Unified and impact treatment of partially overlapping spectral lines

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Abstract. The unified theory of line broadening and its impact limits as well as an 'extended impact theory' are re-investigated with regard to their validity for partially overlapping lines. It is shown that the extended impact theory does not lead to an improved treatment of line coupling, but that it may be used as an interpolating formalism when line coupling is negligible. As an example we present numerical applications to the Stark-broadened fine-structure profile of Balmer-a.

1. Introduction

It has been known for a long time that the core of most atomic or molecular spectral lineshapes can be described by the impact theory if the broadening occurs in a collisional environment (Lorentz 1906, Anderson 1949, Baranger 1958, Kolb and Griem 1958, Griem et al 1962). While for neutral gases such an environment is simply defined as one in which the atom or molecule (hitherto called system) suffers binary collisions, this notion is more complicated for plasmas and may, in some situations, be valid only for some of the charged perturber species (e.g. electrons), while for others (e.g. ions) it is invalid. The requirement for a particle species to constitute a collisional environment is that simultaneous strong interactions between the system and several of the perturbing particles are negligibly rare events (see e.g. Baranger 1958) and that the cumulative effect of weak collisions remains small during the correlation time of the interaction (Capes and Voslamber 1972).

A sufficient condition for having a collisional environment is

\[ w \ll \omega_f \]

where \( w \) indicates the order of magnitude of the linewidth and \( \omega_f \) is the fluctuation frequency (inverse of correlation time) of the interaction. For neutral perturbers, condition (1) just expresses the requirement that the time \( t_c = w^{-1} \) between collisions be long compared with the duration \( \tau_c = \omega_f^{-1} \) of a collision. For charged perturbers, \( \omega_f \) is approximately equal to the plasma frequency \( \omega_p \) of the perturber species considered. This corresponds to the fact that due to plasma screening, the largest collision
durations occur for impact parameters of the order of the Debye length $\lambda_D = v_{th}/\omega_p$ ($v_{th}$ being the thermal velocity).

There are situations where condition (1), though sufficient, is not necessary. This may occur when part of the interactions, e.g. those with impact parameters above a certain critical value $r_{\text{eff}}$, do not become effective. Condition (1) is then to be replaced by

$$w < \omega_{\text{r}}^{\text{eff}} = v_{th}/r_{\text{eff}}.$$  

An example of this is the Stark broadening for the cores of very isolated lines. If typical level separations $\Delta$ greatly exceed $\omega_r$, second-order dipole interactions (assuming states of definite parity) will be important only for impact parameters below $v_{th}/\Delta$ and higher-order or higher multipole interactions only for impact parameters not much larger than the Weisskopf radius $r_w$ or the excited system radius $r_s$. The effective interaction radius is then $r_{\text{eff}} = \max(v_{th}/\Delta, r_w, r_s)$.

The impact theory can be based on a Markovian master equation for the density operator of the radiating system (Blum 1981). Such an equation is characterised by a time-independent collision (or relaxation) operator $\hat{K}$ which is closely related to the collisional $S$ matrix and whose matrix elements (damping or width constants) determine the shape of the line profile. The validity of the master equation is restricted to large times, and consequently that of the line profile to small frequency separations $\Delta \omega$ from some line centre, in a sense which will be made more specific according to different special cases considered below. For values $\Delta \omega$ falling outside the validity domain of the impact theory, the line profile is described by the more general unified theories, which involve a frequency-dependent collision operator $\hat{K}(\omega)$ (Fano 1963, Voslamber 1969, 1972b, Smith et al 1969, Ben Reuven 1975).

Baranger (1958) and Griem et al (1962) have investigated the validity of the impact theory for cases where the line profile originates from a number of neighbouring radiative transitions giving rise to a set of more or less overlapping line components. It is particularly the latter reference which specifies the situations in which a Markovian treatment can be employed. Actually, such a treatment is justified in two limiting cases, characterised by what we shall call 'collisionally degenerate lines' (hereafter referred to as case (a)) and 'isolated lines' (hereafter referred to as case (b)). Each of these cases gives rise to a different formalism.

Case (a) occurs when the sublevels in each of the two level groups corresponding to the radiative transitions show 'collisional degeneracy', in the sense that typical frequency separations $\Delta$ between them are small compared with $\omega_r$. Collisions then occur as if these levels were completely degenerate, so that the effect of the level splitting on the collision operator is negligible. The validity of the Markovian approach is in this case restricted to frequency separations obeying

$$|\Delta \omega| \ll \omega_r,$$  

where $\Delta \omega$ refers to some line centre lying inside the group of line components. Its exact definition does not matter because in the case considered the line components are relatively closely spaced or even overlapping.

Case (b) occurs when the levels are sufficiently isolated to be far from 'shape degeneracy', in the sense that one has $w \ll \Delta$. In that case the cores of the line components are Lorentzians with the widths given by the diagonal elements of the collision matrix, while the off-diagonal elements have significant effects only in the
dips between the components. The corresponding formalism consists of neglecting
the off-diagonal elements altogether, thus renouncing a detailed description of the
dips. The resulting line profile is then just a superposition of a set of Lorentzians.

We note that as long as one has $\Delta < \omega_f$, case \(b\) is included in case \(a\). If the
main purpose is to describe the line profile within a few half widths of each line
component, both formalisms can then be employed equivalently, although, of course,
the one of case \(b\) may be preferred due to its simplicity. If, on the contrary, one is
also interested in accurately describing the dip regions, the formalism of case \(a\) must
be employed in order to include the effect of the off-diagonal part of the collision matrix.

In situations where the level separations $\Delta$ are so large that one has not only \(w \ll \Delta\)
but even $\omega_f \ll \Delta$, the collision operator (and consequently the widths of the line
components) depend on the level spacing; furthermore, the validity of the impact
approach is restricted to the cores of the line components, in a sense which will be
made more specific in § 2. The dip regions between the components as well as the
outer far wings can then only be described by the more complete unified theory
mentioned above (Voslamber 1970). Note that the failure of the impact theory in the
dips occurs because of the frequency dependence of both the diagonal and off-diagonal
elements of the collision operator. The former lead to 'generalised Lorentzians' with
'frequency-dependent widths and shifts', while the latter cause the dip between two
components to be more complicated than just the superposition of the two 'generalised
Lorentzians' associated with them.

The above discussion has, for simplicity, been restricted to situations where 'col-
cisionally degenerate lines' and 'isolated lines' occur as pure cases, i.e. where all levels
are spaced in such a way that one has either case \(a\) or case \(b\). In real situations
both cases may occur simultaneously, i.e. one may have some of the levels so close
together that their spacing is smaller than $\omega_f$, while others are so far away that their
frequency distances exceed $\omega_f$. It is clear that the adequate combination of the
formalisms \(a\) and \(b\) then consists of choosing subgroups of levels in such a way
that different subgroups are isolated from each other but that one has collisional
degeneracy within the same subgroup. Off-diagonal collision matrix elements between
different subgroups will then have to be neglected, while those within a subgroup
(which then depend on the level spacing between subgroups) are retained.

The fact that for $\omega_f \ll \Delta$ the dip regions are not covered by the standard impact
theory (cases \(a\) or \(b\) or combination of both) has led numerous authors to use a
kind of (as we shall call it) 'extended impact theory' (Deutsch et al 1969, 1972, 1974,
al 1986, Boissoles et al 1987, Green et al 1988). This approach consists of taking the
lineshape expression derived for case \(a\) even outside the domain of collisional
degeneracy and accounting for the effect of level spacing by including it in the
calculation of the $S$-matrix elements. Unfortunately, as has previously been pointed
out by one of us (Voslamber 1970) (and as has also been stressed in a recent paper
by Burstein et al (1985)), this method cannot be justified theoretically and provides
no improvement with respect to the standard impact theory mentioned above. We
want to emphasise again (and will give additional support to this in § 2) that valid
corrections to either of the two limiting impact formalisms \(a\) or \(b\) can only be
obtained using a non-Markovian master equation. The result is the lineshape expression
obtained in the unified theory of line broadening already mentioned, with the charac-
teristic feature that the collision operator is no longer a constant but depends on the
frequency variable of the line profile.
Among the various papers quoted in connection with the use of the extended impact theory, most of them belong to one of two groups, the first being concerned with Stark broadening in plasmas (Deutsch et al 1969, 1972, 1974, Barnard et al 1969, Stehlé and Feautrier 1985) and the second with molecular line broadening by neutrals (Lam 1977, Cousin et al 1986, Boissoles et al 1987, Green et al 1988). The main concern of the latter group is an improved treatment of what is usually called 'line coupling' in atmospheric optics, i.e. of the effect of the off-diagonal collision matrix elements on the dips (‘microwindows’) between neighbouring lines of vibration-rotation bands. Considerable effort has been spent in some of these papers to include the energy spacing in the $S$ matrix. Unfortunately, this effort does not seem to be of any worth for an improved treatment of line coupling. Indeed, as already stated above and shown in more detail in § 3, only when it is not affected by the level spacing can the off-diagonal part of the collision operator be expressed in terms of $S$ matrix elements.

