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Enhancement of line broadening in plasmas by penetrating collisions for hydrogenlike lines



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ABSTRACT

Collisions that penetrate the wavefunction extent, which are of increasing importance for more highly correlated plasmas, are not correctly accounted for by the usual long-range dipole approximation. Since the interaction is softened for penetrating collisions, a reduction in line broadening is expected and indeed this is the case with isolated ion lines. Here we report an *enhancement* of broadening for H-like ions due to penetration. This has a simple physical explanation and potentially important applications, for instance in line merging and dense plasmas. In addition, the so-called "strong collision" contribution, usually estimated roughly and actually dominant for highly correlated plasmas, turn out to be often negligible if penetrating collisions are correctly accounted for. It is also shown that for such plasma parameters the expected electronic temperature scaling of widths can be reversed, resulting in widths that increase with temperature.

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1. Introduction

Spectral lines emitted from atomic systems in a medium are influenced by the medium and are effectively imprinted with information about this medium, such as its degree of randomness and the interactions with the atomic system. This information is in principle extractable from the line's broadened and shifted lineshape [1-3].

This work focuses on the electronic, collisional, contribution to the line broadening. This is given by a matrix involving the phase space average

$$\Phi = 2\pi N \int v f(v) dv \int \rho d\rho \{I - S_a S_b^{\dagger}\}$$
(1)

where N is the electron density, I is the unit matrix, S_a and S_b are the S-matrices respectively for the upper and lower levels and $\{\ldots\}$ denotes an angular average. f(v) is the velocity distribution and ρ refers to the impact parameter, with the integration limits for the impact parameter between 0 and the shielding length.

A perturbation approach is provisionally used for $\{I - S_a S_b^{\dagger}\}$:

$$\{I - S_a S^{\dagger}\} = Q_a I_b + Q_b I_a + Q_{ab} \tag{2}$$

with I_a , I_b unit matrices of upper and lower level states respectively and

$$Q_a = \int_{-\infty}^{\infty} dt_1 \frac{V_a(t_1)}{\hbar} \int_{-\infty}^{t_1} dt_2 \frac{V_a(t_2)}{\hbar},$$
(3)

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$$Q_{b} = \int_{-\infty}^{\infty} dt_{1} \frac{V_{b}^{*}(t_{1})}{\hbar} \int_{-\infty}^{t_{1}} dt_{2} \frac{V_{b}^{*}(t_{2})}{\hbar}$$
(4)

and

$$Q_{ab} = \int_{-\infty}^{\infty} dt_1 \frac{V_a(t_1)}{\hbar} \int_{-\infty}^{\infty} dt_2 \frac{V_b^*(t_2)}{\hbar}$$
(5)

with V(t) the emitter- perturber electron interaction and subscripts a and b referring to upper and lower levels respectively. For clarity we ignore Q_b and Q_{ab} in this work, which is justified for Lyman lines, as in the examples.

The interest in this work is radiation from states that have a spatial extent comparable to the shielding length, i.e. states for which the important broadening collisions occur at distances within the relevant wavefunction extent. As a result collisions with plasma electrons cannot be properly treated by the usual dipole, long-range approximation and need to take into account the penetration of the plasma electrons into the wavefunction extent of the levels involved in the line emission [4], which in turn softens the interaction and reduces the widths [5].

Penetration can be taken into account [6] by modifying the interaction by a multiplicative correction factor C_1 which exactly accounts for penetration:

$$C_{\lambda}(R;n,l,n',l') = \frac{\int_{0}^{R} P_{nl}(r) P_{n'l'}(r) r^{\lambda} dr}{\int_{0}^{\infty} P_{nl}(r) P_{n'l'}(r) r^{\lambda} dr} + R^{2\lambda+1} \frac{\int_{R}^{\infty} dr P_{nl}(r) P_{n'l'}(r) r^{-(\lambda+1)}}{\int_{0}^{\infty} P_{nl}(r) P_{n'l'}(r) r^{\lambda} dr}$$
(6)

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with R(t) the position of the plasma electron at time t and λ the multipole order (1 = dipole, 2 = quadrupole). C_1 is a function that is absolutely ≤ 1 as illustrated in Fig. 1, where at long distances it is 1 and at very short distances it vanishes, and as a result the interaction is softened.

