Modeling of hydrogen Stark line shapes with kinetic theory methods

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Abstract. The unified formalism for Stark line shapes is revisited and extended to non-binary interactions between an emitter and the surrounding perturbers. The accuracy of this theory is examined through comparisons with ab initio numerical simulations.

1. Introduction
Since a few years ago, modeling efforts have been carried out in order to provide analytical formulas for the Stark broadening of the first Lyman lines of hydrogen, for opacity simulation purposes in magnetic fusion research [1]. One of the most challenging issues concerns the description of the ion dynamics. At densities and temperatures relevant to tokamak edge and divertors, the impact approximation is not far from being valid for ions, with typically \( b_W/r_0 \leq 0.5 \) for Ly-\( \alpha \) and Ly-\( \beta \) with \( b_W, r_0 \) being the Weisskopf radius and the mean interparticle distance. At such regimes, an approach based on first principles like the unified theory [2,3] is particularly suitable for the description of the ions. In this work, we present an extension of the unified theory applicable beyond the binary limit and suitable for numerical calculations. The theoretical framework is presented in Sec. 2, the model is presented in Sec. 3, and a practical formula for calculations is derived in Sec. 4. Comparisons with numerical simulations are done in Sec. 5.

2. The unified theory
The theoretical development done hereafter follows a previous work reported in [4]. We focus on hydrogen line broadening due to ions. A spectral line shape is determined from the Laplace transform of the average evolution operator \( \Phi_0(t) \):

\[
I(\omega) = \frac{1}{\pi} \text{Re} \sum \left\langle \left[ d \cdot \hat{e} \right] \Phi_0 (-i\omega) \rho \left[ d \cdot \hat{e} \right] \right\rangle.
\]

(1)

Here the double ket notation for Liouville space \( \left\langle \ldots \right\rangle \) has been used, \( \rho \) is the atomic density operator, \( d \cdot \hat{e} \) is the dipole projected onto the polarization vector, and \( \Phi_0 \) is the Laplace transform of the evolution operator averaged over the perturber trajectories (classical path assumption). The latter obeys a Schrödinger-like equation (we set \( \hbar = 1 \))

\[
\left( \frac{\partial}{\partial t} + iH_0 \right) \Phi_0 = -i\mathcal{N} \int d\mathcal{V}(1) \Gamma_1(1),
\]

(2)
with the initial condition $\Phi_0(t = 0) = 1$. $H_0$ is the Liouvillian accounting for the atomic energy level structure and the right-hand side denotes a source term accounting for interactions with the perturbers. The integral is performed over the phase space coordinates $\vec{r}_1, \vec{v}_1$ of one perturber ($d1$ is a shortcut notation for $d^3r_1d^3v_1$), $V(1) = -\vec{d} \cdot \vec{E}(\vec{r}_1)$ denotes the Stark term resulting from the electric field due to the perturber under consideration, and $\Gamma_1(1,1)$ is the atom - perturber 1 correlation function. The correlation function is defined from a cluster representation technique similar to that used in kinetic theory (e.g. [5]). In the most simplified treatment of the plasma, the perturbers can be described as independent particles following straight-line trajectories (weak coupling approximation) and the medium can be assumed uniform and stationary. In this framework, the evolution of $\Gamma_1(1,1)$ is governed by the following equation

$$\left\{ \frac{\partial}{\partial t} + i \left[ H_0 + V(1) \right] \right\} \Gamma_1(1) = -if_1(1)V(1)\Phi_0 - i\mathcal{N} \int d2V(2)\Gamma_2(1,2),$$

(3)

with the initial condition $\Gamma_1(1,1 = 0) = 0$. $f_1(1)$ is the one-particle phase space distribution. The integral in the right-hand side involves $\Gamma_2(1,2,1)$, the atom - particle 1 - particle 2 correlation function. Originally, the unified theory was developed for applications in cases where correlations between the collisions are negligible. $\Gamma_1$ is calculated assuming $\Gamma_2 = 0$. In this framework, the line shape can be written as a sum of generalized Lorentzian functions, whose widths and shifts are frequency-dependent and given by matrix elements of the collision operator

$$K(s) = \mathcal{N} \int_0^{\infty} dt e^{-\omega t} \int d1V(\vec{r}_1 + \vec{v}_1 t)\Phi(1,t)V(\vec{r}_1) f_1(1),$$

