A New Formula for the Spectral Line Broadening in Plasmas with Application to the Asymmetry of Ly-α

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Some time ago, von Waldenfels [4] derived a systematic series expansion of the exact line shape function in case of a single perturber species. In view of the involved mathematics it remained unclear to what physical approximation the first order term of the series corresponds. Here we generalize the approach to two perturber species, one of which is treated quasi-statically (ions), and give a direct physical derivation of the first order term. This term incorporates noncommutativity of ion and electron potentials. In the numerical evaluation for Ly-α it turns out that the noncommutativity effects are washed out to a large extent by the averaging process.

1. Introduction and Results

A spectral line is broadened and deformed if the emitting atoms are placed in a plasma (or gas). This is due to the Doppler shift and to the influence of particles (perturbers) passing by. It is a common approximation to take the influence of the perturbers into account by an external potential [1]. A few calculations treat them quantum mechanically [2].

A main problem is to perform the average over the different perturber configurations without having to make too drastic approximations. A good approximation seems to be to treat the electron collisions as nonoverlapping as in the unified theory [3].

A different approach was proposed by von Waldenfels [4]. It is based on the fact that a perturber configuration can be characterized by velocities, impact parameters and collision times. A systematic series expansion for the electron contribution was given which used in an essential way collision time statistics [5]. The first order term of this series was evaluated by one of us [6] for Lyman-α and good agreement with the experimental data for the line wing was found. It turned out, however, that this series expansion is only applicable to a single species of perturbers. As soon as ions and electrons are both present, as in all realistic cases, this approach has to be modified in some way or other. Furthermore, the very involved mathematics makes it somehow unclear to which physical approximation the first order term corresponds.

In this paper we generalize this approach to include ions in the quasi-static approximation. This is a widespread practice, although recent experiments have indicated the importance of ion dynamical effects in particular for the line centre [7]. Because here we want to stress the physical aspects we give a direct derivation of the first order term which, we hope, will clarify the nature of the approximations involved. We will discuss in section 3 how overlapping of electron collisions is, to some extent, taken into account. The complete series expansion will be published elsewhere [8].

Our result for the line shape function $L(\omega)$ has the following form. By $[\ldots]_e$ we denote the average over impact parameter and velocity of a single electron; by $[\ldots]_i$ the average over the (static) ion configurations and by V_i a corresponding ion potential. For an electron colliding at $t=0$ we denote by $V_I(t)$, $U_I(t)$ and $S_I = U_I(\infty)$ the potential, time development operator from $-\infty$ to t and S-matrix, respectively, in the ion interaction picture. The mean collision frequency is c. Then one has in the line space (or doubled atom) representation of [9]

$$L(\omega_0+\omega) = \mathrm{Tr}\,(D[(\hbar\omega - V_i)^{-1} \cdot \hat{I}_i(\omega)\,(\hbar\omega - V_i)^{-1}]_i) \tag{1.1}$$

with

$$\hat{I}_i(\omega) = \frac{c}{2\pi}[|\int \mathrm{d}t\, e^{i(\omega - V_i/\hbar)t}\, V_I(t)\, U_I(t)|^2]_e + \frac{c^2}{2\pi}\int \mathrm{d}t\, e^{i(\omega - V_i/\hbar)t}[V_I(t)\, U_I(t)]_e \cdot \{-i\omega + iV_i/\hbar + c(1-[S_I]_e)\}^{-1} \cdot \{\int \mathrm{d}t\, e^{i(\omega - V_i/\hbar)t}[V_I(t)\, U_I(t)\, S_I^*]_e\}^* + \mathrm{h.c.}\,. \tag{1.2}$$

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D is the dipole operator (cf. (2.3)) and h.c. means the hermitian adjoint of the second summand of Equation (1.2).

For vanishing ion potential, $V_i = 0$, one recovers the result of Ref. [4]. Equations (1.1/2) can be brought into another form which facilitates the comparison with other approaches. This will be done in section 5.

In Sect. 6 we apply this to Ly-α with particular attention to asymmetry effects and to noncommutativity of ion and electron potentials. We find, as Bacon [10] does, that the line asymmetry is almost completely due to the contribution of the ions and not of the electrons.

The noncommutativity of ion and electron potentials has in this case very pronounced effects for individual configurations. But the averaging process washes out this effect to a large extent so that assuming that the ion and electron potentials commute introduces an error of only about 4%. This explains the good agreement with experiment of the calculations in [7] where this commutativity had been assumed.

Our numerical results are displayed in Figs. 1 to 3. While the agreement with the experimental data for the line wing is good, the line centre shows a behavior similar to that of other calculations based on the quasi-static approximation for the ions.

2. The Classical Path Model in Line Space and Collision Time Statistics

The classical path approximation treats the perturbers as classical point particles. We denote by $t(s, s')$ the time development operator of the atom for a given configuration of perturbers, by $\mathbf{X}$ the position operator of the radiating electron, by $|\mathrm{i}\rangle$ and $|\mathrm{f}\rangle$ the initial and final orthonormal states of the line. Then the normalized line shape function $L(\omega)$ for the intensity of dipole radiation is given by [11]

$$L(\omega) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}s\, e^{i\omega s} \sum_{\substack{\mathrm{i,f} \\ \mathrm{i',f'}}} [\langle \mathrm{i}|\mathbf{X}|\mathrm{f}\rangle \langle \mathrm{f}|t^*(s,0)|\mathrm{f'}\rangle \langle \mathrm{f'}|\mathbf{X}|\mathrm{i'}\rangle \langle \mathrm{i'}|\mathrm{t}(s,0)|\mathrm{i}\rangle]_{\mathrm{av}}$$
$$\equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}s\, e^{i\omega s} C(s) . \tag{2.1}$$

The factor $A = \left[\sum_{\mathrm{i,f}} |\langle \mathrm{i}|\mathbf{X}|\mathrm{f}\rangle|^2\right]^{-1}$ normalizes L, and the averaging is over all perturber configurations. It was noted in Ref. [12] that $C(s)$ is a positive-definite function so that $L(\omega) \geqq 0$, as required.

