Quantum-statistical line shape calculation for Lyman-α lines in dense H plasmas

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Abstract. We present results for the Lyman-α line of hydrogen in dense plasmas. Full line profiles are calculated within a quantum-statistical method, based on thermodynamic Green’s functions. The contributions of plasma ions and electrons are considered separately. Linear and quadratic Stark effect as well as quadrupole effects are taken into account for ions. The model microfield method is used to include ion dynamics. The focus of this work lies on the contribution to broadening and shift by free electrons beyond the Born approximation. The effect of strong collisions can be identified as ladder-like diagrams of the electron-emitter propagator. In an effective two-particle approximation, the electronic self-energy is given in terms of scattering amplitudes, analogous to Baranger’s expressions [Baranger, M 1958 Phys. Rev. 112 855]. We obtained scattering amplitudes from convergent close-coupling calculations including medium effects via Debye screening. Additionally, the electronic coupling between initial and final states is taken care of by a vertex correction. In our examples, the free electron density ranges between $10^{23}$ and $10^{25}$ m$^{-3}$ at a plasma temperature of 1 and 2 eV, respectively.

1. Introduction
Details of spectral lines like width, shift, and asymmetries can be used to determine plasma properties from an electro-magnetic spectrum [1]. The plasma can either be part of an astrophysical object or be created in arc discharges or by laser impact in the laboratory. A sound theory to calculate line profiles is needed in order to obtain accurate information about plasma parameters such as composition, temperature, and density. There exist many approaches to calculate the spectrum of bound-bound electron transitions, emitted from or absorbed by a plasma. No matter, if they use pure quantum mechanics [2], involve a semi-classical view on the perturbers, e.g. [3, 4], or depend on MD simulations, e.g. [5], they are based on the calculation of the dipole-dipole correlation. In our case, the dipole-dipole correlation – namely, the polarization function – is calculated within a many-body theory using thermodynamic Green’s functions.

The theory is briefly described in Sec. 2. The focus of this paper is twofold. At first, we want to improve the perturbative Born approach used so far for the perturbing electrons. It has the shortcoming to overestimate strong electron collisions. Hence, we implement an effective two-particle T-matrix approach, which accounts for strong collisions. This is done at the cost of neglecting dynamical screening for weak collisions. Instead, static screening is used in the calculation of the T-matrix in a convergent close-coupling scheme. The second focus is on the limit of the quasi-static approximation used for ion contributions so far. In this short
communication, we restrict ourselves to theoretical results for the Lyman-α line of hydrogen, see Sec. 3. Lyman lines of hydrogen-like lithium and the application in plasma diagnostics will be discussed in a forthcoming paper.

2. Quantum-statistical approach to line profiles
The quantum-statistical theory for pressure broadening has been described in detail in [6–8]. Here, we give only the key formulas in atomic Rydberg units, i.e \( \hbar = 2m_e = e^2/2 = 1 \). These units are used throughout this paper. The emitted spectral intensity \( I(\Delta \omega) \) at \( \Delta \omega = \omega - \omega_0 \) near the unperturbed transition frequency \( \omega_0 \) is given by

\[
I(\Delta \omega) = \frac{(\omega_0 + \Delta \omega)^4}{8\pi^4 c^3} e^{-\frac{\omega_0 + \Delta \omega}{\hbar n_m}} \text{Im} \left[ \sum_{i'f'} \{ \langle i| \vec{r}|f \rangle \langle f'| \vec{r}|i' \rangle \langle i| < U(\Delta \omega) >_{\text{KP}} |f'| \rangle \langle i' | \rangle \right].
\]

The sum runs over all initial \( i \) and final \( f \) emitter states. The double sum is due to degeneracy. The contributions to the line profile are weighted with the transition probability, which is given by the dipole matrix elements \( \langle i| \vec{r}|f \rangle \). In order to include ion dynamics in the theory, the model microfield method (MMM) based on a kangaroo process (KP) [9, 10] is adapted. Here, the time evolution operator \( < U(\Delta \omega) >_{\text{KP}} \) depends on the jump frequency \( \Omega(E) \) and is given by

\[
< U(\Delta \omega) >_{\text{KP}} = < U(\Delta \omega|\vec{E}) >_s + \frac{\Omega(E) U(\Delta \omega|\vec{E})}{< \Omega(E) >_s} - \frac{\Omega^2(E) U(\Delta \omega|\vec{E})}{< \Omega(E) >_s},
\]

