1}(\theta(t)) W_i^{\tau}(t) D(\theta(t)) D(\Omega) \exp(-iH_0 t/\hbar) \Biggr)
$$

 $\times \exp(iH_0t'/\hbar)D^{-1}(\Omega)D^{-1}(\theta(t'))W_1^r(t')D(\theta(t'))D(\Omega)\exp(-iH_0t'/\hbar)\right]$ .

(42)

The rotations represented by  $D(\Omega)$  and  $D(\theta(t))$ The rotations represented by  $D(\Omega)$  and  $D(\theta(t))$ <br>are similar to those described by Greene *et al*.<sup>15</sup>

For the Lyman- $\alpha$  line of hydrogen, I have found that for the conditions  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T=10000K$ , a value of

$$
\tau = 0.70\hbar\Delta_n^{-1},\qquad(43)
$$

where

$$
\Delta_n = 3n(n-1)e a_0 \bar{\epsilon}/Z \tag{44}
$$

is the full splitting of the  $n$  th quantum level in the mean ion field  $\overline{\epsilon}$ , resulted in 5-10% agreement between Eqs. (40) and (41) for several values of the lower impact-parameter cutoff.

For my calculations I chose  $\bar{\epsilon}$  to be the most probable field strength, determined from the microfields of Hooper.<sup>7</sup> The results of the line shape, however, are not very sensitive to the precise value of the multiplying factor in Eq. (43), as will be seen later. It should be noted that for some impact parameters and velocities the cutoff in the time integral due to Debye shielding may be smaller than that given in Eq. (43). The smaller cutoff, of course, is the appropriate choice.

For the results presented in this paper I have calculated the broadening operator  $\mathfrak{L}(\Delta\omega)$  with a completed-collision assumption by approximating

$$
\langle \hat{U}_{i} - 1 \rangle = \begin{cases} \langle \hat{S}_{i} - 1 \rangle & \Delta \omega < \tilde{\omega}_{pi} \\ 0 & \Delta \omega > \tilde{\omega}_{pi'} \end{cases} \tag{45}
$$

where  $\tilde{\omega}_{pi} = \sqrt{2}\omega_{pi'}$  and  $\omega_{pi}$  is the ion plasma frequency. Thus the ion dynamic correction has been included inside the ion plasma frequency and omitted outside the ion plasma frequency. This discontinuous treatment causes some error This discontinuous treatment causes some  $\alpha$ <br>in the line shape for  $\Delta\omega \sim \tilde{\omega}_{pi}$  (e.g., the lineshape function obtained using (45) is not intrinsically normalized), but is adequate for the purpose of this paper, particularly since  $1/\mathfrak{L}(\Delta\omega)$  $=0$ ) is a good approximation to the line width for the Lyman- $\alpha$  line. The electron average  $\langle U_{\sigma} - 1 \rangle$  is treated in same manner as in Ref. 15. I should emphasize that  $\langle \hat{S}_i - 1 \rangle$  as well as  $\langle U_a - 1 \rangle$ is calculated to all orders in the respective interactions. For details see Ref. 15.

#### B. Results

In Table I the sensitivity of the Lyman- $\alpha$  line shape to the choice of cutoff is illustrated. For the results of this table the cutoff is taken to be

$$
\tau = f\hbar/\Delta_2, \qquad (46)
$$

where  $\Delta_2$  is given by Eq. (44) with  $n=2$ . Four values of f are illustrated. Recall that  $f \approx 0.70$ is expected to be the most nearly correct value. The values of  $I(\Delta \omega = 0)$  for the Lyman- $\alpha$  line at  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T = 10000$  K are tabulated. These peak values are the values that would be obtained from a complete unified calculation (i.e., without a completed-collision assumption), and are approximately inversely proportional to the linewidth. As can be seen, the results are not extremely sensitive to the choice of  $f$ , changing by only  $29\%$  when f is increased by a factor of two, from 0.<sup>5</sup> to 1.