The "line space" or "doubled atom space" is

$$\mathscr{H} \equiv \mathscr{H}_\mathrm{i} \otimes \mathscr{H}_\mathrm{f} . \tag{2.2}$$

In it one defines the operators D and $T(s, s')$ by

$$\langle \mathrm{if}|D|\mathrm{i'f'}\rangle = A \sum_{j=1}^{3} \langle \mathrm{i}|x_j|\mathrm{f}\rangle \langle \mathrm{f'}|x_j|\mathrm{i'}\rangle , \tag{2.3}$$

$$\langle \mathrm{if}|T(s,s')|\mathrm{i'f'}\rangle = \langle \mathrm{i}|t(s,s')|\mathrm{i'}\rangle \langle \mathrm{f'}|t^*(s,s')|\mathrm{f}\rangle . \tag{2.4}$$

Then one finds

$$C(s) = \mathrm{Tr}[DT(s,0)]_{\mathrm{av}} .$$

We define the "intensity operator" $I(\omega)$ by

$$I(\omega) = \frac{1}{2\pi} \int \mathrm{d}s\, e^{i(\omega_0+\omega)s} [T(s,0)]_{\mathrm{av}} . \tag{2.5}$$

Then

$$L(\omega_0 + \omega) = \mathrm{Tr}[DI(\omega)] . \tag{2.6}$$

With the usual "no-quenching" assumption, i.e. the only relevant matrix elements of the perturbing potential V_p are $\langle \mathrm{i}|V_\mathrm{p}|\mathrm{i'}\rangle$ and $\langle \mathrm{f}|V_\mathrm{p}|\mathrm{f'}\rangle$, one defines the operators H_A, $V(t)$ and $H(t)$ in line space by

$$H_\mathrm{A} = (E_\mathrm{i} - E_\mathrm{f})\mathbf{1} = \hbar\omega_0 \mathbf{1} ,$$
$$\langle \mathrm{if}|V(t)|\mathrm{i'f'}\rangle = \langle \mathrm{i}|V_\mathrm{p}(t)|\mathrm{i'}\rangle \delta_{\mathrm{ff'}} - \delta_{\mathrm{ii'}} \langle \mathrm{f'}|V_\mathrm{p}(t)|\mathrm{f}\rangle \tag{2.7}$$
$$H(t) = H_\mathrm{A} + V(t) .$$

Then T satisfies the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} T(t,t') = H(t)\, T(t,t') \tag{2.8}$$

so that T is a time-ordered exponential,

$$T(t,t') = \mathscr{T} \exp\left[-\frac{i}{\hbar} \int_{t'}^{t} H(s)\, \mathrm{d}s\right] . \tag{2.9}$$

We note the relations

$$T(t,0)^* = T(0,t);$$
$$T(t,t') = T(t,t'')\,T(t'',t'). \tag{2.10}$$

Due to time-translation invariance we have a simple expression for $[T(t,0)]''_{\mathrm{av}}$ which we will need later,

$$-\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}t^2}[T(t,0)]_{\mathrm{av}} = [H(t)\,T(t,0)\,H(0)]_{\mathrm{av}}. \tag{2.11}$$

Proof: We have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}[T(t,0)]_{\mathrm{av}} &= -\frac{i}{\hbar}[H(t)\,T(t,0)]_{\mathrm{av}} \qquad (2.12)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}[T(0,-t)]_{\mathrm{av}}\\ &= -\frac{i}{\hbar}[T(0,-t)\,H(-t)]_{\mathrm{av}}\\ &= -\frac{i}{\hbar}[T(t,0)\,H(0)]_{\mathrm{av}},\end{aligned}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}[T(t,0)]_{\mathrm{av}} = -\frac{1}{\hbar^2}[H(t)\,T(t,0)\,H(0)]_{\mathrm{av}}$$

which gives (2.11).

We now introduce the quasi-static treatment of the ions so that

$$H(t) = \hbar\omega_0 \mathbf{1} + V_{\mathrm{i}} + V_{\mathrm{e}}(t).$$

The averaging will be performed first over the electrons for a fixed ion potential V_{i}, and then over the ions,

$$[\ldots]_{\mathrm{av}} = [[\ldots]_{\mathrm{e}}]_{\mathrm{i}}.$$

We put

$$\hat{T}(t,t') = e^{i(\omega_0(t-t')}\,T(t,t'). \tag{2.13}$$

and define the intensity operator for fixed ion configuration by

$$I_{\mathrm{i}}(\omega) = \frac{1}{2\pi}\int \mathrm{d}t\, e^{i\omega t}[\hat{T}(t,0)]_{\mathrm{e}}, \tag{2.14}$$
$$I(\omega) = [I_{\mathrm{i}}(\omega)]_{\mathrm{i}}.$$

Then (2.11/12) hold with T, $H(t)$, $[\ldots]_{\mathrm{av}}$ replaced by $\hat{T}$, $V_{\mathrm{i}}+V_{\mathrm{e}}(t)$, $[\ldots]_{\mathrm{e}}$. Fourier transformation of

$$\begin{aligned}&\frac{\mathrm{d}^2}{\mathrm{d}t^2}[\hat{T}(t,0)]_{\mathrm{e}}\\ &= -\frac{1}{\hbar^2}[(V_{\mathrm{i}}+V_{\mathrm{e}}(t))\,\hat{T}(t,0)\,(V_{\mathrm{i}}+V_{\mathrm{e}}(0))]_{\mathrm{e}}\end{aligned}$$

yields

$$\hbar^2\omega^2 I_{\mathrm{i}}(\omega) = -V_{\mathrm{i}} I_{\mathrm{i}}(\omega)\,V_{\mathrm{i}} + \hbar\omega\,V_{\mathrm{i}} I_{\mathrm{i}}(\omega) + \hbar\omega\, I_{\mathrm{i}}(\omega)\,V_{\mathrm{i}} + \frac{1}{2\pi}\int \mathrm{d}t\, e^{i\omega t}[V_{\mathrm{e}}(t)\,\hat{T}(t,0)\,V_{\mathrm{e}}(0)]_{\mathrm{e}}.$$

By solving for $I_{\mathrm{i}}(\omega)$, we finally obtain

$$I_{\mathrm{i}}(\omega) = (\hbar\omega - V_{\mathrm{i}})^{-1}\frac{1}{2\pi}\int \mathrm{d}t\, e^{i\omega t}[V_{\mathrm{e}}(t)\,\hat{T}(t,0)\,V_{\mathrm{e}}(0)]_{\mathrm{e}}\,(\hbar\omega - V_{\mathrm{i}})^{-1}. \tag{2.15}$$

Averaging this over the ions then gives the intensity operator $I(\omega)$.

