Hydrogen line profiles at low densities

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Résumé - Après une discussion physique des conditions de validité des Différentes approches, nous confrontons la méthode du microchamp modèle (MMM) qui traite les effets dynamiques collectifs provenant de collisions simultanées et l'approximation des impacts valable pour des collisions faibles ou fortes non simultanées. Si l'on néglige la levée de dégénérescence des niveaux, le profil des raies de Lyman et de Balmer est Lorentzien dans le centre aux basses densités et la demi largeur est donnée par une expression analytique. Les effets de levée de dégénérescence et de durée de vie radiative sont ensuite analysés.

Abstract - A physical discussion of the validity conditions of the different approximations allows to compare the Model Microfield Method (MMM) which takes into account the collective dynamical effects resulting from simultaneous collisions and the impact approximation valid for weak or strong non overlapping collisions. Neglecting the level splitting effects, the profile of Lyman and Balmer lines is Lorentzian in the line centre and an analytical formula for the width is given. Then, fine structure and radiative lifetime effects are analysed.

The advent of high monochromatic tunable laser sources and the development of Doppler free spectroscopy allow now a very accurate analysis of hydrogen line profiles at low perturber densities (10^10 to 10^14 cm^-3). Precise low density profiles are also of particular astrophysical interest : indeed, the increase of sensitivity of modern high spectral resolution detectors needs a very accurate analysis of the spectral line shapes.

The line broadening results from the interaction of the radiating H atom with all the surrounding perturbers (electrons and ions) of the plasma. Two distinct problems occur in pressure broadening, the first one is the study of the interaction between the radiating atom and one colliding perturber, the second one is the statistical problem of combining the effect of a large number of perturbers and of averaging over their possible motions. From a field point of view, the states of the H atom are perturbed by the fluctuating electric microfield of the perturbers. The statistical properties of this microfield are function of different characteristic times which are compared in order to understand the physical mechanism of pressure broadening. A particular attention has to be paid to simultaneous strong collisions effects, so we compare the Model Microfield Method (MMM) and the "impact" approach (SCP) (section 1). The comparison of the results obtained by these two methods for the Hα line allows to give the validity condition of an impact treatment (section 2). The radiative lifetime and the fine structure energy separation are not negligible at very low densities. Profiles including these two effects are presented in section 3.

1 - DISCUSSION OF THE FORMALISMS - LIMITING CASES

From a "collisionist" point of view, the main difficulty of the line broadening theory, results from the possibility of simultaneous strong collisions. This problem can be avoided at low perturber densities and it is interesting to determine the
limiting density under which collective effects become negligible. Let us introduce the collisional duration \( \tau_c \) and the time interval \( \Delta T \) between two collisions. If \( \tau_c \ll \Delta T \), the different collisions are separated in time and can be treated independently from each other. At the opposite, if \( \tau_c \gg \Delta T \), simultaneous collisions occur and contribute to the profile. An approximative value of \( \Delta T \) is given by \( \Delta T \approx N_p \langle v \rangle \) where \( N_p \) is the perturber density, \( v \) the mean relative velocity and \( \langle v \rangle \) the collisional cross section. \( v \) is function of the temperature \( T \) and the relative mass of the perturber \( P \)-radiative atom \( A \) system ; \( v \) is low for ionic perturbers. \( \langle v \rangle \) is function of the relative energy (or the temperature) and also of the interaction potential between \( A \) and \( P \). Hence the physical parameters which control the collective effects are:

1. the perturber density
2. the temperature
3. the interaction potential range.

It is interesting to observe that the condition \( \tau_c \ll \Delta T \) can be written \( \tau_c \ll N_p \langle v \rangle \). \( \tau_c \ll \langle v \rangle \) may be interpreted as the collisional volume and \( N_p \langle v \rangle \) the mean volume occupied by one perturber, so that simultaneous strong collisions are negligible if the interaction volume contains one perturber only. Results obtained by Allard /2/ prove that the number of perturbers in the interaction volume is one of the more important parameters in line broadening study.

In the particular case of Stark broadening the Microfield Method Model /1/ takes into account simultaneous collisions effects and we will briefly analyze this method further. In low density case (\( \tau_c \ll \Delta T \)) the Unified Theory /3, 4/ gives a satisfactory description of the broadening and it is interesting to introduce the impact and quasi-static limits in order to facilitate the comparison with the MMH.