The calculated value of f for Lyman- $\alpha$  is surprisingly close to the value that would be obtained  $(f=0.75)$  if a strict average over all possible separations between the Stark states of the  $n=2$  level were used in the right-hand side of (24). This is probably accidental; however, in

TABLE I. Dependence of the peak value of the line-<br>shape function on the static-field cutoff. The first row,  $f=0.0$ , corresponds to no ion dynamics. The plasma conditions are  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T = 10^4$  K.

$I(\Delta\omega=0)$
15.28
10.20
8.68
8.37 ٠
7.24

lieu of more accurate results for f values for other hydrogen lines I will use a cutoff of

$$
\tau_n = f_n \hbar / \Delta_n \,,\tag{47}
$$

where

$$
f_n = \frac{\text{maximum Stark splitting for level } n}{2 \times \text{average Stark splitting for level } n}
$$
 (48)

The numerator on the right-hand side of (48) is  $\Delta_n$ . All other results to be shown in this paper will use the cutoff given in Eqs. (47) and (48)—or the Debye cutoff if it is smaller.

In Table II is given the line shape  $S(\alpha)$  as a function of the reduced wavelength  $\alpha = \Delta \lambda / 2.61 \text{ cm}^2/\text{m}^3$ for plasma conditions  $n_e = 10^{17}$  cm<sup>-3</sup> and T =10000K. The results with and without the ion dynamic correction are shown, along with those dynamic correction are shown, along with those<br>of Vidal *et al*.<sup>16</sup> Because of the approximation of Eq. (45), the line shape with the ion dynamic correction is not normalized to unit area as are the other two, although the value at line center is the result that a full unified theory based on Eq. (31) would give. It can be seen that the theory with ion dynamics leads to a decrease in the value at the line center of  $45\%$ . The halfwidth is increased by a factor of 1.<sup>8</sup> when ion dynamics is included. The "with ion dynamics" half-width is increased by about 2.0 when compared to the results of Vidal et al. (which do not include time ordering). This factor is somewhat larger than that found by Voslamber<sup>5</sup> and in remarkably good agreement with that found by Seidel. $6$  The comparison between these results and those of Lee<sup>4</sup> will be discussed in Sec. IV.

The factor of 2.0 increase in width is somewhat smaller than the approximately 2.5 increase obtained by Grützmacher and Wende<sup>1</sup> in experiments on the Lyman- $\alpha$  line of hydrogen, but does show that, in agreement with previous authors,  $4-6$  much of the discrepancy between theory and experiments can be removed by the inclusion of ion dynamics. Although some of the remaining discrepancy is due to the neglect of inelastic collisions in this treatment, it is likely that there is another broadening mechanism which has not been included —perhaps the screening fluctuations proposed by Griem.<sup>10</sup>

I illustrate the reduced-mass effect calculated from the theory in Table III. The peak values  $S(0)$  of the Lyman- $\alpha$  line are presented for four different radiator-perturber reduced masses, along with the static-ion result. The five cases are (radiator given first)  $H - H^*$ ,  $\mu = \frac{1}{2}$ ;  $H - D^*$ ,  $\mu = \frac{2}{3}$ ; H - He<sup>+</sup>,  $\mu = \frac{4}{5}$ ; H - Ar<sup>+</sup>,  $\mu \approx 1$ ; and D - Ar<sup>+</sup>,  $\mu$  $\simeq$  2, where the reduced masses are in units of the proton mass. The peak values (and thus the halfwidths) are linearly dependent on the inverse of