To manifestly exhibit the positivity properties of the r.h.s. of (2.15), we rewrite the square bracket as a convolution. By $\chi_{[a,b]}(t)$ we denote the characteristic function of the interval [a, b], which is 1 on [a, b] and 0 outside. Then we claim

$$\begin{aligned}&[V_{\mathrm{e}}(t)\,\hat{T}(t,0)\,V_{\mathrm{e}}(0)]_{\mathrm{e}}\\ &= \lim_{T\to\infty}\frac{1}{T}\left[\int_{-\infty}^{+\infty}\mathrm{d}s\,\{\chi_{[0,T]}(t-s)\,V_{\mathrm{e}}(t-s)\,\hat{T}(t-s,0)\}\,\{\chi_{[0,T]}(-s)\,V_{\mathrm{e}}(-s)\,T(-s,0)\}^*\right]_{\mathrm{e}}.\end{aligned} \tag{2.16}$$

The Fourier transform of the square bracket on the r.h.s. is of the form $k(\omega)k(\omega)^*$. The proof of (2.16) is straightforward if one uses (2.10) and time-translation invariance.

Now it is possible, and this is the crucial point, to replace the time limit in (2.16) by a limit over electron numbers. To this end we introduce the concept of collision times and their statistics for the electrons. Perturber correlations are taken into account by a cut-off of the electron potentials at the Debye length, i.e. only electrons inside the Debye sphere contribute. Since in a finite time

interval only a finite number enters, and if by collision time we mean the time of closest approach, it makes sense to speak, for a given configuration, of collision times τ_1, τ_2 ... of the first, second etc. electron collision after $t=0$ [13] and similarly of τ_0, τ_{-1} etc. for collisions before $t=0$. These collision times obey a statistical law which depends upon the correlations between the electrons (and ions). If, as usual, the perturbers are treated as an ideal gas, then the interarrival (intercollision) times

$$u_i = \tau_{i+1} - \tau_i \tag{2.17}$$

are mutually independent and are exponentially distributed according to $c e^{-cu} du$ where c is the mean collision frequency,

$$c = 1/[u]_e = \bar{v}_e \pi \varrho_D^2 \nu_e . \tag{2.18}$$

An electron configuration can then be characterized by a collection of collision times τ_i, velocities $\boldsymbol{\upsilon}_i$ and $\boldsymbol{\varrho}_i$ where $\boldsymbol{\varrho}_i$ is the position of the i-th electron at $t=\tau_i$; obviously $\boldsymbol{\upsilon}_i \perp \boldsymbol{\varrho}_i$.

For a given configuration, $V_e(t)$ can then be written as

$$V_e(t) = \sum_{k=-\infty}^{+\infty} V(k; t-\tau_k) ,$$

where $V(k;t)$ denotes the potential of an electron with $\boldsymbol{\upsilon}_k$, $\boldsymbol{\varrho}_k$, which collides at $t=0$. We set

$$\begin{aligned} V_e(1 \dots N; t) &:= \sum_{k=1}^{N} V(k; t - (\tau_k - \tau_1)) \\ &= V(1;t) + V(2; t-u_1) + \cdots + V(N; t-u_1 - \cdots - u_{N-1}) , \end{aligned} \tag{2.19}$$

i.e., the contribution of the first N electrons shifted in time to the past by τ_1, so that the first collision is at $t=0$. By $T(1 \dots N; t, t')$ we denote the time development operator belonging to $V_i + V_e(1 \dots N; t)$,

$$i\hbar \frac{\partial}{\partial t} T(1 \dots N; t, t') = \{V_i + V_e(1 \dots N; t)\} T(1 \dots N; t, t') . \tag{2.20}$$

We now claim that (2.16) can be rewritten as

$$\begin{aligned} &[V_e(t)\, \hat{T}(t,0)\, V_e(0)]_e \\ &= \lim_{N\to\infty} \frac{c}{N} \left[\int_{-\infty}^{+\infty} ds \{V_e(1 \dots N; t-s)\, T(1 \dots N; t-s, t')\} \{V_e(1 \dots N_i - s)\, T(1 \dots N; -s, t')\}^* \right]_e , \end{aligned} \tag{2.21}$$

identically in t'; later t' will be taken to $-\infty$. A rigorous proof will be given elsewhere. But intuitively this is seen as follows. The average time between two collisions is $[\tau_{i+1} - \tau_i]_e = [u_i]_e = 1/c$ so that $T = [Nu]_e = N/c$ approximates the time during which the N electrons contribute to the potential. $V_e(1 \dots N; t)$ and $T(1 \dots N; t, t')$ approximate $V_e(t+\tau_1)$ and $\hat{T}(t+\tau_1, t'+\tau_1)$, respectively. Since $\hat{T}(t,t')\hat{T}(s,t')^* = \hat{T}(t,0)\hat{T}(s,0)^*$ for all t, s and t', the second argument of $\hat{T}(\cdot,\cdot)$ in Eq. (2.16) can be changed from 0 to $t'+\tau_1$ and by changing the integration variable from s to $s-\tau_1$ one sees that the r.h.s. of (2.16) and (2.21) agree in the limit.

Basic for the following will be the still exact equations (2.15) and (2.21). In the next section it will be shown that the limit $N \to \infty$ can be performed if one uses the exact potential $V(1 \dots N; t)$ and an approximation for $T(1 \dots N; t, t')$.

3. The Approximation

The curly brackets in (2.21) are the sum of terms of the form

$$V(k; t - \sum_{j=1}^{k-1} u_j)\, T(1 \dots N; t, t') . \tag{3.1}$$

The first factor, the potential of the k-th electron, has its main contribution for t in the vicinity of its collision time $\sum_{j=1}^{k-1} u_j$, and it vanishes sufficiently far away from that. For these t-values we now approximate $T(1 \dots N; t, t')$ by treating the contribution of the first $k-1$ electrons as nonoverlapping and complete.