where the average \( < \cdots >_s \) is over the static ion microfield with the distribution function \( W(E) \). For hydrogen, we use Hooper’s low frequency tables [11] to determine \( W(E) \). In our theory, the time evolution operator is constructed in the following way to include electron contributions

\[
U(\Delta \omega|\vec{E}) = \{ \Delta \omega - \text{Re} [\Sigma_i(\Delta \omega) - \Sigma_f(\Delta \omega)] + i\Omega(E) + i \text{Im} [\Sigma_i(\Delta \omega) + \Sigma_f(\Delta \omega)] + \Gamma_{if}(\Delta \omega) \}^{-1}.
\]

Here, \( \Sigma_i \) and \( \Sigma_f \) are the self-energies, i.e. broadening and shift, of energy level \( i \) and \( f \) due to the surrounding plasma, respectively, and \( \Gamma_{if} \) is the upper-lower level coupling term. Due to different interaction time scales, the self-energy can be split into an E-field-dependent ionic part and a frequency-dependent electronic part

\[
\Sigma_{i,f}(E, \Delta \omega) = \Sigma_{i,f}^e(E) + \Sigma_{i,f}^e(\Delta \omega).
\]

The perturbation of the emitter by the plasma ions is mainly given by the linear and quadratic Stark effect. Furthermore, quadrupole contributions are taken into account from [12]. In the quasi-static limit, i.e. with \( \Omega(E) \rightarrow 0 \), the second term of Eq. (2) vanishes.

2.1. Contribution of electron-emitter collisions
Two approaches have been developed to account for the contribution by free electrons. They are either considered within a dynamically screened Born approximation (1st order) or within an effective two particle T-matrix approach. While the former includes the dynamical screening of weak collisions, it overestimates strong collisions. This can be rectified to some extend by a cut-off procedure introduced by Griem [3]. The effective T-matrix approach is a simplified version of the T-matrix approach presented in [13]. It can describe weak and strong collisions equally well, but does so far only include static screening [14]. For a non-degenerate plasma, the electronic self-energy, evaluated at \( \Delta \omega = 0 \), is then given by

\[
\Sigma_{i,f}^e = -\frac{2}{\pi} n_e \Lambda_{\text{th}}^3 \int_0^\infty dk \ k^2 e^{-k^2/2k_B T} f_{i,f}(0, k).
\]
Plasma properties enter via the electron density $n_e$ and the thermal wavelength $\Lambda_{th} = \sqrt{4\pi/k_B T}$ as well as the forward scattering amplitude $f_{i,f}(0,k)$ for elastic electron scattering at the emitter in state $i$ and $f$, respectively. This expression was also found by Baranger in [2]. There, a level coupling term is derived, which is given by

$$\Gamma_{if} = \frac{2i}{\pi} n_e \Lambda_{th}^3 \int_0^\infty dk \frac{k^3 e^{-k^2/k_B T}}{k_B T} \int_0^\pi d\theta \sin(\theta) f_f(\theta,k) f_i^*(\theta,k).$$

(6)

2.2. Scattering amplitudes from Debye screened convergent close-coupling

The scattering amplitudes, which enter Eqs. (5) and (6), are obtained from a convergent close-coupling calculation (CCC). It is modified to include Debye screening in the interaction potentials. Details of the CCC method and its modification can be found in [15] and [16], respectively. Here, we use 54 (Sturmian) Laguerre functions as a basis for bound and continuous emitter states. With this choice, the emitter states up to 4f are reproduced with the correct energies. The electron-electron potential is expanded in partial waves, where the first partial waves (up to 70) are considered directly, for larger numbers of partial waves extrapolation formulas are used. The coupled equations are solved in momentum space and lead to the scattering amplitude. Our method gives separate results for singlet and triplet scattering channels as well as for scattering at the emitter with initial and final states $n_i, l_i, m_i \rightarrow n_f, l_f, m_f$. Here, we consider only elastic scattering $n_i, l_i, m_i \rightarrow n_i, l_i, m_i$ for the self-energies.

3. Lyman-α line of H

To illustrate the T-matrix approach, we consider the simplest line of hydrogen, namely Lyman-α. As the lower level 1s gives a small contribution, we focus on shift and broadening of the 2p level due to electrons in the discussion. In Fig. 1, the convergence with the number of partial waves is presented for $k_B T = 1$ eV and $n_e = 2 \cdot 10^{23}$ m$^{-3}$, and $n_e = 1 \cdot 10^{25}$ m$^{-3}$, respectively. The self-energies are given for different magnetic quantum numbers $m$ of the emitter. Singlet and triplet scattering results are averaged.