$\log_{10}(\alpha)$	$S(\alpha)$ Vidal et al. <sup>a</sup>	$S(\alpha)$ Static ions	$S(\alpha)$ Dynamic ions
$-5.0$	$2.342 \times 10^{3}$	$2.06 \times 10^{3}$	$1.14 \times 10^{3}$
$-4.8$	$2.304 \times 10^{3}$	$2.03 \times 10^{3}$	$1.13 \times 10^{3}$
$-4.6$	$2.213 \times 10^{3}$	$1.97 \times 10^{3}$	$1.12 \times 10^{3}$
$-4.4$	$2.015 \times 10^{3}$	$1.83 \times 10^{3}$	$1.10 \times 10^{3}$
$-4,2$	$1.650 \times 10^{3}$	$1.55 \times 10^{3}$	$1.05 \times 10^{3}$
$-4.0$	$1.147 \times 10^{3}$	$1.13 \times 10^{3}$	$9.32 \times 10^{2}$
$-3,8$	$6.749 \times 10^{3}$	6.93 $\times$ 10 <sup>2</sup>	$7.39 \times 10^{2}$
$-3.6$	$3.713 \times 10^{2}$	$3.89 \times 10^{2}$	$3.89 \times 10^{2}$
$-3.4$	$2.227 \times 10^{2}$	$2.34 \times 10^{2}$	$2.34 \times 10^{2}$
$-3.2$	$1.508 \times 10^{2}$	$1.58 \times 10^{2}$	$1.58 \times 10^{2}$
$-3.0$	$9.256 \times 10^{1}$	$9.65 \times 10^{1}$	$9.65 \times 10^{1}$
$-2,8$	$4.293 \times 10^{1}$	$4.43 \times 10^{1}$	$4.43 \times 10^{1}$
$-2.6$	$1.593 \times 10^{1}$	$1.64 \times 10^{1}$	$1.64 \times 10^{1}$
$-2.4$	$5.419 \times 10^{0}$	$5.57 \times 10^{0}$	$5.57 \times 10^{0}$
$-2.2$	$1.816 \times 10^{0}$	$1.87 \times 10^{0}$	$1.87 \times 10^{0}$
$-2.0$	$6.116\times10^{-1}$	$6.28 \times 10^{-1}$	$6.28 \times 10^{-1}$

TABLE II. Lyman- $\alpha$  line shape for  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T = 10^4$  K. The difference between the "Static ions" column and the Vidal et  $al$ , results is that the time ordering of electron collisions has been. included in the former.

<sup>a</sup> Reference 16.

the square root of the reduced mass, as found by the square root of the reduced mass, as found<br>Seidel,  $\binom{6}{6}$  and assumed by Wiese *et al*.<sup>17</sup> for H<sub>α</sub>.

The line shape  $S(\alpha)$  for the Lyman- $\beta$  line of hydrogen for plasma conditions  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T = 10000$  K is given in Table IV. The results of Vidal et  $al$ <sup>16</sup> are also given for the sake of comparison. As can be seen, the effect of ion dynamics and the time ordering of electron collisions is to raise the line center by about 8%. Time ordering is responsible for about half of this effect  $\left[ S(0)=1.02 \times 10^2 \right]$  at these conditions if ion motion is neglected]. Thus the effect of including ion dynamics is to partially fill in the dip in Lyman- $\beta$ . Recent experiments of Grutzmacher and Wende<sup>18</sup> on the Lyman- $\beta$  line, however, show a larger effect than presented here, which again might indicate an additional broadening mechanism.

Application of the theory to the case of  $H_{\alpha}$  at  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T = 10^4$  K yields a value of S(0) =17.0, compared to 23.1 found by Vidal et al.<sup>16</sup> This lowering of the line center (and consequent increase in the half-width) due to ion dynamics (and time ordering) is about the same size as the discrepancy between the results of Vidal  $et$   $al$ . and Kepple and Griem.<sup>3</sup> This latter discrepancy is due to the different treatment of the so-called interference terms. This must be viewed with caution, however, since the cutoff time  $\tau$  given by (48) may not be accurate for lines in which lower-state broadening is important. Work is presently underway to determine correct cutoffs for lines other than Lyman  $\alpha$ .