For greater clarity we first consider the case $V_i = 0$. Then with this approximation (3.1) becomes

$$V\left(k; t - \sum_{j=1}^{k-1} u_j\right) \cdot T\left(k; t - \sum_{j=1}^{k-1} u_j, -\infty\right) \prod_{j=k-1}^{1} S(j), \tag{3.2}$$

where $T(k; t, t')$ belongs to $V(k, t)$, the potential of the k-th electron colliding at $t = 0$, and where $S(j) = T(j; \infty, -\infty)$.

If $V_i \neq 0$, then $T(1 \ldots N; t, t')$ is no longer constant between two complete and nonoverlapping electron collisions but develops with V_i. We therefore go to the interaction picture for V_i and define

$$V_I(k; t) = e^{(iV_i/\hbar)t} V(k; t) e^{(-iV_i/\hbar)t}, \tag{3.3}$$

$$U_I(k; t, t') = e^{(iV_i/\hbar)t} T(k; t, t') e^{(-iV_i/\hbar)t'}, \tag{3.4}$$

where $T(k; t, t')$ now belongs to $V_i + V(k; t)$. One has

$$\dot{U}_I(k; t, t') = -i/\hbar\, V_I(k; t)\, U_I(k; t, t'). \tag{3.5}$$

Then (3.2) is replaced by

$$\exp\left\{-i V_i\left(t - \sum_1^{k-1} u_j\right)/\hbar\right\} V_I\left(k_i t - \sum_1^{k-1} u_j\right) \cdot U_I\left(k; t - \sum_1^{k-1} u_j, -\infty\right) \cdot \prod_{k-1}^{1} e^{-iV_1 u_j/\hbar} S_I(j)\, e^{-iV_1 \Delta_1/2\hbar} \tag{3.6}$$

where $S_I(j)$ is the S-matrix of the j-th electron in the interaction picture and Δ_1 is the collision duration of particle 1.

Equation (3.6) is our basic approximation for (3.1) and also, after summing over k from 1 to N and after replacing t by $t - s$ and $-s$ respectively, for the curly brackets in (2.21). It should be noted that in (2.21) we have kept the full electron potential $V_e(1 \ldots N; t)$ and have made the non-overlapping assumption for $T(1 \ldots N; t, t')$ only. When summing (3.6) over different k's, a certain overlapping will still result, due to the exact treatment of $V_I(k; t)$ and because for $U_I\left(k; t - \sum_1^{k-1} u_j, -\infty\right)$ we take the exact 1-electron time-development operator in the interaction picture.

Besides taking the electron overlapping partially into account, this approximation has the further advantage that it yields an evidently positive line shape function because the r.h.s. of (2.21), after Fourier transform, is a positive operator. In addition, and this will be shown elsewhere, it gives the first order contribution in a systematic series expansion.

4. The Limit $N \to \infty$

We now insert the approximation of (3.1) given in (3.6) into the curly brackets of (2.21), the first of which then becomes the sum over k of the expressions in (3.6) with t replaced by $t - s$ while the second curly bracket becomes the same sum with t replaced by $-s$. The resulting double sum in (2.21) is then decomposed into a sum over the diagonal terms and two sums over off-diagonal terms, $\sum_{k>k'}$ and $\sum_{k>k'}$.

The sum over the diagonal terms becomes, after replacing the integration variable s by $s - \sum_1^{k-1} u_j$,

$$\frac{c}{N} \sum_{k=1}^{N} \Big[\int \mathrm{d}s\, e^{-iV_i(t-s)/\hbar}\, V_I(k; t - s) \cdot U_I(k; t - s, -\infty)\, U_I(k; -s, -\infty) \cdot V_I(k; -s)\, e^{-iV_i s/\hbar} \Big]_e \tag{4.1}$$

where the S-matrices and other factors have canceled each other. Since the electron velocities and impact parameters are identically distributed, the averages for different k all coincide. Hence the sum over the diagonal terms becomes, after Fourier transforming,

$$c\left[\left| \int \mathrm{d}t\, e^{i(\omega - V_i/\hbar)t}\, V_I(1; t)\, U_I(1; t, -\infty) \right|^2\right]_e. \tag{4.2}$$

Turning to the off-diagonal terms, we first regard $k > k'$. We put $k = k' + m$ and write

$$\sum_{N \geqq k > k'} = \sum_{k'=1}^{N-1} \sum_{m=1}^{N-k'}.$$

We replace the integration variable s by $s - \sum_1^{k'-1} u_j$ and use the independence of the interarrival times to renumber $u_{k'+m-1}$ by u_m. This yields

$$\frac{c}{N} \left[\sum_{k'=1}^{N-1} \sum_{m=}^{N-k'} \int \mathrm{d}s \exp\left\{-i V_i\left(t - s - \sum_1^m u\right)/\hbar\right\} V_I\left(k' + m; t - s - \sum_1^m u_j\right) U_I\left(k' + m; t - s - \sum_1^m u_j, -\infty\right) \cdot \prod_{j=1}^{m} e^{-iV_1 u_j/\hbar} S_I(k' + j - 1)\, U_I(k'; -s, -\infty)^* V_I(k'; -s)\, e^{-iV_i s/\hbar} \right]_e. \tag{4.3}$$

Except for the u_j's each summand would be a product of three mutually independent factors, namely

$$V_I(k'+m)\, U_I(k'+m), \quad \prod_2^m S_I(k'+j-1)$$

and

$$\{V_I(k')\, U_I(k')\, S_I(k')\}^*.$$

But Fourier transformation of (4.3) brings about just this because one gets, in each summand, phase factors $\prod^m e^{i\omega u_j}$ which can be combined with those in front of the S-matrices to the product

$$\left(\prod_2^m e^{i(\omega - V_i/\hbar)u_j} S_I(k'+j-1)\right) e^{i(\omega - V_i/\hbar)u_1}, \quad (4.4)$$

and now one has indeed three independent factors. The averages of the first and the third are independent of k' and m. Thus the sum over k' and m is only over the average of the terms in (4.4), which are seen to be independent. Since

$$[e^{i(\omega - V_i/\hbar)u_j}]_e = c\int_0^\infty du\, e^{-cu}\, e^{i(\omega - V_i/\hbar)u} \quad (4.5)$$
$$= c\{i(V_i/\hbar - \omega) + c\}^{-1} =: A$$

one obtains, by partial summation of a geometric series,

$$\frac{c}{N}\sum_{k'=1}^{N-1}\sum_{m-1}^{N-k'} A^{m-1}[S_I(1)]_e^{m-1} A$$
$$\xrightarrow[N\to\infty]{} c\{1 - A[S_I(1)]_e\}^{-1} A\,. \quad (4.6)$$