(4)

with $s = -i\omega$. Here $\Phi(1,t)$ is the propagator of the atom under the influence of one perturber. It obeys the time-dependent Schrödinger equation

$$\left\{ \frac{\partial}{\partial t} + i \left[ H_0 + V(\vec{r}_1 + \vec{v}_1 t) \right] \right\} \Phi(1,t) = 0,$$

(5)

with the initial condition $\Phi(1,t = 0) = 1$, and it is proportional to a time-ordered exponential (Dyson series)

$$\Phi(1,t) = e^{-iH_0t} \mathcal{T} \exp \left[-i \int_0^t \right] d\tau e^{iH_0\tau} V(\vec{r}_1 + \vec{v}_1 \tau) e^{-iH_0\tau}.$$  

(6)

3. Multiple collisions

We go beyond the binary approximation by assuming $\Gamma_2$ finite. We consider the following truncature relation, similar to that proposed by Kirkwood in kinetic theory [6]

$$\tilde{\Gamma}_2(\vec{k}_1, \vec{v}_1, \vec{k}_2, \vec{v}_2; s) = \tilde{\Gamma}_1(\vec{k}_2, \vec{v}_2, s + i\vec{k}_1 \cdot \vec{v}_1) \tilde{\Phi}_0(s + i\vec{k}_1 \cdot \vec{v}_1) \tilde{\Gamma}_1(\vec{k}_1, \vec{v}_1; s) + 1 \leftrightarrow 2.$$  

(7)

This expression can be obtained formally from solving the evolution equation for $\Gamma_2$ perturbatively, assuming $V$ small [4]. Here, the hat denotes Fourier transform with respect to the $\vec{r}$-variable and $1 \leftrightarrow 2$ denotes permutation between the variables. This closure relation provides a closed nonlinear evolution equation for $\Gamma_1$. A practical simplification for numerical calculations is provided by neglecting the second term in Eq. (7). We obtain a collision operator similar to that obtained within the binary approximation [Eq. (4)] in terms of an effective propagator $\Gamma_{\text{eff}}(1,t)$ accounting for multiple collisions

$$K(s) = \mathcal{N} \int_0^{\infty} dt e^{-\omega t} \int d1V(\vec{r}_1 + \vec{v}_1 t)\Gamma_{\text{eff}}(1,t)V(1) f_1(1),$$

(8)

$$\left\{ \frac{\partial}{\partial t} + i \left[ H_0 + V(\vec{r}_1 + \vec{v}_1 t) \right] \right\} \Gamma_{\text{eff}}(1,t) + \int_0^t d\tau M(\tau) \Gamma_{\text{eff}}(1,t - \tau) = 0.$$  

(9)

$\Gamma_{\text{eff}}(1,t)$ can be interpreted as describing the evolution of the atom under the influence of one collision represented by the interaction term $V$, given a set of collisions occurring in its past history. These
collisions are characterized by the kernel \( M(t) \). This term is identical to the inverse Laplace transform of the collision operator. In contrast with the binary case, Eq. (8) is not a closed expression for the collision operator because the evolution equation of \( Q_{\text{eff}} \) involves the collision operator, through the \( M \) term. In practice, a calculation should be done by iterations. A further simplification is provided by assuming \( M(t) = K_0 \delta(t) \) with \( K_0 = K(-i\omega_0) \) in Eq. (9). This leads to a simple relation between \( Q_{\text{eff}} \) and \( \gamma(s) \),

\[
Q_{\text{eff}}(1,t) = e^{-K_0 \gamma(s)} Q(1,t)
\]  

(10)

As in the binary case, the multiple integral in Eq. (8) can be evaluated with the use of cutoffs accounting for the oscillatory behavior of \( Q_{\text{eff}} \) at small impact parameters (strong collisions). The special case of hydrogen can be treated analytically following the same method as that used for obtaining the exact solution of the binary problem (e.g. [7] and Refs. therein). In the following we consider the first approach and derive an analytical formula for the collision operator suitable for numerical calculations.