The situation is similar in Stark broadening, where the inclusion of level splitting in the off-diagonal collision matrix elements (see e.g. Deutsch et al 1969, Barnard et al 1969) has led to unnecessary analytical complications (for more details see Voslamber 1970). In an application to He I lines in plasmas of medium density, Deutsch et al (1972, 1974) have compared their results for the 4471 Å line with corresponding results obtained from the unified theory. The agreement was found to be satisfactory; however, in the particular case investigated this has a very simple explanation: for the plasma parameters chosen, the $4^3D$, $F$ levels happen to be collisionally degenerate, which implies that both the extended impact theory and the unified theory just reproduce the results of the standard impact theory for case (a).

Although the extended impact theory is unable to reach its goal of improving the standard impact theory, it may yet be of some use in practical applications. Since it reproduces correctly cases (a) and (b) in the appropriate limits, it may indeed be considered as an interpolating formalism for those situations where the intensity in the dip regions is too small to be of experimental interest, or where these regions are little influenced by off-diagonal elements not described by the standard impact theory. The extended impact theory may then be preferred over both the standard impact theory (which, though simpler in structure, requires nonetheless some switchover between cases (a) and (b) in their common domain $w < \Delta < \omega_r$) and the unified theory (which, though more correct, is rather computer-time consuming because it not only requires a matrix inversion for each frequency considered but also involves complicated transient collision effects to evaluate the collision operator). An example where the extended impact theory has led to satisfactory results because of the interpolation properties mentioned has been the application to the fine-structure profile of Balmer-$\alpha$ (Stehlé and Feautrier 1985, hereafter referred to as I). This example will be analysed again in § 5 of the present paper.

The purposes of the remaining part of this paper are the following. In §§ 2–4 we will present a brief account of the formal aspects of unified and impact theories; we will show how and under what conditions the latter can (or cannot) be obtained as limiting cases of the former. Some of the results will be exemplified numerically by application to a four-level model atom (§ 4). In § 5 we will report and analyse the results of calculations which have been carried out for the Stark-broadened fine-structure profile of the Balmer-$\alpha$ line of hydrogen. Calculated profiles obtained on the basis of the unified theory and of the standard impact theory will be compared with each other and with those obtained in I on the basis of the extended impact theory. Densities varying between $10^{12}$ and $10^{14}$ cm$^{-3}$ will be considered so that our
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investigation will encompass the main typical cases characterising the transition from isolated to collisionally degenerate lines.

2. Formalism of the unified theory

2.1. Unified lineshape expression

We take as a starting point the unified theory, whose validity is assured by condition (1) or (2), depending on the case considered. Apart from unimportant factors, this theory yields the lineshape expression

\[ L(\omega) = \frac{1}{\pi} \text{Re} \sum_{\alpha \beta} D^\alpha_{\alpha'} D^\beta_{\beta'} \langle (a\beta)(i(\hat{H}_0/h - \omega) + \hat{K}(\omega) + \hat{R})^{-1} |a\beta'\rangle \rangle. \] (4)

Here, \( \omega \) denotes the angular frequency; \( \alpha, \alpha' \ldots \) and \( \beta, \beta' \ldots \) label, respectively, the upper and lower states of the radiative transitions; the corresponding dipole moments are denoted by \( D_{\alpha \beta} \) etc; double kets \( |a\beta\rangle \rangle \) designate states in Liouville space (see e.g. Ben Reuven 1975), which is acted on by superoperators (denoted by a caret on top of them) such as the commutator \( \hat{H}_0 \) of the unperturbed Hamiltonian \( H_0 \), the collision operator \( \hat{K}(\omega) \) and the radiative damping operator \( \hat{R} \).

To write the collision operator, we choose the classical path description as given e.g. in Voslamber 1972a, but use a slightly more general form in allowing for arbitrary (instead of straight) paths. This form reads

\[ \hat{K}(\omega) = \frac{N_p}{\hbar^2} \int_0^\infty \delta(t) \exp(-i\hat{H}_0 t/h) \hat{U}(t, 0) \hat{U}(0) \langle \hat{V}(t) \rangle \langle \hat{V}(0) \rangle \rangle dt \] (5)

where \( N_p \) is the total number of perturbers, \( \hat{V}(t) \) the interaction potential at time \( t \) between the system and a given perturber, \( \hat{U}(t, t') \) the interaction representation of the time evolution operator associated with this perturber (describing the evolution of the system from time \( t' \) to time \( t \)), and the average is over all initial \( (t = 0) \) perturber positions and velocities.

We note two simplifications introduced deliberately into the above formalism of the unified theory. First, for Stark broadening, equation (5) is not quite complete because it does not contain the plasma dielectric function accounting for dynamic Debye screening. (For a more complete treatment see Capes and Voslamber (1972).) We have still chosen this formula for the sake of simplicity, bearing in mind that screening effects must now be introduced artificially, e.g. by cutting integrations over the impact parameter at the Debye length. Second, in establishing equation (4) we have assumed, without loss of generality for a stationary system, that

\[ \langle \hat{V}(t) \rangle \rangle = \langle \hat{V}(0) \rangle \rangle = 0. \] (6)

Actually, non-vanishing parts of the average potential, whenever existing, might be incorporated in the unperturbed Hamiltonian \( \hat{H}_0 \) as well as in the corresponding basis states. \( \hat{H}_0 \) would then be supplemented by the term \( N_p \langle \hat{V}(0) \rangle \rangle \).

Since the average in equation (5) is defined in the one-perturber phase space, it contains additive contributions from all types of collisions which may occur. We roughly distinguish between 'weak' collisions where \( \hat{U}(t, 0) \) stays close to the unity operator for all times \( t \), and 'strong' collisions where it does not. Consequently, the collision operator can be written as the sum of two contributions,

\[ \hat{K}(\omega) = \hat{K}^{(s)}(\omega) + \hat{K}^{(w)}(\omega) \] (7)
where superscripts s and w refer to strong and weak collisions respectively. The relative importance of the two contributions depends on the \( \omega \) region of the line profile considered and is also rather different according to whether one is dealing with neutral pressure broadening or with Stark broadening in plasmas.

In neutral pressure broadening, the weak collision contribution is usually unimportant because of the rapid fall-off of the interatomic potentials. It is actually the strong collision part in (7) which prevails all over the line profile. (For exceptions see Lobb and McCartan (1988).)

The contrary occurs for Stark broadening where, due to the long range of the Coulomb potential, it is usually the weak collision part which dominates the line body. Strong collisions are there of minor importance (except for very isolated lines) but these determine essentially the behaviour of the far wings (see e.g. Griem 1974, Voslamber 1972a, Lisitsa and Sholin 1972, Caby et al 1975, Le Quang Rang and Voslamber 1981). It is important to notice that on the far line wings the classical path approximation becomes questionable; it may then be more appropriate to employ the quantum version of the unified theory (Fano 1963, Van Regemorter 1969, Tran Minh and Van Regemorter 1972, Voslamber 1972b, Tran Minh et al 1975, 1976, 1980, Feautrier et al 1976, Feautrier and Tran Minh 1977).

2.2. Functional behaviour of collision operator

Since it will be our aim to elaborate the impact limits of the unified theory, it is important to know how rapidly the collision operator varies with the frequency \( \omega \). To answer this question, we first look at the time dependence of the average operator product

\[
\hat{C}(t) = \langle \hat{V}(t) \exp(-i\hat{H}_c t/\hbar) \hat{U}(t,0) \hat{V}(0) \rangle_{av}
\]  

(8)

occurring in (5). It is easily seen that this expression drops to zero at the latest after times \( t > T \), indeed, for such times the two \( \hat{V} \) factors in (8) correspond to perturber positions separated by more than the effective range of the potential, implying that at least one of the two factors and thus their product vanishes.