Using

$$\{1 - AB\}^{-1}A = \{A(A^{-1} - B)\}^{-1}A$$
$$= \{A^{-1} - B\}^{-1}$$

and inserting for A from (4.5) one gets for the r.h.s. of (4.6)

$$c^2\{i(V_i/\hbar - \omega) + c(1 - [s_I(1)]_e)\}^{-1}. \quad (4.7)$$

Thus the off-diagonal, $k > k'$, part written in (4.3) becomes after Fourier transform in the limit $N\to\infty$

$$c^2 \int dt\, e^{i(\omega - V_i/\hbar)t}[V_I(1;t)\, U_I(1;t,-\infty)]_e$$
$$\cdot\{-i\omega + iV_i/\hbar + c(1 - [s_I(1)]_e\}^{-1}$$
$$\cdot\{\int dt\, e^{i(\omega - V_i/\hbar)t}$$
$$\cdot[V_I(1;t)\, U_I(1;t,-\infty)\, S_I^*(1)]_e\}^*. \quad (4.8)$$

The remaining, $k < k'$, part is just the hermitian conjugate of (4.8). Combining this with (4.2) and suppressing the lable 1 as well as the lower bound $-\infty$ in U_I gives the result announced in (1.1/2).

5. Equivalent Alternative Form of Basic Result. Discussion

The formula for $L(\omega)$ which was derived in the preceding sections can be brought into an alternative form as we indicate now. The original form of the line shape function was

$$L(\omega_0 + \omega) = \mathrm{Tr}\, D[(\hbar\omega - v_i)^{-1} \quad (5.1)$$
$$\cdot \hat{I}_i(\omega)(\hbar\omega - v_i)^{-1}]_i$$

with $\hat{I}_i(\omega)$ given by (1.2). Here i refers to ions and $[\ldots]_i$ to averaging over ion configurations. As in Sect. 1, $U_I(t)$ denotes the time development operator from $-\infty$ to t for an electron colliding at $t=0$ (in the ion interaction picture) and $S_I = U_I(\infty)$ the corresponding S-matrix. By $\chi_{(-\infty,0)}(t)$ we denote the step function which is 1 on $(-\infty, 0)$ and zero elsewhere; analogously for $\chi_{(0,\infty)}(t)$.

Inserting (1.2) for $\hat{I}_i(\omega)$ into (5.1) one can show by partial integration and a little algebra that

$$L(\omega_0 + \omega) = \frac{1}{2\pi}\mathrm{Tr}\, D[c[\,|\int dt\, e^{i(\omega - V_i/\hbar)t}(U_I(t) - \chi_{(-\infty,0)}(t) - \chi_{(0,\infty)}(t) S_I)\,|^2]_e$$
$$+ \{c\int dt\, e^{i(\omega - V_i/\hbar)t}[U_I(t) - \chi_{(-\infty,0)}(t) - \chi_{(0,\infty)}(t) S_I]_e + 1\}$$
$$\cdot\{-i\omega + iV_i\hbar^{-1} + c[1 - s_I]_e\}^{-1}$$
$$\cdot\{c\int dt\, e^{i(\omega - V_i/\hbar)t}[U_I(t) S_I^* - \chi_{(-\infty,0)}(t) S_I^* - \chi_{(0,\infty)}(t)]_e + 1\}^* + \mathrm{h.c.}]_i \quad (5.2)$$

where h.c. stands for hermitian conjugate of the second summand. The step functions insure that for $t\to\pm\infty$ the integrands vanish; without them the integrals would not exist. We note that the individual terms of (1.1/2) and (5.2) do not correspond to each other, it is only an overall equality. For $c\to 0$, (5.2) trivially reduces to the result for quasi-static ions.

Equation (5.2) can also be directly derived from (2.6) without differentiation, using a convolution expression for $[T(t,s)]_{av}$ analogous to (2.16) and similar reasoning as in Sects. 3 and 4. In this con-

text the step functions correspond to a special choice of integration constant. Smoother choices are possible [14].

The mathematically equivalent expressions, (1.1/2) and (5.2), have their merits in different regions of ω, and the latter approaches a simple well known form for small ω as will now be discussed.

Large ω. In (1.2) the second and third term fall off with a higher power than the first. Hence in the far line wing they can be neglected and (1.1/2) become

$$L(\omega_0+\omega)=\frac{c}{2\pi}\operatorname{Tr} D \cdot[(\hbar\omega - V_\mathrm{i})^{-1}[|\int \mathrm{d}t\, e^{i(\omega - V_\mathrm{i}/\hbar)t} \cdot V_\mathrm{I}(t)\, U_\mathrm{I}(t)|^2]_\mathrm{e}(\hbar\omega - V_\mathrm{i})^{-1}]_\mathrm{i}\,. \tag{5.3}$$

On the other hand, for large ω (5.2) is the difference of two large quantities (as seen by computer calculations), and hence difficult to evaluate. Numerically one can use (5.3) for $\Delta\lambda \geqq 2$ Å.

Small ω. Now (1.2) is a difference of large quantities. This is most easily seen for $V_\mathrm{i}=0$, since then (1.1) contains a factor ω^{-2} so that $\hat{I}_\mathrm{i}(\omega)$ in (1.2) has to go to zero as ω^2. But since

$$\int_{-\infty}^{+\infty}\mathrm{d}t\, V_\mathrm{I}(t)\, U_\mathrm{I}(t) = -i\hbar^{-1}\int_{-\infty}^{+\infty}\mathrm{d}t\, \dot{U}_\mathrm{I}(t) = -i\hbar^{-1}(S_\mathrm{I}-1)\,,$$

the first term in (1.2) remains finite for $\omega\to 0$. On the other hand, (5.2) becomes quite simple. It turns out, that for $\Delta\lambda \leqq 0.5$ Å all integrals can be neglected so that one obtains

$$L(\omega_0+\omega)=\frac{1}{\pi}\operatorname{Tr} D\,\Re\mathrm{e} \cdot[\{-i\omega + iV_\mathrm{i}\hbar^{-1} + c[1-S_\mathrm{I}]_\mathrm{e}\}^{-1}]_\mathrm{i} \tag{5.4}$$

which leads to the result of the impact approximation below.