It is easy to understand the physical basis of these two limits by introducing the typical evolution time \( \tau(\omega) \) of the atomic dipole, often called the radiative time of interest. \( \tau(\omega) \) depends on the detuning \( \Delta \omega \) from the line center through the relation \( \tau(\omega) = \text{Min} (\Delta \omega_{1/2}, \Delta \omega_{1/2}^{-1}) \) where \( \Delta \omega_{1/2} \) is the halfwidth of the line. Two situations may occur:

1. \( \tau_c \ll \tau(\omega) \) (figure 1). This condition is verified in the line centre.

\[ \begin{array}{c}
\text{collisions} \\
\Downarrow \\
\tau(\omega)
\end{array} \]

\[ Fig.1 - \text{Comparison between the radiative time of interest } \tau(\omega) \text{ and the collisional duration in the impact limit.} \]

It is possible to neglect the dynamics of the system on time scales smaller than \( \tau(\omega) \). Therefore the profile results in the effect of a large number of complete collisions and can be expressed in terms of collisional S-matrix elements. This domain corresponds to the "impact" limit.

ii. \( \tau_c \gg \tau(\omega) \) (figure 2). This condition is verified in the wings.

It is now necessary to take into account radiative processes during the collision. It is usual to consider the atom-perturber system as a quasimolecule which absorbs or emits radiation. In the far wings, \( \tau(\omega) \) becomes so small in comparison with \( \tau_c \) that it is possible to consider the absorption or emission processes as instantaneous : this corresponds to the "quasistatic" approximation. Many theoretical works
have been devoted recently /5, 6, 7, 8/ to the departures from this limit but it is not the purpose of this paper to discuss this problem.

![Diagram of collisions](image)

**Fig. 2** - Comparison between the radiative time of interest $\tau(\nu)$ and the collisional duration in the wings.

For a care of simplicity, we will adopt further a semi-classical description of the collisions. Owing to the long range of interaction potential between the radiating H atom and each perturber $P$ at distance $r(t)$, the major effect comes from its dipolar part:

$$V_p(t) = -\frac{e^2}{r^2(t)}$$

The potential is proportional to $\vec{E}$ so that it is possible to speak in terms of electric fields.

In the semi-classical impact approximation valid at low densities, the profile calculation is obtained in two steps. At first the contribution of each collision to the time evolution operator is calculated from the $S$-matrix elements. Then an average over all the relative orientations and velocities is performed. From the Dyson series expansion of the $S$-matrix, we obtain:

$$S = 1 - \sum_{l=1}^{\infty} \int_{-\infty}^{t_1} dt_1 \int_{-\infty}^{t_2} dt_2 \frac{\nabla_p(t_1) \nabla_p(t_2)}{E_p(t_1) E_p(t_2)} + \ldots$$

where $V_p$ is the potential in the interaction picture.

From symmetry considerations, it is easy to prove that the first non zero contribution comes from the second order term. This term is proportional to

$$\int_{-\infty}^{t_1} dt_1 \int_{-\infty}^{t_2} dt_2 \frac{\nabla_p(t_1) \nabla_p(t_2)}{E_p(t_1) E_p(t_2)}$$

which represents the covariance of the electric field. The following terms, negligible for distant collisions, are important for the determination of the strong collisions contribution.

Instead of looking at the detailed mechanism of each collision, the MMM adopts a field point of view. This method proceeds in two steps also. The Schrödinger equation for the total electric field $\vec{E} = \sum_p \vec{E}_p$ (resulting from interactions with all the surrounding perturbers) is first solved at fixed time. Then the time evolution of $\vec{E}$ is given by its statistic properties. The true microfield is replaced by a model field (kangaroo process) which incorporates the true electric field distribution function and the time covariance. The MMM leads to the usual limits (impact and quasistatic) when the corresponding physical conditions are realized. It is important to note that the dynamics of the microfield is taken into account through the time covariance. Consequently, as was before noticed by Smith et al. /9/ the impact approach and the MMM coincide at low densities up to the second order moment of the electric field. Therefore these two methods may differ by strong collisions contributions only. These physical considerations will be illustrated in the next section with results on Balmer line profiles.
Assuming that the impact approximation is valid in the line center, we prove elsewhere /10, 11/ that the Balmer and Lyman lines have Lorentzian shapes. The half-width is given by:

\[ \Delta \omega_{1/2} = N_p \int_{0}^{\infty} v f(v) dv \int_{0}^{b_c} 2 \pi b P(b, v) db \]

where \( f(v) \) is the velocity distribution of the relative motion \( (M = m_p/(1+m_p) \) reduced mass), \( b \) the impact parameter of the rectilinear trajectory, and \( b_D \) the Debye radius. The electronic contribution to the halfwidth is negligible (10%) in comparison with the ionic one. At large values of the angular momentum \( \ell = M b v \) (weak collisions) we adopt a second order perturbative calculation of the S-matrix and we neglect the inelastic collisions between states of different \( n \) quantum numbers (no-quenching approximation). The probability \( P(b, v) \) varies as \((M/\ell)^2\). At small \( \ell \) values (strong collisions) a non perturbative approach is necessary. Thus we have shown /10/ in a quantum description of the relative motion that \( P(b, v) \) oscillates around 1 for \( b \leq r_c(v) \); with

\[ r_c(v) = k_n e^2/\hbar v \]

\( k_n = 0.5 (3n^4 - 27n^2 + 36) \) for the Balmer line \( H_n \) and \( k_n = 1.5 n^2 (n^2 - 3) \) for the Lyman line \( L_n \). Taking \( P(b, v) \approx 1 \) for \( b \leq r_c(v) \) we obtain the following analytical expression for the halfwidth:

\[ \Delta \omega_{1/2} = N_p \times 3.69 \times 10^4 k_n (M/T)^{1/2} [22.22 + \ln(T^2/N_p M) - \ln k_n] \]

\[ \left( \text{Hz, K, cm}^{-3} \right) \]

The corresponding Lorentzian profiles are in good agreement with the MMM results in the \( H_n \) case for the low densities \((N_p < 10^{13} \text{ cm}^{-3}) /11/\). The relative contribution of the strong collisions to the halfwidth \([22.22 + \ln(T^2/N_p M) - \ln k_n]^{-1}\) is negligible in this density range and the broadening is approximatively given by the field covariance only (weak collisions). This explains the similitude between the results of the MMM and SCP approaches. Small divergency between the profiles at \( 10^{14} \text{ cm}^{-3} \) in the \( H_n \) case can be imputed partly to differences in the strong collisions description, partly to an eventual small departure from the impact regime.

The validity of the impact assumption in the line center requires that the collision duration \( \tau_c(b, v) \) is smaller than the time of interest \( \tau(\omega) = \omega_0^{-1} \) with \( \omega = \omega_{1/2} \). We define thus a mean collision time \( \langle \tau_c \rangle \) as:

\[ \Delta \omega_{1/2} \langle \tau_c \rangle = N_p \int_{0}^{\infty} v f(v) dv \int_{0}^{b_c} 2 \pi b \tau_c(b, v) P(b, v) db \]

Taking \( \tau_c(b, v) = b/v \) for \( b > r_c(v) \) and \( \tau_c(b, v) = r_c(v)/v \) for \( b < r_c(v) \) we obtain the following validity condition:
\[ \Delta \omega_{\alpha} < \tau_c > \approx 4.97 \times 10^{-7} k_B \frac{M\sqrt{N_p/T}}{T} \quad (K, cm^{-3}) \] (6)

As it appears from the application of this condition an impact treatment is still valid at \( T = 10 \times 10^4 K \) up to \( 10^{14} \text{ cm}^{-3} \) \((\text{H}_\alpha), 10^{12} \text{ cm}^{-3} \) \((\text{H}_\beta), 10^{15} \text{ cm}^{-3} \) \((\text{L}_\alpha), 10^{13} \text{ cm}^{-3} \) \((\text{L}_\beta)\), for protons perturbers.

However, the impact approximation fails in the line wings since the collisional duration becomes smaller than the time of interest \( \tau (\omega) \).

The quasistatic model becomes approximatively suitable at first for the ions and further in the wings for the electrons leading to an approximately dependance in \( \Delta \lambda^{-5/2} \). This is shown in figure 3 by the comparison between the results of Vidal et al. (VCS /12/) corresponding to the quasistatic approximation for the ionic contribution, the MMM results and the impact SCP results.