The convergence is faster for the imaginary part and at the higher density, where the screening is stronger. The plasma conditions correspond to a Debye length of 314 $a_0$ and 44 $a_0$, respectively, where $a_0$ is the Bohr radius. Assuming our T-matrix results as benchmark, the cut-off Born approximation overestimates the shift (real part), especially for the higher density of $n_e = 1 \cdot 10^{25}$ m$^{-3}$. The width (imaginary part) agrees within 10% with the average.
Figure 2. Hydrogen Lyman-α line calculated for quasi-static ions and electrons in either Born approximation (- - - -), Born approximation supplemented with a cut-off procedure (——) or with T-matrix approach (×——×). For $k_B T = 1$ eV and $n_e = 2 \cdot 10^{23} \text{ m}^{-3}$ (left) and $n_e = 1 \cdot 10^{25} \text{ m}^{-3}$ (right). All profiles are area normalized.

Figure 3. Same as Fig. 2 but with ion dynamics considered within the model microfield method, the scale is identical to Fig. 2.

Over $m$. However, as the central component of the Lyman-α line is given by the transition $2p_{m=\pm 1} \rightarrow 1s$, the line width is dominated by the width of the $2p_{m=\pm 1}$ level. Thus, in Fig. 2, the Born approximation with cut-off underestimates the width by up to 35% compared to the T-matrix approach. There, ions are only considered quasi-statically. In Fig. 3, the lines are further broadened by up to 50% for the lower density, and up to 30% for the higher density due to the ion dynamics (MMM). The importance of ion dynamics for H Lyman-α has been known from measurements [17] since 1977. Our full line profiles include Stark broadening by the plasma surroundings and are convoluted with a Gaussian to account for Doppler broadening.

In Tab. 1, we compare the width and shift due to electron collisions with an older close-coupling calculation [18]. There, Debye screening is included by restricting the calculation of isolated e-H scattering to a certain number of partial waves. When we average the self-energy and vertex term of different line components, our results agree within few percent with [18]. However, when we calculate the full line profile without ion effects and Doppler broadening, the line is 50% narrower and up to 40% less shifted. Thus, it is not appropriate to average width and shift over different scattering channels in line shape calculations.

Table 1. Width and shift of H Lyman-α from electron collisions compared with results from [18] for two plasmas with the same Debye length $\lambda_D = 314 a_0$. Conditions are 1) $k_B T = 1$ eV, $n_e = 2 \cdot 10^{23} \text{ m}^{-3}$ and 2) $k_B T = 2$ eV and $n_e = 4 \cdot 10^{23} \text{ m}^{-3}$. All values are given in Å.

| shift:     | averaged | full line [18] | HWHM: | averaged | full line [18] |
|------------|----------|----------------|-------|----------|----------------|
| 1)         | 0.0087   | 0.0051         | 0.0087| 0.062    | 0.031          |
| 2)         | 0.021    | 0.014          | 0.021 | 0.098    | 0.048          |
4. Conclusions
Full Lyman-α line profiles have been calculated for H plasmas within a quantum-statistical theory using a perturbative Born approximation as well as an effective two particle T-matrix approach for the electronic contributions. The latter needs scattering amplitudes as an input. They are obtained from convergent close-coupling calculations with Debye screening. The T-matrix approach can intrinsically treat strong electron-emitter collisions, whereas the Born approximation compensates the overestimation of strong collision contributions by an artificial cut-off procedure.

We show, that for a density of $n_e = 1 \cdot 10^{25} \text{ m}^{-3}$ and a temperature of $k_B T = 1 \text{ eV}$, the Born approach overestimates the shift even after cut-off by a factor of three, whereas the width agrees to the average obtained in the T-matrix approach within 10%. However, the line shape is significantly different between both approaches, because the self-energy is strongly dependent on the magnetic quantum number. This feature cannot be reproduced within the Born approximation. Ion contributions have been taken into account quasi-statically, and dynamically within the model microfield method. The ion dynamics leads to further line broadening.

Results for hydrogen Lyman-α were presented as a test case in comparison to older results. The method can be applied for other lines of hydrogen and hydrogen-like ions, as well.

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