In case of the impact approximation — negligible interaction time between electrons and radiator — (5.2) goes over to the usual expression. Indeed, in this case $U_\mathrm{I}(t)$ equals 1 for $t<0$ and S_I for $t>0$ so that the integrals in (5.2) vanish, leading to (5.4). Now one has for the one-electron potential $V(1;t)$

$$e^{iV_\mathrm{i}t/\hbar}\, V(1;t)\, e^{-iV_\mathrm{i}t/\hbar} = V(1;t)$$

since only $t\approx 0$ matters, and hence S_I can be replaced by the pure electronic S-matrix $S^{(\mathrm{e})}$ (without ion interaction picture). This gives the usual impact result.

The limiting forms, (5.3/4), are much simpler than (1.1/2) and (5.2). However, in the intermediate region the additional terms become important and have to be taken into account in a numerical evaluation.

When one analyses the derivation of (1.1/2) one notices that the first term in (1.2) arose from the diagonal terms, whose contribution is independent of N (cf. (4.1/2)).

6. Application to Ly — α

In order to exploit rotation symmetry more easily we use angular momentum eigenstates $|nlm\rangle$. The lower level space, $\mathscr{H}_\mathrm{f}$, is spanned by $|100\rangle$ and the upper one, $\mathscr{H}_\mathrm{i}$, by $|200\rangle$, $|21\text{-}1\rangle$, $|210\rangle$, $|211\rangle$. We number the basis vectors of $\mathscr{H}_\mathrm{i}\otimes\mathscr{H}_\mathrm{f}$ in this order,

$$|1\rangle \equiv |200\rangle|100\rangle, \ldots, \quad |4\rangle \equiv |211\rangle|100\rangle\,. \tag{6.1}$$

Then all operators in line space, $\mathscr{H}_\mathrm{i}\otimes\mathscr{H}_\mathrm{f}$ of Sect. 2, become 4×4-matrices, and in it one has a reducible four-dimensional representation of the rotation group which decomposes into $l=0$ and $l=1$ parts, just as in $\mathscr{H}_\mathrm{i}$. From (2.3) one calculates

$$D_{jk}=\begin{cases}\frac{1}{3} & \text{for } j=k=2,3,4\,,\\ 0 & \text{otherwise}\,.\end{cases} \tag{6.2}$$

To obtain the matrices for the potential $V_\pm$ of a single perturber in line-space we use the Coulomb potential of a point charge $\pm e$ at (instantaneous) position $\mathbf{r}=(x,y,z)$ and the analog of (2.7). Let $a_0=\hbar^2/me^2$ be the Bohr radius. Neglecting terms containing $\exp(-a_0/r)$, one finds

$$V_\pm(\mathbf{r}(t)) = \pm 3e^2a_0\begin{pmatrix} 0 & 2^{-1/2}r^{-3}(x-iy) & r^{-3}z & -2^{-1/2}r^{-3}(x+iy)\\ \cdot & a_0r^{-3}(3r^{-2}z^2-1) & 3a_0r^{-5}z(x+iy) & 3a_0r^{-5}(x+iy)^2\\ \cdot & \cdot & -2a_0r^{-3}(3r^{-2}z^2-1) & -3a_0r^{-5}z(x+iy)\\ \cdot & \cdot & \cdot & a_0\tau^{-3}(3r^{-2}z^2-1)\end{pmatrix}, \tag{6.3}$$

where the remaining matrix elements are determined by hermitian conjugacy. The omitted $\exp(-a_0/r)$-terms can be found in [14].

If one describes a collection of perturbers in the dipole approximation with resulting field strength $\mathbf{F}(t)$ at the origin, then one has to insert $V_p = e\mathbf{X}\cdot\mathbf{F}$ in (2.7). This yields the hermitian matrix

$$V_{\mathbf{F}}(t) = 3a_0 e 2^{-1/2}\begin{pmatrix} 0 & -F_x + iF_y & -2^{1/2}F_z & F_x + iF_y \\ \cdot & 0 & 0 & 0 \\ \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}. \tag{6.4}$$

We note that $V_\pm(\mathbf{r})$ and $V_{\mathbf{F}}$ have simple transformation properties under rotations. If $U(R)$ is the operator in line space corresponding to the rotation R, then

$$V_\pm(R\mathbf{r}) = U(R)\, V_\pm(\mathbf{r})\, U(R)^* \tag{6.5}$$

and similarly for $V_{R\mathbf{F}}$.

For large field strength of an ion configuration it is known that the nearest-neighbor approximation is sufficient [15], so in this case we use for the ion potential V_i the expression in (6.3) with V_+ and $\mathbf{r}(t) = \mathbf{r}_i$. In the remaining region we use for V_i the dipole approximation, (6.4), with the Holtsmark distribution for $\mathbf{F}$.

The potential for an electron is given by (6.3) also, with V_- and $\mathbf{r}(t) = \boldsymbol{\varrho} + \mathbf{v}t$. In the ion interaction picture we then have

$$V_I(t) = \exp\{i V_i t/\hbar\}\, V_-(\boldsymbol{\varrho} + \mathbf{v}t) \cdot \exp\{-i V_i t/\hbar\}. \tag{6.6}$$