Since we have shown in this way that \( T \) is an upper bound of the decay time of (8), it follows that \( \omega_T = \tau_c^{-1} \) is a lower bound to the characteristic frequency intervals over which \( \hat{K}(\omega) \) varies appreciably. To demonstrate this explicitly, we first write equation (5) in terms of matrix elements:

\[
\langle \alpha \beta | \hat{K}(\omega) | \alpha' \beta' \rangle = \sum_{\gamma \delta} K_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(\omega)
\]  

(9)

where

\[
K_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(\omega) = \frac{N_p}{\hbar^2} \int_0^\infty \exp[i(\omega - \omega_{\gamma \delta})t] F_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(t) \, dt
\]  

(10)

and

\[
F_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(t) = \langle \langle \alpha \beta | \hat{V}(t) | \gamma \delta \rangle \rangle \langle \gamma \delta | \hat{U}(t,0) \hat{V}(0) | \alpha' \beta' \rangle \rangle_{av}
\]  

(11)

and where the summation is over a complete basis of eigenvectors |\( \gamma \delta \rangle \rangle of \( \hat{H}_c \), \( \omega_{\gamma \delta} \) denoting the energy difference, in angular frequency units, between states \( \gamma \) and \( \delta \).
Next we observe that equation (10) may also be written as
\[ K_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(\omega) = \frac{N_p}{\hbar^2} \int_0^\infty \exp[i(\omega - \omega_i) t] \exp[i(\omega_i - \omega_{\gamma \delta}) t] F_{\alpha \beta \alpha' \beta'}^{\gamma \delta}(t) \, dt \] (12)
where \( \omega_i \) is any frequency of interest in the spectral range considered. If \( \omega \) lies in the vicinity of \( \omega_i \) such that \(|\omega - \omega_i| \approx \omega_i\), the argument of the first exponential in (12) remains smaller than unity for \( t \ll \tau_c \); hence this exponential does not really start to oscillate before the integration in (12) is terminated, and the value of the integral does not differ much from what one obtains when putting exactly \( \omega = \omega_i \). Since \( \omega_i \) was chosen arbitrarily, we conclude that the collision operator \( K(\omega) \) is everywhere 'locally constant' over a scale of order \( \omega_c \).

As for more details about the functional behaviour of the collision operator, no general statement seems possible without further specification. One such specification is the assumption of weak collisions which will be considered in the next subsection.

2.3. Weak collision contribution

2.3.1. General considerations. Because of its importance for Stark broadening (our field of application in § 5), we pay particular attention to the weak collision contribution \( K^{(w)}(\omega) \). This contribution is obtained from equation (5) by putting there \( \tilde{U} = 1 \), which yields
\[ \hat{K}^{(w)}(\omega) = \frac{N_p}{\hbar^2} \int_0^\infty \exp[i(\omega_i - \omega_{\gamma \delta}) t] \exp(-i \tilde{H}_c t/\hbar) \tilde{V}(0)_{\omega} \, dt \] (13)
where the average is now over weak collisions only. Correspondingly, the weak collision part in equation (11) takes the simpler form
\[ F_{\alpha \beta \alpha' \beta'}^{(w)\gamma \delta}(t) = \langle \langle \alpha \beta | \tilde{V}(t) | \gamma \delta \rangle \langle \gamma \delta | \tilde{V}(0) | \alpha' \beta' \rangle \rangle_{\omega} \]. (14)
This expression can be assumed real by virtue of an appropriate choice of the basis \( \{ |\gamma \delta \rangle \} \). It has the meaning of a correlation function of potential matrix elements. When this correlation function is everywhere positive, the real part of the weak collision contribution \( K^{(w)\gamma \delta}(\omega) \) of (10) has a maximum at \( \omega = \omega_{\gamma \delta} \), shows negligible variation as long as \(|\omega - \omega_{\gamma \delta}| \ll \omega_c \), and tends to zero for \(|\omega - \omega_{\gamma \delta}| \to \infty \). According to what has been stated in § 2.2, the decrease is slow over a scale which has \( \omega_c \) as a lower bound. Actually for the case of weak collisions we are considering, the true scale becomes larger than this bound to the extent that \(|\omega - \omega_{\gamma \delta}| \) exceeds \( \omega_c \). As can be seen when inserting (14) into equation (10), the RHS of the latter equation varies little as long as the relative change of the frequency variable \( \omega - \omega_{\gamma \delta} \) is small compared with unity. Therefore, it is this frequency variable which, when it exceeds \( \omega_c \), defines the scale of variation and not \( \omega_c \).

In contrast to the real part, the imaginary part of \( K^{(w)\gamma \delta}(\omega) \) vanishes for \( \omega = \omega_{\gamma \delta} \) and varies linearly in the vicinity of this frequency. As compared with the real part, this term is there, in order of magnitude, smaller by a factor of about \(|\omega - \omega_{\gamma \delta}|/\omega_c \); therefore, if the interest is not focused on frequency separations \(|\omega - \omega_{\gamma \delta}| \) approaching of exceeding \( \omega_c \), the imaginary part may be neglected.

We conclude that the \( \omega \) dependence of \( \hat{K}^{(w)}(\omega) \) as a whole is rather involved. According to equations (9) and (10) (written for weak collisions) a matrix element of this operator taken between the two 'transitions' \( (\alpha \beta) \) and \( (\alpha' \beta') \) is a sum of terms associated with these and all other transitions \( (\gamma \delta) \). The \( \omega \) dependence of the term...
associated with \((\gamma \delta)\) is centred about the frequency \(\omega_{\gamma \delta}\), where the real part of the term is approximately \(\omega\) independent in a range of order \(\omega\), and the imaginary part varies there linearly about zero. Since in the general case the \(\omega_{\gamma \delta}\) may be spread over a wide range of frequencies, the total sum of terms shows various maxima and minima and can generally not be expected to show any regular behaviour. It is only in special limits that one may demonstrate, e.g., the validity of the impact theory which requires that all terms in (9) (or at least those contributing significantly to the line profile) are \(\omega\) independent in the total frequency domain under consideration.

2.3.2. Weak collision contribution for Stark broadening. In the case when the broadening is due to the charged particles of a plasma, the validity condition (1) (or (2)) must be checked for each particle species separately. While these conditions are usually fulfilled for electron perturbers, they are often not for ion perturbers unless the plasma density takes rather small values (typically \(n_e < 10^{14}\) cm\(^{-3}\) for the lower hydrogen lines).

For distant collisions with charged point charges (electrons or ions) the potential in (14) can be written in the dipole approximation, \(\hat{V}(t) = -D \cdot E\), where \(E\) is the electric field (at the location of the system) of the perturber under consideration. Assuming the perturbers to move on classical straight paths, the weak collision contribution in equation (10) has been evaluated previously (Voslamber 1970) with the result (written here in SI units and in the Liouville space language)

\[
K_{\alpha \beta}^{(\omega) \gamma \delta}(\omega) = \frac{n_p q^2}{3e_0 \hbar^2} \langle \alpha \beta | \hat{D} | \gamma \delta \rangle \langle \gamma \delta | \hat{D} | \alpha' \beta' \rangle 
\times \int_0^\infty \frac{f(v)}{v} \left[ g \left( \frac{r_w}{v} (\omega - \omega_{\gamma \delta}) \right) - g \left( \frac{\lambda_D}{v} (\omega - \omega_{\gamma \delta}) \right) \right] dv. \tag{15}
\]

Here, \(n_p\) and \(q\) are the density and the charge of the perturber species considered, \(f(v)\) is the distribution of the velocity module \(v = |v|\) (assumed isotropic and normalised to unit area), and the function \(g(z)\) is defined as

\[
g(z) = a(z) + ib(z) \tag{16}
\]

with

\[
a(z) = |z| K_0(|z|) K_1(|z|) \quad \text{and} \quad b(z) = \frac{1}{\pi} \int_\infty^z \frac{a(z')}{z' - z} dz' \tag{17}
\]

where \(K_0\) and \(K_1\) are modified Bessel functions (Abramowitz and Stegun 1965).

The difference appearing in the integrand of equation (15) arises from an integration over the impact parameter from its lower limit \(r_w\) to its upper limit \(\lambda_D\), the Debye length. The lower limit (Weisskopf radius) is the impact parameter below which collisions are considered as being strong. In our application to the Stark broadened \(H_n\) line (§ 5) we will fix its value in accordance with the calculations performed in I.

When \(|\omega - \omega_{\gamma \delta}| > \omega = v_{th}/\lambda_D = \omega_p\), there is partial cancellation between the two terms forming the difference in (15). Only collisions with impact parameters below \(v_{th}/|\omega - \omega_{\gamma \delta}|\) then become really effective and the real part of the RHS of (15) decreases as \(\log(v_{th}/r_w|\omega - \omega_{\gamma \delta}|)\) (as long as the argument of the logarithm remains large compared with unity) while the imaginary part behaves like \(\arctan((\omega - \omega_{\gamma \delta})/\omega_p)\) (Voslamber 1970).
For still larger frequency separations, such that $|\omega - \omega_{\gamma\delta}|$ exceeds the Weisskopf frequency $\omega_{W} = v_{\gamma\delta}/r_{W}$, the weak collision part $K^{(w)}_{\alpha\beta\alpha'\beta'}(\omega)$ becomes negligible. The only significant contribution then comes from the strong collision part $K^{(s)}_{\alpha\beta\alpha'\beta'}(\omega)$ which, in the framework of the dipole approximation mentioned above, has the well known quasistatic $|\omega - \omega_{\gamma\delta}|^{-1/2}$ asymptote for both the real and the imaginary part.