4. An analytical formula for the collision operator

We assume that collisions with a small impact parameter give no significant contribution to the integrals in Eq. (8). On the other hand, we consider that the atomic wavefunction is not sensitive to perturbers located at large distance. In this framework, an approximation for the evolution operator is provided by

\[
Q(1,t) = \begin{cases} 0 & \text{if } r_i < r_m \\ 1 & \text{otherwise} \end{cases}
\]  

(11)

where \( r_m \) is a characteristic radius that remains to be determined. A possible approach consists in estimating the matrix elements of the integral \( \int dt V(\vec{r}_i + \vec{v}_i \tau) \) that appears in the Dyson series and comparing them to unity [8]. Such a procedure yields the following relation

\[
r_m = \begin{cases} b_w & \text{if } b_w \leq v_t t \\ \sqrt{b_w v_t t} & \text{otherwise} \end{cases}
\]  

(12)

where \( b_w = n^2/m v_1 \) is the Weisskopf radius. This relation exhibits the separation between the short and long time regimes, which correspond to incomplete and complete collisions, respectively. The interaction term has been estimated as \( V \sim H(r_m/v_1 - \tau b_w v_1/r_m^2) \), \( H \) being the Heaviside function. From the approximation Eq. (11), the space integral in Eq. (8) can be calculated analytically, in a fashion similar to what is done for the electric field autocorrelation function (e.g. [9]). We assume a Coulomb field and retain Debye screening through a cut-off at \( \lambda_D \). Hence,

\[
\int d^3r_i V(\vec{r}_i + \vec{v}_i t)Q_{\text{eff}}(1,t) = \frac{4\pi(b_w v_1)^2}{3(n^2e\alpha_0)^2} \vec{d} \cdot e^{-K_0 \gamma(s)} \vec{d} \times \begin{cases} \frac{1}{r_m} - \frac{1}{\lambda_D} & \text{if } v_t t \leq r_m \leq \lambda_D \\ \frac{1}{v_t t} - \frac{1}{\lambda_D} & \text{if } r_m \leq v_t t \leq \lambda_D \\ 0 & \text{otherwise} \end{cases}. 
\]  

(13)

The time integral in Eq. (8) can be evaluated analytically. We focus on Ly-\( \alpha \) and we choose a system of units such that \( \lambda_D = 1 = v_T \) (thermal velocity). The matrix element \( \gamma(s) = \langle 210 | K(s) | 210 \rangle \), which provides the line width and shift, is given by
\[
\gamma(s) = \frac{3\pi Nb_{WT}^2}{4} \left[ \text{erf}(b_{WT}) - \frac{2b_{WT}}{\sqrt{\pi}} e^{-b_{WT}^2} \right] \left( \frac{\pi}{s' b_{WT}} \right) - \frac{1}{s'} - \frac{1}{v} E_1\left( \frac{s' b_{WT}}{v} \right)
\]

\[
= \left[ \text{erf}(b_{WT}) - \frac{2b_{WT}}{\sqrt{\pi}} e^{-b_{WT}^2} \right] \left( \frac{\pi}{s' b_{WT}} \right) - \frac{1}{s'} - \frac{1}{v} E_1\left( \frac{s' b_{WT}}{v} \right)
\]

\[\gamma(s) = \frac{3\pi Nb_{WT}^2}{4} \left[ 2 + E_1\left( b_{WT}^2 \right) \right]. \tag{15}\]