Group theoretical reduction. The transformation properties of $V_\pm$ and $V_{\mathbf{F}}$, (6.5), allow the reduction of $[\ldots]_i$ and $[\ldots]_e$ by standard group theoretical methods. Physically it is quite clear that in the case of the one-ion approximation only the distance should enter and, in case of the dipole approximation, only $|\mathbf{F}|$. For $[I_i(\omega)]_i$ one obtains a diagonal matrix [14] with

$$[I_i(\omega)_{kk}]_i = \int_0^\infty \mathrm{d}\beta\, W(\beta)\, \tfrac{1}{3}\sum_{l=2}^{4} I_z(\beta,\omega)_{11} \quad \text{for} \quad k = 2,3,4, \tag{6.7}$$

where $W(\beta)$ denotes the Holtsmark distribution, whose argument $\beta = F/F_0$ is defined in terms of the normal field strength $F_0 = 2.6023\, e\, \nu_{\mathrm{ion}}^{2/3}$. The intensity operator $I_z(\beta,\omega)$ is defined as the intensity operator $I_i(\omega)$ for a particular configuration: the ion is on the z-axis (in the nearest neighbor approximation) or the ion field is parallel to the z-axis (in the dipole approximation). We change from dipole to nearest neighbor approximation at $\beta = 8$. Then, in Eq. (6.3), $x = y = 0$, $z = -r_i$ and

$$r_i = r_i(\beta) = (e/F_0\beta)^{1/2}. \tag{6.8}$$

From (2.6/14) and (6.2/7) one finds immediately for $\varkappa = 2,3,4$

$$L(\omega+\omega_0) = [I_i(\omega)_{\varkappa\varkappa}]_i.$$

In the case of pure electron broadening one has the special form

$$L(\omega+\omega_0) = \tfrac{1}{3}\sum_{l=2}^{4} I_z(0,\omega).$$

With the ion field along the z-axis or the ion on the z-axis, respectively, one has still a rotational degree of freedom around this axis. Together with the transformation properties of the potentials this can be used to eliminate one integration in the electron averaging. Physically this means that the point of closest approach is rotated into the $x-z$-plane. This leaves four integration variables, $0 \leqq \varrho \leqq \varrho_D$, the polar angle $0 \leqq \theta \leqq \pi$ of ϱ, v, and the angle $0 \leqq \varphi_1 \leqq 2\pi$ between $\mathbf{v}$ and the projection of $\mathbf{v}$ onto the $x-z$-plane. Since the number of electrons entering the Debye sphere is proportional to v and since the $\boldsymbol{\varrho}$'s were, originally, uniformly distributed in the Debye sphere, the weight factor becomes

$$2(m_e/2\pi k_B T)^{3/2}(\bar{v}\varrho_D^2)^{-1} v^3 \cdot \exp\{-m_e v^2/2k_B T\}\, \varrho \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\varphi_i\, \mathrm{d}\varrho\, \mathrm{d}v. \tag{6.9}$$

The transformation properties, (6.5), imply that the only nonvanishing matrix elements are those with (total) $L_z = 0$, i.e., the diagonal ones and those with $(j,k) = (1,3), (3,1)$; they are also independent of the angles θ, φ_1.

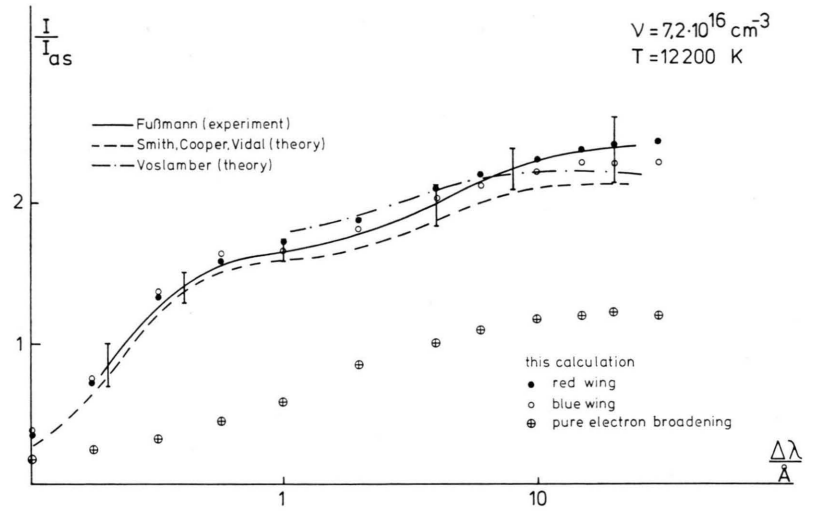

Fig. 1. Expected asymmetry effects for the line wing of Ly-α and comparison with experiment [18] and with other calculations (without asymmetry). The pure electron part belongs to the blue wing.

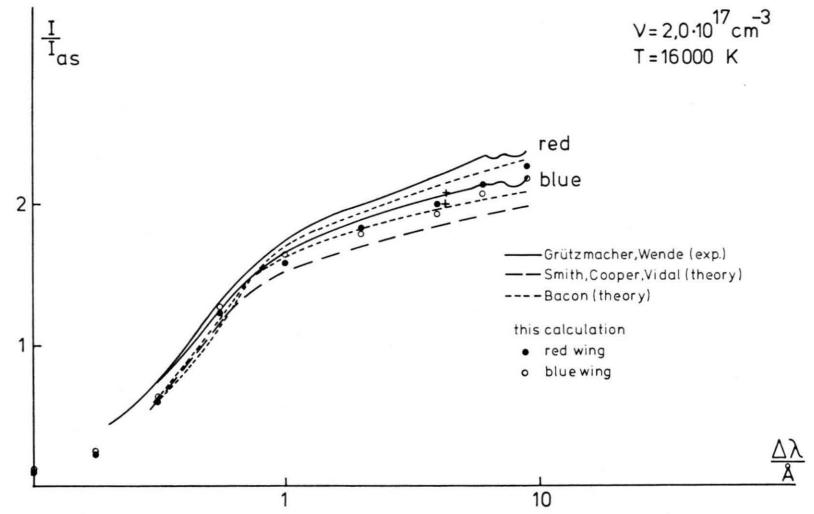

Fig. 2. Asymmetry of the line wing of Ly-α and comparison with experiment [18] and the calculations of Bacon [10]. Smith, Cooper, Vidal [20] do not consider asymmetry effects. The two "crosses" at $\Delta\lambda = 4$Å represent our formula with a more elaborate numerical evaluation (including noncommutativity effects). We find a crossover between red and blue wing at about $\Delta\lambda = 1$ Å.