3. Impact limits of the unified theory

The fact that the collision operator $\hat{K}(\omega)$ does not vary over a scale less than $\omega_{r}$ (see § 2.2) implies that the impact formalism can be employed at any point $\omega_{r}$ of the spectrum, provided that the use of the constant operator $K(\omega)$ is restricted to a domain of order $\omega_{r}$ around $\omega_{r}$. This has consequences of practical interest essentially in the two situations corresponding to cases (a) (collisionally degenerate line-components) and (b) (isolated line-components) mentioned in § 1. We will again simplify the discussion by considering only ‘pure’ cases (a) or (b), because situations where these cases are combined can be discussed in an analogous manner (see the corresponding paragraph in § 1).

3.1. Impact limit for case (a)

In case (a), the line components are so closely spaced that they lie all in a common narrow range much smaller than $\omega_{r}$. Since also their widths are small compared with $\omega_{r}$ (see equation (1)), the main portion of the line profile (extending to frequency separations of about $\omega_{r}$ on the wings) is covered by the impact theory with one and the same $\omega$-independent collision operator. The corresponding formalism consists of taking equation (4) and replacing $\hat{K}(\omega)$ by $\hat{K}(\omega_{0})$ where $\omega_{0} (= \omega_{\alpha\beta} = \omega_{\alpha'\beta'} = \ldots)$ denotes some line centre within the group of line components considered. The (sufficient) conditions of validity may then be summarised by the inequalities

$$\max_{\alpha\beta\alpha'\beta'} |\omega_{\alpha\beta} - \omega_{\alpha'\beta'}| \ll \omega_{r}$$

and

$$|\omega - \omega_{0}| \ll \omega_{r}.$$  (19)

The analytical expression for $\hat{K}(\omega_{0})$ simplifies considerably if one makes the ‘no-quenching’ approximation, i.e. if one neglects the influence of far-lying levels (those not included in the group of transitions $(\alpha\beta)$ considered). In that case, the basis $\{|\gamma\delta\rangle\}$ is restricted to states $|\alpha''\beta''\rangle$ belonging to the group, and the impact limit of equations (9) and (10) yields

$$\langle \alpha\beta | \hat{K}(\omega_{0}) | \alpha'\beta' \rangle = \sum_{\alpha''\beta''} K^{\alpha''\beta''}_{\alpha\beta\alpha'\beta'}(\omega_{0})$$  (20)

$$K^{\alpha''\beta''}_{\alpha\beta\alpha'\beta'}(\omega_{0}) = \frac{N_{0}}{\hbar^{2}} \int_{\infty}^{\infty} F_{\alpha''\beta''}(t) \, dt.$$  (21)

Equation (21) is obtained from equation (10) by a reasoning analogous to that following equation (12). Manifestly, equation (21) shows no explicit dependence on the position of the energy levels. Actually, there is no implicit dependence either, as can be seen by writing the Schrödinger equation for $\hat{U}(t, 0)$,

$$\left(\frac{\partial}{\partial t}\right) \hat{U}(t, 0) = -\left(i/\hbar\right) \exp(i\hat{H}_{0t}/\hbar) \hat{V}(t) \exp(-i\hat{H}_{0t}/\hbar) \hat{U}(t, 0)$$  (22)
and taking matrix elements on both sides of this equation. If these are evaluated in
the projected basis \(\{|\alpha'\beta'\}\), the two exponentials in (22) involve arguments of the
type \((\omega_{\alpha\beta} - \omega_{\alpha'\beta'}) t\) which remain small compared with unity for
\(t < \tau_c\). Hence, during the times which contribute to the integration in (21), \(\hat{U}\) and thus \(F_{\alpha'\beta' \alpha\beta}, K_{\alpha'\beta' \alpha\beta}\) and
finally \(\hat{K}\) (see equations (11), (21) and (20)) do not depend on the level positions.
Consequently, the impact limit of the collision operator can, in case (a), be calculated
as if there were complete degeneracy of the two level groups involved in the radiative
transitions.

The fact that one is allowed to use a formalism based on complete degeneracy
greatly simplifies the calculations. For example, if the level splitting arises from
spin–orbit interaction, the collision operator may be evaluated in the \(|LM\rangle\)
representation first and then transformed to the \(|LSJM\rangle\) representation by exploiting rotational
invariance (Omont 1973). Note also that degeneracy leads to a particularly simple
form for the weak collision part of the collision operator whose matrix elements then
read

\[
\langle \alpha\beta | \hat{K}^{(\omega)} | \alpha'\beta' \rangle = \frac{N_p}{\hbar^2} \sum_{\alpha'\beta'} \int_0^\infty \langle \langle \alpha\beta | \hat{V}(t) | \alpha''\beta'' \rangle \langle \alpha''\beta'' | \hat{V}(0) | \alpha'\beta' \rangle \rangle_\omega \, dt.
\]  

(23)

3.2. Impact limit for case (b)

3.2.1. General situation. In case (b), the line components are separated by frequency
distances much larger than the line widths, i.e. we have

\[
\min_{\alpha\beta\alpha'\beta'} |\omega_{\alpha\beta} - \omega_{\alpha'\beta'}| \gg w
\]  

(24)

where \(w\) stands for the order of magnitude for the matrix elements of the width operator
\(\hat{K} + \hat{\Delta}\). If the interest is not focused on the troughs between the components, the
impact formalism can be employed ‘piecewise’ by replacing \(\hat{K}(\omega)\) with \(\hat{K}(\omega_{\alpha\beta})\) for
the component \((\alpha\beta)\), with \(\hat{K}(\omega_{\alpha'\beta'})\) for the component \((\alpha'\beta')\) etc. Note that these
operators are significantly different only if \(|\omega_{\alpha\beta} - \omega_{\alpha'\beta'}| \gg \omega_f\), otherwise case (b)
is included in case (a). According to our discussion at the beginning of § 3, a sufficient
validity condition for employing the approximation mentioned is

\[
|\omega - \omega_{\alpha\beta}| \ll \omega_f
\]  

(25)

for any of the transitions \((\alpha\beta)\) of the group.

As in case (a), a significant simplification of the lineshape expression is obtained
by the use of an additional approximation. In the present case this is the secular
approximation which consists of neglecting the off-diagonal matrix elements of the
collision operator. The line profile is then simply a sum of Lorentzians, obtained from
equation (4) as

\[
L(\omega) = \frac{1}{\pi} \text{Re} \sum_{\alpha\beta} \frac{|D_{\alpha\beta}|^2}{i(\omega_{\alpha\beta} - \omega) + K_{\alpha\beta} + R_{\alpha\beta}}
\]  

(26)

with the width and shift parameters

\[
K_{\alpha\beta} + R_{\alpha\beta} = \langle \alpha\beta | \hat{K}(\omega_{\alpha\beta}) + \hat{\Delta} | \alpha\beta \rangle.
\]  

(27)

If condition (24) is fulfilled, the secular approximation is valid around each line
component \((\alpha\beta)\) in a domain restricted by the inequality

\[
|\omega - \omega_{\alpha\beta}| \ll \min_{\alpha'\beta'} |\omega_{\alpha\beta} - \omega_{\alpha'\beta'}|.
\]  

(28)
This condition may be less restrictive or more restrictive than (25), according to whether the level separations are larger or smaller than $\omega_r$. To encompass both possibilities, the (sufficient) validity condition for the impact formula (26) may be written as

$$|\omega - \omega_{\alpha\beta}| \ll \min_{\alpha'\beta'} (\omega_r, |\omega_{\alpha\beta} - \omega_{\alpha'\beta'}|)$$  \hspace{1cm} (29)$$

which has to be considered in addition to the condition (24) required for having isolated line components.

3.2.2. Special case of weak collisions. The impact limit of the weak collision contribution $\tilde{K}^{(w)}$ for isolated line components deserves particular attention not only because it is applied in part of the calculations presented in § 5, but also because it provides an example where the validity condition (29) is only sufficient but not necessary.

We recall that the validity conditions for the impact formula (26) are imposed by two approximations. One of them is the secular approximation (neglect of off-diagonal collision matrix elements) which is valid under conditions (24) and (28). The other one consists of replacing the frequency variable $\omega$ by the constant frequencies $\omega_{\alpha\beta}$ associated with the various line components $(\alpha\beta)$. For the latter approximation we have established, so far, the sufficient validity condition (25). In the following we will show that there may be special situations where this condition is not necessary. To demonstrate this, it is convenient to start again from the general formalism of the unified theory.