where \( b_{WT} \) is the Weisskopf radius evaluated at the thermal velocity, \( s' = -i\Delta\omega + \gamma(0) \) with \( \Delta\omega \) being the frequency detuning, \( F(v) = 4v^2\exp(-v^2)/\sqrt{\pi} \) is the Maxwellian velocity distribution function, and \( \text{erf} \), \( E_1 \) are the error and first exponential integral functions, respectively. Equation (14) is suitable for numerical calculations. The binary approximation (“usual” unified theory) corresponds to setting \( s' \equiv -i\Delta\omega \), and the complete collision approximation (“impact” theory) corresponds to setting \( s' \rightarrow 0 \). An explicit calculation for \( b_{WT} << \lambda_D \) yields

\[\gamma(s) = \frac{3\pi Nb_{WT}^2}{4} \left[ 2 + E_1\left( b_{WT}^2 \right) \right]. \tag{15}\]

which corresponds to the standard result for hydrogen [10].

5. Application

We have applied the collision operator formula Eq. (14) to calculations of hydrogen line shapes in ideal cases. Figures 1 and 2 present a plot of Ly-\( \alpha \) broadened due to ions at \( b_{WT}/r_0 = 0.01 \) and 0.5, respectively, assuming \( r_0/\lambda_D = 0.5 \) in both cases. The calculations have been carried out using the unified theory (binary approximation) and the non-binary model (referred to as “Q_{eff}-model”). A numerical result from an ab initio simulation code is also shown in the figure. This code uses the “collision-time technique”, which has been developed and designed in the past so as to provide correct statistics at near-impact regimes where \( b_{WT}/r_0 << 1 \) [11]. Both the binary and non-binary models are in good agreement with the simulation in the first case (the small deviation visible at the line center falls within the typical uncertainty range of the simulation). This confirms the applicability of the unified theory at conditions where the atom-perturber interactions are supposed binary, typically when \( b_{WT}/r_0 << 1 \). It also illustrates that the non-binary model includes the binary limit. In contrast, the second case shows a strong discrepancy between the unified theory and the simulation. The binary assumption leads to an overestimate of the line width and predicts a different structure, with a dip at the line center. This deviation stems from an improper use of the unified theory. The non-binary model yields a better result, with no dip and an overestimate of the width no larger than 25%. A plot of \( |I(\Delta\omega = 0) - I_{\text{sim}}(\Delta\omega = 0)|/I_{\text{sim}}(\Delta\omega = 0) \) in terms of \( b_{WT}/r_0 \) is presented in Fig. 3 and shows the trend of the deviation in terms of the non-binarity.
**Figure 1.** Plot of the Ly-α profile obtained within the unified theory (dashed line), the non-binary $Q_{\text{eff}}$ model (solid line) and a simulation method (circles), at conditions where the atom - perturber interactions are binary. The analytical models are both in a good agreement with the simulation.

**Figure 2.** Plot of the Ly-α profile at conditions where the interactions are no longer binary. The $Q_{\text{eff}}$ model gives a correct estimate of the line shape whereas using the unified theory yields an overestimate of the width and predicts an incorrect structure.

**Figure 3.** Plot of the deviation to the simulation results. The $Q_{\text{eff}}$ model provides a good estimate of the line shape, even for a value of $b_{WT}/r_0$ as large as 0.5, whereas the unified theory gives a significant overestimate of the width as soon as $b_{WT}/r_0$ exceeds 0.1.
6. Conclusion
We have demonstrated the possibility of retaining non-binary effects in Stark broadening models through a simple approach inspired from kinetic theory. The average atomic evolution operator is calculated from a hierarchy of equations similar to that of Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY), able to account for many-particle correlations with arbitrary accuracy. When one single collision is considered, the correlations result in an alteration of the atom evolution due to cumulative collisions [12]. The model developed in this work provides results in a very good agreement with numerical simulations. The method can be applied either to ions or electrons, and it can be generalized to isolated lines. Also, the kinetic theory treatment is transposable to quantum plasma [13]. Further work would address the study of multiple correlations in the presence of a strong magnetic field like in tokamak plasmas. In this case the Zeeman effect can be important, so that the detailed structure of the levels should be retained.

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