#### IV. DISCUSSION AND SUMMARY

## A. Comparison with second-order theory

The theory presented in Sec. I of this paper is more closely allied to the method of Lee $4$ (which is basically that proposed by  $Dufty^{19}$ ) than to those of Voslamber<sup>5</sup> or Seidel.<sup>6</sup> Although there is some difference as to how the staticion interactions are removed from  $\mathcal{L}(\Delta \omega)$  of Eq. (31) (or Lee's  $H$  operator), the primary difference in the two methods is that Lee's calculations are quantum mechanical and second order in the atom-perturber interaction, whereas the theory of this paper assumes classical paths for the perturbers and treats the atom-perturber interaction to all orders in the time-development operators. The second-order theory must introduce a \*\*strong-collision cutoff" to ensure convergence, and at the present time there is no clear-cut way of selecting what this cutoff should

TABLE III. Dependence of the peak value of the Lyman- $\alpha$  line shape on the reduced mass of the perturbing ions. The reduced mass  $\mu$  is in terms of the proton mass. Plasma conditions are  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T=10^4$  K.



TABLE IV. Lyman- $\beta$  line shape for  $n_e = 10^{17}$  cm<sup>-3</sup> and  $T=10^4$  K. The "Dynamic ions" column includes both ion dynamics and the time ordering of electron collisions.

$log_{10} (\alpha)$	$S(\alpha)$ Vidal et al. <sup>a</sup>	$S(\alpha)$ Dynamic ions
$-5.0$		$1.06 \times 10^{2}$
$-4.8$		$1.06 \times 10^{2}$
$-4.6$		$1.06 \times 10^{2}$
$-4.4$	$9.813 \times 10^{1}$	$1.07 \times 10^{2}$
$-4.2$	$9.927 \times 10^{1}$	$1.08 \times 10^{2}$
$-4.0$ .	$1.020 \times 10^{2}$	$1.10 \times 10^{2}$
$-3.8$	$1.085 \times 10^{2}$	$1.15 \times 10^{2}$
$-3.6$	$1.221 \times 10^{2}$	$1.28 \times 10^{2}$
$-3.4$	$1.463 \times 10^{2}$	$1.53 \times 10^{2}$
$-3.2$	$1.745 \times 10^{2}$	$1.80 \times 10^{2}$
$-3.0$	$1.782 \times 10^{2}$	$1.78 \times 10^{2}$
$-2.8$	$1.344 \times 10^{2}$	$1.29 \times 10^{2}$
$-2.6$	$7.324 \times 10^{1}$	$6.75 \times 10^{1}$
$-2.4$	$3.076 \times 10^{1}$	$2.77 \times 10^{1}$
$-2.2$	$1.103 \times 10^{1}$	$9.90 \times 10^{0}$
$-2.0$	$3.694 \times 10^{0}$	$3.36 \times 10^{0}$

<sup>a</sup> Reference 16.

be. The method does have the advantage of treating perturber correlations in a more realistic manner than the straight Debye cutoff that I have used; however, the line shape is in general less sensitive to the upper (Debye) cutoff than to the strong- collision cutoff.

Another difference in our calculations lies in the fact that I have incorporated an upper cutoff due to ion field splitting which Lee has not used. Calculations without this cutoff (which cannot be justified in the manner of Sec. II B) result in significantly larger effects of ion dynamics, which are not seen experimentally. For example, the peak value S(0) of the Lyman- $\alpha$  line at  $n_e = 10^{17}$ 

~Permanent address: Dept. of Physics, University of Southwestern Louisiana, Lafayette, La. 70504.