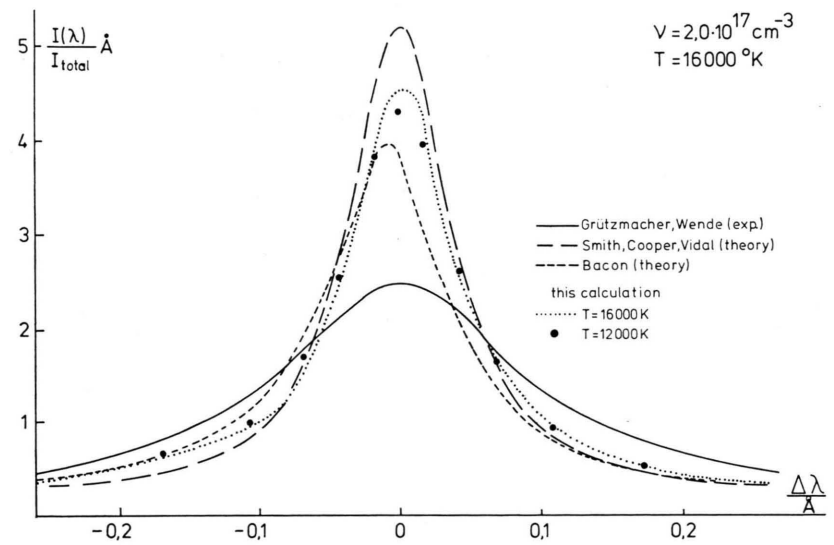

Fig. 3. Experiment and some calculations in the line center (relative units). The "fat dots" show that the temperature dependence is small.

Numerical evaluation. For given values of the parameters ϱ, θ, v, φ_1 and β one has to determine the time development operator in the ion interaction picture from the differential equation (3.5). This is easily achieved by a predictor-corrector subroutine. To reduce the numerical effort for the integration, one can make a further approximation. Dividing the β-integration into two subregions, $0 \leqq \beta \leqq 20$ and $20 \leqq \beta \leqq \infty$, one can neglect V_i in $V_\mathrm{I}(t)$ within the first region so that V_i appears only in the denominators of (1.2) and (5.2). This does not mean that the ion and electron potential commute in this region, but it is rather an effect of the angular averaging as apparent in the numerical analysis. The integrations over φ_1 and θ can now be performed analytically, and the closed form of Pfennig [16] for the time development operator can be used.

The β-integration over the second region contributes only if $\Sigma_j I_z(\beta, \omega)_{jj}$ has an extremum there, since $W(\beta)$ falls off rapidly. For small ω, $|\hbar\omega| \leqq 3ea_0F_0 \cdot 20$, there is no extremum in the region $20 \leqq \beta < \infty$ so that we need integrate over $0 \leqq \beta \leqq 20$ only.

For the line wing, $|\hbar\omega| \gg 3ea_0F_0 \cdot 20$, the situation is different. In the first β-region, V_i can now be neglected in the denominators also, since $|\hbar\omega|$ is much larger than the matrix elements of V_i, leading to

$$\begin{aligned}
&\int_0^{20} \mathrm{d}\beta\, W(\beta)\, \tfrac{1}{3} \sum_{k=2}^{4} I_z(\beta, \omega)_{kk} \\
&\approx \tfrac{1}{3} \sum_{k=2}^{4} I_z(0, \omega)_{kk} \int_0^{20} \mathrm{d}\beta\, W(\beta) \\
&\approx \tfrac{1}{3} \sum_{k=2}^{4} I_z(0, \omega)_{kk} =: L_\mathrm{e}(\omega + \omega_0)\,, \qquad (6.10)
\end{aligned}$$

the pure electron contribution to the broadening. In the second β-region, however, $\det(\omega - V_z(\beta)/\hbar)$ has zeros. If one approximates the resulting steep maxima by δ-functions one obtains [21]

$$\begin{aligned}
&\tfrac{1}{3} \int_{20}^{\infty} \mathrm{d}\beta\, W(\beta)\, \{2\,\delta(\omega - V_z(\beta)_{22}/\hbar) \\
&\qquad + |\omega|\, \delta(D(\beta))\} \\
&=: L_\mathrm{i}(\omega + \omega_0)\,, \qquad (6.11)
\end{aligned}$$

where

$$\begin{aligned}
D(\beta) = {} & (V_z(\beta)_{13}/\hbar)^2 \\
& + \omega\, V_z(\beta)_{33}/\hbar - \omega^2\,. \qquad (6.12)
\end{aligned}$$

$L_\mathrm{i}(\omega + \omega_0)$ is a contribution due to the ions only. Thus with the above approximations one obtains for the line wing the well known form

$$\begin{aligned}
L(\omega + \omega_0) = {} & L_\mathrm{e}(\omega + \omega_0) \\
& + L_\mathrm{i}(\omega + \omega_0) \qquad (6.13)
\end{aligned}$$

since the trace is trivial now.

To check the above approximations in the numerical evaluation we have calculated the β-integral in the region $20 \leqq \beta < \infty$ without them for $\Delta\lambda = 4$ Å (cf. Figure 2). The result is only about 4% higher than with the approximations. These 4% thus include effects of the noncommutativity of electron and ion-potential as well as the replacement of maxima by δ-functions.

Discussion of Results

In our approach we have used the non-quenching assumption throughout, thus disregarding higher order perturbation effects. Hence the resulting asymmetries are due entirely to the quadrupole moments of the interaction potentials. The essential asymmetry contribution comes from the ions via (6.11), where the first term gives a contribution proportional to ω^{-2} to the blue wing, while in the second term quadrupole moments displace the δ-function and yield a stronger red wing. In the line center, however, we obtain a higher intensity of the blue part. This reversal is due to the lectrons.

In Figs. 1, 2 and 3 we have compared our results with measurements of Fußmann [17] and of Grützmacher and Wende [18] as well as with calculations of Voslamber [19], Smith, Cooper and Vidal [20], and Bacon [10], quoted from Refs. [17] and [18], respectively. On the line wing the agreement is good. In the center we have the same discrepancies as other calculations. This is probably due to the quasi-static treatment of the ions [7].

Neglecting Doppler broadening the dependence of the line shape on the plasma temperature is rather small. Figure 3 shows the results for two different temperatures. Noticible dependence occurs only in the inner line center.

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