3 - SCP PROFILES INCLUDING ENERGY SPLITTING AND SPONTANEOUS EMISSION EFFECTS

In order to make the preceding calculations more tractable we have neglected the energy separation of the \((n \ell j)\) states with the same \( n \) numbers and the spontaneous emission effects.

We restrict us hereafter to the \( \text{H}_\alpha \) case only. In the low density range \((N_p < 10^{12} \text{ cm}^{-3})\) the profile splits in seven components as showed in figure 4.

The energy splitting leads to some modifications in the profile expression with the exact wavelength position of the unshifted components and in the calculation of the S-matrices.

The range of the dipolar potential is reduced with the introduction of natural cutoff radii, similar to the Lewis cutoff /13/. The Debye cutoff becomes of no avail. These natural cutoffs \( b_{N\ell j} (v) = v/2|\omega_{ab}| \) lead to a collisional shift and broadening of each line component \((a a)\) which vary linearly with the perturber density \( N_p \). This is of practical interest for density diagnostics in Doppler free experiments /14, 15/.
The spontaneous emission leads to an additional broadening $R_{\alpha\alpha} = 0.5 \left( \tau^{-1} + \tau^{-1} \right)$ where $\tau_a$ ($\tau^R_a$) are the natural lifetimes of the states $a$ ($a^R$). At $10^{12}$ cm$^{-3}$ both collisional and radiative broadenings are of the same order of magnitude.

The seven components are gradually mixed for increasing densities, resulting in two resolved components at $10^{13}$ cm$^{-3}$ and in an unresolvable profile at $10^{14}$ cm$^{-3}$ (figure 5).

At $10^{14}$ cm$^{-3}$ the profile is asymmetric. The omission of the energy splitting effects would lead to a halfwidth of 0.08 Å instead of 0.14 Å. These splitting effects are naturally lesser in the near line wings.

In the figure 6 we compare our results (full triangles) with the experimental results of Ehrich et al. /16/.

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**Fig. 4** - $H_\alpha$ line ($10^4$ K, $N_p = 10^{12}$ cm$^{-3}$, $M = 0.5$) including electron and proton contributions and the natural broadening.

**Fig. 5** - Same as Fig. 4, with $N_p = 10^{14}$ cm$^{-3}$
- full line: profile including the energy splitting effects
- dashed line: profile without the energy splitting effect
Fig. 6 — Full half-width of $H_\alpha$ vs electron density.
0 : experiment of Ehrich et al. /14/. The hatched area indicates the estimated $H_\alpha$ half-width without Doppler and experimental broadenings. Dashed line: Kepple and Griem /17/. Solid line: Vidal et al. /12/.
▲: impact SCF calculation ($T_e = 17000$K, $T_i = 4000$K, $M = 0.5$). ▼ MMM results (after correction in order to include the energy splitting effects, Nollez and Masure, private communication).

The energy splitting effects enhances the full half-width of 0.122 Å for $N_p = 10^{14}$ cm$^{-3}$ and 0.086 Å for $N_p = 4 \times 10^{14}$ cm$^{-3}$, in comparison with a calculation excluding this effect. At these densities however, same departures from the impact regime appear. We have thus plotted (see fig. 6) the MMM results after an additional correction of 0.122 Å for $N_p = 10^{14}$ cm$^{-3}$ and 0.086 Å for $N_p = 4 \times 10^{14}$ cm$^{-3}$ in order to include qualitatively the energy splitting effects.

CONCLUSION

We have presented here the physical basis of the various approximations usually made in line broadening problems. The comparison between the impact and the MMM results for the $H_\alpha$ profile proves that the broadening is correctly described within the frame of the impact approximation in the line center up to $N_p = 10^{14}$ cm$^{-3}$. We have shown also that the ions yield the essential contribution to the Stark broadening and that fine structure and radiative lifetime effects are important at these low densities. An extensive analysis of the strong collisions contribution in the MMM and semi-classical impact formalisms is in progress. It seems that the exact calculation lie between the two preceding results. This is in a good agreement with the experimental profiles. Moreover the theories using the quasistatic assumption for the ionic broadening are to be avoided in the line center at low densities, as shown in figure 6.