- <sup>1</sup>K. Grützmacher and B. Wende, Phys. Rev. A 16, 243 (1977).
- ${}^{2}$ Earl W. Smith, J. Cooper, and C. R. Vidal, Phys. Rev. 185, 140 (1969).
- $3\overline{P}$ . Kepple and Hans R. Griem, Phys. Rev. 173, 317 {1968);P. Kepple, University of Maryland, Report No. 831, 1968 {unpublished).
- ${}^{4}$ R. W. Lee, J. Phys. B 11, L167 (1978).
- 5Dietrich Voslamber, Phys. Lett. <sup>A</sup> 61, 27 (1977). 6Joachim Seidel, Z. Naturforsch. Teil. <sup>A</sup> 32, 1207
- (1977). <sup>7</sup>C. F. Hooper, Jr., Phys. Rev. 165, 215 (1968); 169,
- 193 {1968).
- ${}^{8}$ Hans R. Griem, Spectral Line Broadening by Plasmas (Academic, New York, 1974).
- ${}^{9}$ Earl W. Smith, C. R. Vidal, and J. Cooper, J. Res. Natl. Bur. Stand. Sec. A 73, 389 (1969).

cm<sup>-3</sup> and  $T = 10^4$  K is decreased by 68% compared to the results of Vidal et  $al.^{15}$ . This corresponds to an increase in the half-width by a factor of 2.7, larger than what has been seen experimentally, despite the fact that several known broadening mechanisms have not been included.

## B. Summary

I have presented a theory of Stark broadening of hydrogenic radiators which adds ion-dynamics corrections to the basic unified theory of Smith  $et \ al.<sup>2</sup>$  The validity of the theory requires the assumption that strongly dynamic ion collisions do not overlap in time. This requirement results in the condition on density and temperature given in expression (39). For hydrogen at moderate temperatures  $($   $\sim$  1 eV), the condition requires  $n_e > 10^{17} [n(n-1)]^{-3}$  cm<sup>-3</sup>, where *n* is the upper-state principal quantum number.

Sample calculations were performed for the  $L_{\alpha}$ ,  $L_{\beta}$ , and H<sub> $\alpha$ </sub> lines in hydrogen. For the Lyman- $\alpha$  line the half-width increased by a factor of about 2.0, which compared reasonably well with previous calculations and the experiment of Grützmacher and Wende.<sup>1</sup> The filling of the dip in the Lyman- $\beta$  line, however, is not as large as is found experimentally.<sup>18</sup> This may indicate an additional broadening mechanism which has not been included.

#### ACKNOWLEDGMENTS

It is with pleasure that I acknowledge a number of helpful discussions with Dr. C. F. Hooper, Jr. and Dr. J. W. Dufty. This work was supported in part by a U. S. Department of Energy grant to the University of Florida.

 $^{10}$ Hans. R. Griem, Phys. Rev. A 17, 214 (1978).

- <sup>11</sup>Earl W. Smith, J. Cooper, and Larry Roszman, J.
- Quant. Spectrosc. Radiat. Transfer 13, 1523 (1973).  $^{12}$ Earl W. Smith and C. F. Hooper, Jr., Phys. Rev. 157, 126 {1967).
- $^{13}V.$  S. Lisitsa and G. V. Sholin, Zh. Eksp. Teor. Fiz. 61, 921 (1971) [Sov. Phys. JETP 34, 484 (1972)].
- $^{14}$ A. R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University, Princeton N. J., 1960).
- $^{15}R.$  L. Greene, J. Cooper, and E.W. Smith, J. Quant. Spectrosc. Radiat. Transfer 15, 1025 (1975); R. L. Greene, Phys. Rev. <sup>A</sup> 14, 1447 (1976).
- $^{16}$ C. R. Vidal, J. Cooper, and E.W. Smith, Astrophys. J. Suppl. Ser. 25, 37 (1973).
- $17W$ . L. Wiese, D. E. Kelleher, and V. Helbig, Phys. Rev. <sup>A</sup> 11, 1854 (1975).
- $18K$ . Grützmacher and B. Wende, Phys. Rev. A 18, 2140  $(1978)$ .
- $19J$ ames W. Dufty, Phys. Rev. 187, 305 (1969).