According to equations (9), (10) and (14), the diagonal elements of the weak collision contribution to the unified collision operator are given by

$$\langle \alpha\beta | \tilde{K}^{(w)} | \alpha\beta \rangle = \frac{N_f}{\hbar^2} \sum_{\gamma \delta} \int_0^\infty \exp[i (\omega - \omega_{\gamma\delta}) t] \langle \langle \alpha\beta | \hat{V}(t) | \gamma\delta \rangle \langle \gamma\delta | \hat{V}(0) | \alpha\beta \rangle \rangle_\omega \ dt.$$  \hspace{1cm} (30)$$

Assuming the correlation function of the potential matrix elements to be positive, the various terms of the sum in (30) are centred around the frequencies $\omega_{\gamma\delta}$, where they are about maximal. It is convenient at this stage to distinguish between the term with $\omega_{\gamma\delta} = \omega_{\alpha\beta}$, which represents elastic collisions, and the terms with $\omega_{\gamma\delta} \neq \omega_{\alpha\beta}$, which represent inelastic collisions. According to the general discussion in § 2.3.1, the first term is approximately $\omega$ independent for

$$|\omega - \omega_{\alpha\beta}| \ll \omega_r.$$  \hspace{1cm} (31)$$

As for the remaining terms, these have their ‘central frequencies’ $\omega_{\gamma\delta}$ far apart from the line component $(\alpha\beta)$ considered, since for $\omega = \omega_{\alpha\beta}$ and $|\omega_{\alpha\beta} - \omega_{\gamma\delta}| > \omega_r$ the characteristic scale of variation of such a term is $|\omega - \omega_{\gamma\delta}|$ (see the discussion following equation (14)) rather than $\omega_r$, the condition for replacing $\omega$ by $\omega_{\alpha\beta}$ in these terms is

$$|\omega - \omega_{\alpha\beta}| \ll \min_{\gamma\delta} |\omega_{\alpha\beta} - \omega_{\gamma\delta}|.$$  \hspace{1cm} (32)$$

instead of (31). Apart from the unimportant fact that (32) may involve pairs of states $(\gamma\delta)$ not initially counted in the group of transitions $(\alpha\beta)$, this condition is the same as (28) which was required for making the secular approximation. Taking both conditions (31) and (32) together is equivalent to the condition (29) already established for the impact limit in the general situation of case (b). However, condition (31) is associated with the occurrence of elastic collisions (terms with $\omega_{\gamma\delta} = \omega_{\alpha\beta}$) and is thus relevant only when elastic collisions provide a significant contribution. If this is not the case, as often occurs when weak collisions are dominant, condition (31) need not
be considered and condition (29) may be replaced by (32) which is less restrictive. Thus, when the level spacing largely exceeds $\omega_r$, application of the impact formalism may then be extended far beyond $\omega_r$ on the wings of the line components, provided that the distance from line centre remains small compared with the distance from neighbouring line components.

An important instance of the situation just described occurs in Stark broadening, when weak collisional dipole transitions between far-lying states of definite parity provide the most important contribution to the line profile. To a certain extent this will also play a role in our application to Balmer-$\alpha$ which we will present in § 5.

3.3. Connection with the $S$ operator

The purpose of this section is to establish the relationship between the impact limit of the collision operator $\hat{K}$ and the scattering ($S$) operator known in collision theory. To this end we pass to different forms of the expression given in (5), which we will obtain under the assumption that the frequency $\omega$ and the matrix elements $\langle \alpha\beta | \hat{K} | \alpha'\beta' \rangle$ are chosen such that $\omega = \omega_{\alpha\beta} = \omega_{\alpha'\beta'}$. This equality encompasses the formalisms of both cases (a) and (b) of the standard impact theory; it is indeed exact for the diagonal collision matrix elements required for case (b) (see equation (16)) and holds formally also for case (a) as pointed out in § 3.1.

As a first step we note that $\hat{U}(t, t')$ obeys the Schrödinger equation (22) and use this to write equation (5) in the form

$$\hat{K}(\omega) = \frac{i N_D}{\hbar} \int_0^\infty \exp[i(\omega - \hat{\tilde{H}}_0/\hbar)t] \left\langle \frac{\partial \hat{U}(t, 0)}{\partial t} \hat{V}(0) \right\rangle_{av} dt.$$  \hspace{1cm} (33)

The exponential in this expression can be set equal to the unity operator. Indeed, applying $\hat{K}(\omega)$ to the bra $\langle \alpha\beta |$ leads to the frequency $\omega - \omega_{\alpha\beta}$ in the exponent, which vanishes according to the assumptions made above. The integration in (33) can then be readily carried out and yields

$$\hat{K} = \frac{i N_D}{\hbar} \langle \hat{U}(\infty, 0) \hat{V}(0) \rangle_{av}$$  \hspace{1cm} (34)

where we have used equation (6) at the lower integration limit $t = 0$. For further evaluation we write the average in (34) as

$$\langle \hat{V}(0) \hat{U}(\infty, 0) \rangle_{av}^\dagger = \langle \hat{V}(0) \hat{U}(0, \infty) \rangle_{av}^\dagger$$

$$= \lim_{t' \to 0} \langle \exp[i\tilde{H}_0 t'/\hbar] \hat{V}(t') \exp[-i\tilde{H}_0 t'/\hbar] \hat{U}(t', \infty) \rangle_{av}^\dagger$$

$$= -i\hbar \lim_{t' \to 0} \frac{\partial}{\partial t'} \langle \hat{U}(t', \infty) \rangle_{av}$$

$$= -i\hbar \lim_{t' \to 0} \frac{\partial}{\partial t'} \langle \hat{U}(\infty, t') \rangle_{av}$$  \hspace{1cm} (35)

where the superscript $\dagger$ designates the adjoint of an operator. In the above chain of equations we have used that $\hat{V}$ is self-adjoint, and that $\hat{U}$ is unitary ($\hat{U}^\dagger(t', t) = \hat{U}(t, t')$) and obeys the Schrödinger equation (22).

The last expression in equation (35) can be expressed in terms of the (angle-averaged) collisional $S$ operator $\langle \hat{S}(v, b) \rangle$ associated with a perturber having speed $v$.
and impact parameter \( b \). A detailed derivation of this is given in the appendix. Combining the result (A10) derived there with equations (34) and (35) we obtain

\[
\hat{K} = 2\pi n_p \int f(v) v \, dv \int_0^\infty b \, db (1 - \hat{S}(v, b))_{\text{ang}}
\]

(36)

where \( n_p \) is the perturber density, \( f(v) \) the distribution function of the speed \( v = |v| \) and the average is now over all velocity and position angles.

Equation (36), obtained here as a limit from the more general unified theory, is well known as one of the possible forms which the collision operator may be given in the framework of the impact theory. If correctly applied, it just reproduces the results of what we have called the standard impact theory. Indeed, it follows from the above derivation that in case (a) all matrix elements of the \( \text{RHS} \) of (36) are equivalent to those given in equation (21) and that in case (b) the diagonal elements are equal to the quantities \( K_{\alpha\beta} \) entering equation (26). On the other hand, it is essential to notice that off-diagonal matrix elements of the \( \text{RHS} \) of (36) outside the validity domain of case (a) have not been included in the above derivation (nor have they been obtained in previous Markovian treatments) and are there indeed incorrect, as will be demonstrated in the following section.

4. Extended impact theory

As stated at the end of § 3, when one leaves the validity domain of case (a), in particular when the separations \( |\omega_{\alpha\beta} - \omega_{\alpha'\beta'}| \) between line components exceed \( \omega_f \), equation (36) no longer provides correct expressions for the off-diagonal part of the collision operator. It is this fact which has obviously been overlooked in the numerous papers employing the formalism which we have named ‘extended impact theory’ (see references quoted in § 1) and which consists of extending the use of equation (36) outside the validity domain of case (a). Unfortunately, the emphasis in most of the papers quoted was precisely on the off-diagonal part of the collision operator, as the original motivation of the extension was to improve the dip regions by a more sophisticated treatment of the coupling between line components.

The extent to which the off-diagonal part in (36) becomes incorrect can be seen by comparing it with the corresponding result of the unified theory. An illustrative example is provided by the weak collision part \( \hat{K}^{(\omega)} \) which is amenable to easy quantitative evaluation. Let us consider \( \text{Re} K^{(\omega)}_{\alpha\beta\alpha'\beta'} \), which represents the contribution of a given perturbing transition \( (\gamma\delta) \) to the real part of \( \langle \alpha\beta | \hat{K}^{(\omega)} | \alpha'\beta' \rangle \) (see equations (9)-(11) for \( \hat{U} = 1 \)). In the extended impact formalism, this term is affected by the two ‘energy cut-offs’ \( |\omega_{\alpha\beta} - \omega_{\gamma\delta}| \) and \( |\omega_{\alpha'\beta'} - \omega_{\gamma\delta}| \), but does not depend on the frequency variable \( \omega \). In the unified theory, it is affected by only one energy cut-off \( |\omega - \omega_{\gamma\delta}| \) which, moreover, varies with \( \omega \) and does not become effective when \( |\omega - \omega_{\gamma\delta}| \leq \omega_f \). The corresponding differences become particularly manifest for large level separations. While in the extended impact theory \( \text{Re} K^{(\omega)}_{\alpha\beta\alpha'\beta'} \) remains constant, it may undergo dramatic changes in the unified theory when the frequency varies from one (isolated) line component to a neighbouring one. Indeed, if \( \omega \) varies, say, between \( \omega_{\alpha\beta} \) and \( \omega_{\gamma\delta} \), this term changes from the small value \( \text{Re} K^{(\omega)}_{\alpha\beta\alpha'\beta'} (\omega_{\alpha\beta}) \) (affected by an ‘energy cut-off’ at \( |\omega_{\alpha\beta} - \omega_{\gamma\delta}| \) which arises from the rapidly oscillating exponential in the weak collision part of (11)) to the much larger value \( \text{Re} K^{(\omega)}_{\alpha\beta\alpha'\beta'} (\omega_{\gamma\delta}) \) (affected by no energy cut-off
It is obvious that this variation is of primary importance for describing the dip regions between the line-components.

As a numerical example, let us consider a four-level atom with one lower state $\beta$ and three excited states $\alpha, \alpha', \alpha''$. Let us assume that $\alpha$ and $\alpha'$ correspond to allowed transitions while $\alpha''$ corresponds to a forbidden transition. For simplicity, we take equal dipole strengths for the allowed transitions and assume the forbidden level to lie midway between the two allowed ones (see figure 1). The collision operator is assumed to be due to weak collisions and is taken in the dipole approximation as in equation (15) to represent the unified theory, and as in equation (6) of I to represent the extended impact theory. For further simplification we assume that the dipole matrix elements connecting $\alpha$ and $\alpha'$ vanish, and that the non-vanishing elements between excited states are all equal. The thermal average is accounted for roughly by replacing the velocity variable with the thermal velocity. To be far from case (a) (where all formalisms yield essentially the same results), we choose $\omega_w = |\omega_{\alpha''}| = 100 \omega_f$. The width of the two line components is assumed much smaller than $\omega_f$ (by an appropriate choice of the density), so that the line profile can be expanded to first order in the collision operator, except in the immediate vicinity of the two allowed components. The resulting profiles of the unified theory (full curve) and the extended impact theory (broken curve) are shown in figure 2. It is seen that in about half of the frequency interval between the two line components (namely for $0.25 \omega_{\alpha''} \leq \omega - \omega_{\alpha\beta} \leq 0.75 \omega_{\alpha''}$) the two profiles deviate significantly. In particular, while the unified theory predicts that the intensity drops to zero at the location of the forbidden component, the extended impact theory does not. According to the latter, the trough

---

**Figure 1.** Four-level atom with two allowed and one forbidden transition. The latter ($\alpha'\beta$) is assumed to lie midway between the former ($\alpha\beta$ and $\alpha'\beta$).

**Figure 2.** Line-profiles of the four-level atom presented in figure 1. Unified theory: full curve; extended impact theory: broken curve.
between the two components would be filled by an intensity which is still about half
of the intensity taken at $\omega - \omega_{aB} = 0.3 \omega_{aB}$. We would like to mention in this connection
that similar results have been obtained in a recent paper by Burstein et al (1985).

It is noteworthy that in contrast to the weak collision part $\hat{K}^{(w)}$, no differences
between the unified theory and the extended impact theory are expected for the strong
collision part $\hat{K}^{(s)}$. Indeed, the latter is usually insensitive to the level splitting and is
thus not only correctly provided by the unified theory but also by the impact limit of
case (a) and by the extended impact theory. Therefore, in cases where the strong
collision part contributes significantly, errors due to the use of the extended impact
theory are expected to play a minor role.

We conclude from all the foregoing considerations that if the interest is focused
on an improved treatment of line coupling (as is particularly the case in molecular
line broadening, see the corresponding references in §1), the extended impact theory
is entirely worthless. Indeed, either it reproduces the results of the standard impact
theory (case (a)), in which case the additional complications inherent in its formalism
are superfluous, or it does not (outside case (a)), in which case it leads to incorrect
results. Since line coupling is precisely the effect which arises from the off-diagonal
part of $\hat{K}$, any improvement accounting for the influence of level separations can only
be achieved by using the unified theory.

On the other hand, the extended impact theory may be of appreciable practical
use if the aim is not an accurate description of the troughs between isolated line
components. The off-diagonal part of the collision operator is then of minor import-
ance, and the extended impact formalism provides a valuable interpolation between
cases (a) and (b), with the advantage that equation (4) in connection with the unique
formula (36) requires no change between different lineshape expressions. This is of
particular interest when the diagonal and off-diagonal elements of the $S$ matrix are
computed together from a common numerical procedure.

It should be noticed, however, that interpolation may also be achieved by various
other expressions for $\hat{K}$. What really matters is that the diagonal part coincides with
that of (36), while it suffices that the off-diagonal part just reproduces the correct limit
for case (a). Thus, instead of employing the extended impact formalism, it may in
some cases be simpler to use equation (36) only for the diagonal part (which has a
simple structure because it involves essentially only one energy difference $\omega_{aB} - \omega_{aB}$
in each term of expressions like (30)), while for the off-diagonal matrix elements one
may take those calculated for case (a) (e.g. from equation (23)), where no energy
differences are involved at all. This kind of interpolation would be particularly useful
in calculations employing the weak collision part $\hat{K}^{(w)}$ of the collision operator.

5. Application to Balmer-$\alpha$

We have performed calculations for the Stark-broadened fine-structure profile of the
Balmer-$\alpha$ line of hydrogen. Typical conditions of astrophysical plasmas were con-
sidered; the temperature was taken to be $T = 10000 \text{ K}$ and the density $n_p$ was chosen
to vary from $10^{12}$ to $10^{14} \text{ cm}^{-3}$. Under such conditions, the broadening is essentially
due to the proton perturbers, the electrons providing a minor contribution. Further-
more, since the electron plasma frequency is large compared with the fine-structure
splitting, the electron collision operator is independent of the latter and can thus be
described in the impact limit of case (a). Note that condition (1) for having a collisional
environment is well fulfilled for the electrons in the total density range under consideration.

As for the protons, the fulfilment of condition (1) becomes marginal when going to the upper end of the density range considered. To show this quantitatively, we express the fluctuation frequency \( \omega_r \) associated with the proton perturbers as \( \omega_r = v_r / \lambda_D \), where \( v_r = \sqrt{2} v_{th} = (6kT/m_p)^{1/2} \) is the thermal relative perturber-atom velocity and \( \lambda_D = (kT_{ee}/2n_p)^{1/2} \) the Debye length of the two-component plasma. Comparing this with the halfwidth \( w \) of the main line components (see figures 5–7), we find \( \omega_r = 4w \) for \( n_p = 10^{12} \text{ cm}^{-3} \), \( \omega_r = 1.5w \) for \( n_p = 10^{13} \text{ cm}^{-3} \) and \( \omega_r = w \) for \( n_p = 10^{14} \text{ cm}^{-3} \). The fact that, at least for the higher densities, \( \omega_r \) is scarcely larger than \( w \), indicates that the effects of distant multiple collisions (i.e. with impact parameters approaching the Debye length) are no longer strictly additive. As a consequence, the broadening is likely to be overestimated by our numerical results. We expect the error to be tolerable, however, because condition (1) may be thought of as written separately for different ranges of impact parameters \( b \), and it is only for the most distant ones \( (b \approx \lambda_D) \) that it is but marginally met. Moreover, for the two lower densities considered, those contributions to the broadening which arise from far-lying levels are subject to the less restrictive condition (2) rather than to condition (1).

The fine structure of the two level groups corresponding to principal quantum numbers \( n = 2 \) and \( n = 3 \) produces a splitting of the line into seven components of different line strengths, five of them being sufficiently strong to be visible in the spectrum (see table 1 and figure 5). At the lowest density considered \( (n_p = 10^{12} \text{ cm}^{-3}) \), the components are rather well resolved and can be considered as isolated except, perhaps, for the two pairs of transitions around \( \Delta \lambda = -0.08 \text{ Å} \) and \( \Delta \lambda = 0.06 \text{ Å} \) whose components are partially overlapping. At the intermediate density \( n_p = 10^{13} \text{ cm}^{-3} \) (see figure 6), the two components of each pair overlap completely and the profile is essentially formed of two separated line bodies. For the highest density \( n_p = 10^{14} \text{ cm}^{-3} \) all line components merge together to form one body of completely overlapping transitions.

<table>
<thead>
<tr>
<th>Transition</th>
<th>( \Delta \omega \times 10^{-14} \text{ rad s}^{-1} )</th>
<th>( \Delta \lambda ) (Å)</th>
<th>Line strength (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2s_{1/2} - 3p_{1/2} )</td>
<td>0.111</td>
<td>-0.0254</td>
<td>21.3</td>
</tr>
<tr>
<td>( 2s_{1/2} - 3p_{3/2} )</td>
<td>0.316</td>
<td>-0.0721</td>
<td>42.7</td>
</tr>
<tr>
<td>( 2p_{1/2} - 3s_{1/2} )</td>
<td>0.198</td>
<td>-0.0452</td>
<td>2.0</td>
</tr>
<tr>
<td>( 2p_{1/2} - 3d_{3/2} )</td>
<td>0.382</td>
<td>-0.0872</td>
<td>102.0</td>
</tr>
<tr>
<td>( 2p_{1/2} - 3s_{3/2} )</td>
<td>-0.492</td>
<td>0.112</td>
<td>4.0</td>
</tr>
<tr>
<td>( 2p_{3/2} - 3s_{3/2} )</td>
<td>-0.308</td>
<td>0.0703</td>
<td>20.5</td>
</tr>
<tr>
<td>( 2p_{3/2} - 3d_{3/2} )</td>
<td>-0.240</td>
<td>0.0548</td>
<td>184.0</td>
</tr>
</tbody>
</table>

In addition to the results obtained in I in the framework of the extended impact theory, we have evaluated the collision operator \( \hat{K}(\omega) \) using the unified theory and its impact limits for cases (a) and (b). To minimise the numerical effort, no combined application of cases (a) and (b) (as described in § 1) has been made, although this would have been appropriate for the medium density \( n_p = 10^{13} \text{ cm}^{-3} \) and possibly even for the lowest density \( n_p = 10^{12} \text{ cm}^{-3} \). The weak collision contribution to the collision operator has been calculated to second order in the atom-perturber potential, as indicated in § 2.3.2, while the strong collision contribution, which is insensitive to the
level splitting, has been evaluated in the impact limit (a), along the lines of I. An analysis of the numerical results shows that the strong collision part is negligible for the off-diagonal elements of $\hat{K}(\omega)$, but that it is quite important for the diagonal elements where it contributes about 30%.

Figures 3(a–d) present some typical matrix elements of the proton collision operator as functions of the wavelength $\lambda$. The wavelength separation $\Delta \lambda$ is referred to the wavelength $\lambda_0 = 6564.610$ Å, which corresponds to a mean energy difference $E_3 - E_2$ with

$$E_2 = \frac{1}{2} [2E(s_{1/2}) + 2E(p_{1/2}) + 4E(p_{3/2})]$$
$$E_3 = \frac{1}{2} [2E(s_{1/2}) + 2E(p_{1/2}) + 4E(p_{3/2}) + 4E(d_{3/2}) + 6E(d_{5/2})].$$

In each of the figures the expression obtained from the unified theory (full curve) is compared with the corresponding constant value obtained from the extended impact formalism (broken curve). For the diagonal element presented in figures 3(a) (real part) and (b) (imaginary part) both results coincide at the wavelength of the transition considered, while no such systematic coincidence occurs for the off-diagonal element presented in figures 3(c) and (d). The latter fact is in agreement with the circumstance that the off-diagonal elements cannot be treated in the framework of the extended impact theory. It is noteworthy that the real part of the diagonal element presented in figure 3(a) runs through a maximum at $\Delta \lambda = -0.04$ before decreasing definitely for $\Delta \lambda \to \infty$. This can be interpreted with the help of equation (15) whose RHS is maximal at the position of the perturbing transition $\omega_{5h}$. A corresponding transition in figure 3(a) is the forbidden component $3p_{1/2} - 2p_{1/2}$ at $\Delta \lambda = -0.041$ Å, which provides a particularly strong contribution to the diagonal element $K_{a\beta a\beta} (a\beta = 3d_{3/2}2p_{1/2})$.

In figure 4, the real part of the diagonal element $K_{a\beta a\beta}/n_p (a\beta = 3p_{3/2}2s_{1/2})$ is plotted for two different densities. The difference gives an account of the effect of Debye screening. It is seen that in the far wings (beyond the largest of the two fluctuation frequencies $\omega_f$ concerned) the two functions converge to a common curve.

![Figure 3](image-url)

**Figure 3.** Real parts (a, c) and imaginary parts (b, d) of matrix elements $K_{a\beta a\beta}/n_p$ of the collision operator divided by the proton density; the units are $10^9$ rad s$^{-1}$ cm$^{-1}$. (a) and (b) present the case $a\beta = a'\beta' = 3d_{3/2}2p_{1/2}$; (c) and (d) present the case $a\beta = 3p_{3/2}2s_{1/2}$, $a'\beta' = 3d_{3/2}2p_{1/2}$. Full curve: unified theory; broken curve: extended impact theory.
which is no longer affected by the screening. For such large detunings $\Delta \lambda$ the collision operator thus becomes purely proportional to $n_p$, which confirms that when $\Delta \lambda$ is also large compared with the level splitting (so that the line profile is linear in the collision operator), the unified theory leads to the one-perturber limit.

Our results for the Stark-broadened Balmer-$\alpha$ profiles are presented in figures 5-7. For the lowest density considered ($n_p = 10^{12} \text{ cm}^{-3}$), the differences between the various theories do not become apparent on the intensity scale of figure 5(a). The enhanced scale chosen for figure 5(b) displays slight differences in the dips between the line components. While the profiles obtained from the impact theory for case (b) and the extended impact formalism (both represented by the dotted curve) still coincide, even on this scale, the profile of the unified theory (full curve) lies slightly apart.

The fact that even in the dip regions there is such a good agreement between the different results can be traced to several causes. One of them (and probably the most significant one) is the circumstance that due to the large fine-structure separation between the lower ($n = 2$) $j = \frac{1}{2}$ and $j = \frac{3}{2}$ levels, most of the (allowed and forbidden) Balmer-$\alpha$ transitions form two well separated groups, each of them being almost collisionally degenerate and thus providing intense wing contributions in the trough between them. These contributions arise from matrix elements $K_{\alpha \beta \alpha' \beta'}$ with $\alpha \beta$ and $\alpha' \beta'$ belonging to the same group. Their evaluation depends little on the formalism employed, because their frequency dependence, as indicated by the unified theory, is slow in the domain where they contribute significantly to the line profile. To see this, we note that terms $K_{\alpha \beta \alpha' \beta'}^{(l)}$ with $\alpha'' \beta''$ belonging to the same group as $\alpha \beta$ and $\alpha' \beta'$ show a slow logarithmic variation in the region where their contribution to the line profile is not yet hidden by the two transitions $3p_{1/2} - 2s_{1/2}$ and $3s_{1/2} - 2p_{1/2}$ in the dip region between the groups and by the wing contribution of the neighbouring group. Similarly, also terms $K_{\alpha \beta \alpha' \beta'}^{(r)}$ with $\alpha'' \beta''$ not belonging to the same group vary slowly in this region. This can be seen from the discussion in § 3.2.2 according to which the scale of variation of these terms is of the order of the frequency separation between the groups (RHS of (32) with $\alpha \beta$ and $\gamma \delta$ referring to different groups) and not $\omega_r$ (RHS of (29)).

In comparison to the wing contributions mentioned, there is only a small part of the intensity arising from the coupling between the groups. Indeed, the off-diagonal
elements of $\hat{K}$ connecting transitions of different groups are small, not only because the two groups are rather far apart, but also because they are unaffected by strong collisions.

As a further reason for the agreement we note that the treatment of the rather important contribution of strong collisions to the diagonal elements of the collision operator is the same in the various formalisms employed.

We now turn to the results obtained for the intermediate density $n_0 = 10^{15} \text{ cm}^{-3}$, which are presented in figure 6. For reasons analogous to those indicated for figure 5, the various approaches, and in particular those of the unified theory and the extended impact theory, lead to rather similar profiles. As mentioned earlier, the curves representing the impact limits for the pure cases (a) and (b) do not make much sense in the present case; indeed, since some of the components are collisionally degenerate and

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**Figure 5.** Fine-structure profiles (normalised to unit area) of Balmer-$\alpha$ for $n_0 = 10^{12} \text{ cm}^{-3}$. For the intensity scale chosen in (a) differences between the unified theory, the impact theory (case (b)) and the extended impact theory do not become apparent. On the enhanced intensity scale chosen in (b) slight differences appear between the unified theory on the one hand (full curve) and the impact theory (case (b)) and the extended impact theory on the other hand (broken curve).
Figure 6. Fine-structure profiles (normalised to unit area) of Balmer-$\alpha$ for $n_p = 10^{15}$ cm$^{-3}$. Unified theory: full curve; impact theory (case (a)): broken curve; impact theory (case (b)): dotted curve; extended impact theory: chain curve.

Figure 7. Profiles of Balmer-$\alpha$ (normalised to unit area) for $n_p = 10^{14}$ cm$^{-3}$. Unified theory: full curve; impact theory (case (a)): broken curve; extended impact theory: chain curve; impact theory (case (b)): dotted curve.

others isolated, the appropriate application of the impact theory would have consisted of combining the formalisms (a) and (b) as indicated in § 1. We have still presented the pure limits (a) and (b) to illustrate that even far outside their validity domains these approaches do not lead to very large errors.

For $n_p = 10^{14}$ cm$^{-3}$, the highest density considered, the Balmer-$\alpha$ profiles obtained from the various approaches are significantly different, as illustrated in figure 7. We draw attention to the fact, however, that precautions must be taken to interpret these results because the validity of all the formalisms employed is restricted by condition (1) which, as stated above, is met only marginally for the density under consideration. Although this leads to a common overestimation of the widths of all profiles, it is interesting to analyse how these profiles compare with each other, as this displays the effects of the different approximations used.
Since for the density considered all transitions are rather close to collisional degeneracy, the impact limit for case (b) is, of course, inappropriate for describing the line profile. We have, nevertheless, plotted the corresponding curve in order to illustrate the effect of the off-diagonal part of the collision operator. Since this curve does not contain the off-diagonal part (it just represents a superposition of Lorentzians), it is seen that introducing off-diagonal collision matrix elements leads to a narrowing of the line. Obviously, this can be understood as an interference between the different transitions composing the line. The fact that the remaining three profiles deviate from each other even at the line centre demonstrates that there is no complete collisional degeneracy. In fact, according to table 2, the fluctuation frequency $\omega_f$ corresponds to a wavelength interval of about 0.1 Å, which is of the order of but not large compared with the splitting between the outer transitions. Consequently one still expects an influence of the splitting on the collision operator, and in particular on its off-diagonal elements which, as we have seen, are important in the present case. It is noteworthy in this connection that the extended impact theory, as compared with the impact theory of case (a), does not improve but spoil the situation; instead of approaching the profile of the unified theory it goes in the opposite direction and leads to a still broader profile.

Table 2. Fluctuation frequency (in frequency and wavelength units) for different densities.

<table>
<thead>
<tr>
<th>$n_0$ (cm$^{-3}$)</th>
<th>$\omega_f$ (10$^{11}$ rad s$^{-1}$)</th>
<th>$\Delta\lambda_f$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{12}$</td>
<td>0.046</td>
<td>0.010</td>
</tr>
<tr>
<td>$10^{13}$</td>
<td>0.14</td>
<td>0.033</td>
</tr>
<tr>
<td>$10^{14}$</td>
<td>0.46</td>
<td>0.10</td>
</tr>
</tbody>
</table>

6. Conclusion

We have given an analysis of the formal and practical aspects of line-broadening theories as applicable in a collisional environment. A study of the validity domains of the unified theory and its impact limits for isolated and collisionally degenerate line components has been presented together with a critical investigation of the 'extended impact theory'. In spite of its more sophisticated structure, the latter does not provide line profiles which are more accurate than those obtained from the standard impact theory. In particular, as illustrated by the numerical example presented in § 4, it is unable to improve the treatment of line coupling, which is of particular importance for describing the troughs between isolated line components as encountered in molecular line broadening and also in Stark broadening. The extended impact theory is nonetheless of appreciable practical use as an interpolating formalism in cases where certain off-diagonal elements of the collision operator have no significant influence on the line profile. An example of this is the fine-structure profile of the Balmer-α line of hydrogen for which we have presented various numerical results.

As for a possible comparison with measurements, it seems that, unfortunately, the very few experiments done at low densities have been performed under conditions which prohibit a direct confrontation with our calculations (see I for a more detailed discussion of this point). The main field of application of the results obtained in § 5 therefore remains the line broadening in astrophysical plasmas (Stehlé et al 1983).
Acknowledgments

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Appendix

In order to evaluate the average time evolution operator \( \langle \hat{U}(\infty, t') \rangle_{av} \), occurring in equation (35), it is convenient to introduce cylindrical coordinates \( \rho, \varphi, z \) for the initial \((t = 0)\) position of the perturber relative to the radiating system. Let the \( z \) axis traverse the location of the system and point along the perturber's initial velocity \( v \). Let us further write \( \hat{U}(v, \rho, \varphi, z; \infty, t') \) to characterise \( \hat{U}(\infty, t') \) for a perturber with a given initial position in phase space. The average of this operator can then be written as

\[
\langle \hat{U}(\infty, t') \rangle_{av} = \frac{1}{1 + V} \int F(v) \, dv \int_0^{\infty} \rho \, d\rho \int_0^{2\pi} \varphi \, d\varphi \left[ \hat{U}(v, \rho, \varphi, z; \infty, t') - 1 \right] \tag{A1}
\]

where \( F(v) \) denotes the velocity distribution and \( V \) the vessel volume (extended to infinity such that the perturber density \( N_p/V = n_p \) keeps a finite value).

The integration over \( z \) is conveniently carried out after taking the time derivative of (A1) as required in equation (35). We may then take advantage of a relation which exists between this time derivative and a corresponding derivative with respect to \( z \). To establish this relation we transform from the time evolution operator in the interaction representation, \( \hat{U} \), to the corresponding operator in the Schrödinger representation, \( \hat{T} \):

\[
\hat{T}(v, \rho, \varphi, z; t, t') = \exp(-i\hat{H}_0 t' / \hbar) \hat{U}(v, \rho, \varphi, z; t, t') \exp(i\hat{H}_0 t' / \hbar). \tag{A2}
\]

Obviously, an infinitesimal time translation \( dt \) has the same effect on \( \hat{T} \) as the infinitesimal displacement \( v \, dt \) of the initial position of the perturber along its trajectory (which need not be a straight path). One therefore has

\[
\hat{T}(v, \rho, \varphi, z; t + dt, t' + dt) = \hat{T}(v, \rho, \varphi, z + v \, dt; t, t') \tag{A3}
\]

or equivalently

\[
\frac{\partial}{\partial t} \hat{T} + \frac{\partial}{\partial t'} \hat{T} = v \frac{\partial}{\partial z} \hat{T}. \tag{A4}
\]

This relation may be used to express the time derivative occurring in (35); with the help of equation (A2) we obtain

\[
\lim_{t' \to 0} \frac{\partial}{\partial t'} \hat{U}(\infty, t')
\]

\[
= \lim_{t' \to 0} \frac{\partial}{\partial t'} \exp(i\hat{H}_0 t' / \hbar) \hat{T}(t, t') \exp(-i\hat{H}_0 t' / \hbar)
\]

\[
= -\frac{i}{\hbar} \hat{U}(\infty, 0) \hat{H}_0 + \lim_{t' \to 0} \exp(i\hat{H}_0 t / \hbar) \left( v \frac{\partial}{\partial z} - \frac{\partial}{\partial t} \right) \hat{T}(t', t) \exp(-i\hat{H}_0 t' / \hbar). \tag{A5}
\]

Since \( \hat{T} \) obeys the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \hat{T}(t, t') = (\hat{H}_0 + \hat{V}(t)) \hat{T}(t, t') \tag{A6}
\]
where $\hat{V}(t)$ vanishes in the limit $t \to \infty$, its derivative with respect to $t$ is to be replaced with $-i\hat{H}_0 \hat{T}/\hbar$. We thus obtain

$$\lim_{t \to 0} \frac{\partial}{\partial t'} \hat{U}(\infty, t') = \frac{i}{\hbar} (\hat{H}_0 \hat{U}(\infty, 0) - \hat{U}(\infty, 0) \hat{H}_0) + v \frac{\partial}{\partial z} \hat{U}(\infty, 0). \quad (A7)$$

Here we make again use of our assumption that matrix elements of the collision operator are only to be taken between double states corresponding to the same frequency difference. The above commutator then vanishes and we are left with the last term in (A7) which permits an easy integration in equation (A1). At the lower integration limit $z = -\infty$, $\hat{U}$ represents a completed collision, so that we have

$$\hat{U}(\nu, \rho, \varphi, -\infty; \infty, 0) = \hat{S}(\nu, \rho, \varphi) \quad (A8)$$

where $\hat{S}(\nu, \rho, \varphi)$ is the $S$ operator associated with a perturber having velocity $\nu$, impact parameter $\rho$ and azimuthal angle $\varphi$. At the upper integration limit $z = +\infty$, $\hat{U}$ represents a collision which never takes place and we have

$$\hat{U}(\nu, \rho, \varphi, +\infty; \infty, 0) = 1. \quad (A9)$$

Putting equation (A1), (A7) (with the commutator omitted), (A8) and (A9) together finally leads to

$$\lim_{t \to 0} \frac{\partial}{\partial t'} (\hat{U}(\infty, t'))_{av} = \frac{1}{V} \int F(\nu)|\nu| d\nu \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi [1 - \hat{S}(\nu, \rho, \varphi)]$$

$$= \frac{2\pi}{V} \int f(\nu) \nu d\nu \int_0^\infty \rho d\rho (1 - \hat{S}(\nu, \rho))_{ang} \quad (A10)$$

where $f(\nu) = 4\pi F(\nu)|\nu|^2$ is the distribution function of the velocity module $\nu = |\nu|$ and the average is now over all velocity and position angles.

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