We define the eccentricity

$$\epsilon = \sqrt{1 + \left(\frac{\rho}{s}\right)^2} \tag{7}$$

with ρ the impact parameter,

$$s = \frac{(Z-1)e^2}{4\pi\epsilon_0 mv^2} \tag{8}$$

and a dimensionless parameter ξ , related to the asymptotic velocity v, spectroscopic charge number Z and principal quantum number n as follows:

$$\xi = \frac{Z(Z-1)e^2}{2\pi\epsilon_0 m n a_0 v^2} \tag{9}$$

As shown in Fig. 2, ζ determines how fast the asymptotic limit $C_1(\infty)$ is approached, with small ζ (large velocities) leading to a slow transition and large ζ (small velocities) to a fast transition. Specifically, $C_1(u) = 1 - e^{-x}P_{2n+1}(x)$ where $x = \zeta(\epsilon coshu - 1)$ and $P_k(x)$ is a polynomial of degree k with the 0th and first term being 1. The polynomial coefficients are given in [7]. The asymptotic limit is reached for $\zeta(\epsilon \cosh u - 1) \gg \alpha$, i.e. $u \gg arcosh\left(\frac{1+\alpha/\zeta}{\epsilon}\right)$ where $\alpha > 3$ is a parameter to mark when the decaying exponential is small enough to render the correction from 1 negligible. C_1 is identically zero for $\zeta = 0$ and is $\theta(u)$ for infinite $\zeta(v = 0, \epsilon = 1)$. Thus, for large $\zeta(\epsilon - 1), C_1 = 1$ even at u = 0 and penetration makes no difference.

2. Atomic collision aspects

Defining

$$I(n, l, n', l') = \frac{1}{2} \int_{-\infty}^{\infty} du C_1 \left(R(t); n, l, n', l' \right) \frac{\epsilon(\epsilon - \cosh u)}{(\epsilon \cosh u - 1)^2}, \tag{10}$$

with *u* defined in terms of time *t* by

 $t = s(\epsilon sinhu - u)/v$,

a matrix element of Q_a may be written as:

$$\langle \mathbf{n}_{a}\mathbf{lm}|\mathbf{Q}_{a}|\mathbf{n}_{a}\mathbf{l'm'}\rangle = \frac{2}{3} \left(\frac{\mathbf{mv}}{\epsilon(\mathbf{Z}-1)\hbar}\right)^{2} \mathbf{I}(\mathbf{n}_{a},\mathbf{l},\mathbf{n}_{a},\mathbf{l''})$$

$$\mathbf{I}(\mathbf{n}_{a},\mathbf{l''},\mathbf{n}_{a},\mathbf{l'})\langle \mathbf{n}_{a}\mathbf{lm}|\mathbf{r}|\mathbf{n}_{a}\mathbf{l'm''}\rangle \cdot \langle \mathbf{n}_{a}\mathbf{l''m''}|\mathbf{r}|\mathbf{n}_{a}\mathbf{l'm}\rangle$$
(12)

I essentially includes the atomic collision physics, while the eccentricity and velocity integrations represent the plasma parameter phase space average. Note that a large *I* does not necessarily indicate a breakdown of the perturbation expansion, which is essentially checked by Eq. (12) [8]. I may be expressed in terms of modified Bessel functions K_0 and K_1 [9], but it is not numerically safe to do so.

When C_1 is identically 1 (i.e. no penetration) I = 1. However, note that because of the field changing direction this (I = 1) result arises from a positive, small $u \le arcosh(\epsilon)$ contribution of $\frac{\epsilon}{\sqrt{\epsilon^2-1}}$ and a negative, large *u* contribution. For large eccentricities ϵ , the positive contribution is approximately 1 and the negative approximately zero as illustrated in Fig. 3.

For small eccentricities however, the positive contribution can be $\gg 1$ and the negative contribution is then also absolutely very large, to give a net result of 1, as illustrated in Fig. 4. As a result, for large ϵ , account for penetration which suppresses the small R(t) and hence u, as $R(t) = s(\epsilon \cosh u - 1)$, contributions will decrease the positive contribution and give a smaller I^2 and hence width, as expected. For small ϵ however the positive contribution may be substantially suppressed, leaving a net large negative result and, since I^2 matters, a large *enhancement* of the broadening contribution. In Fig. 5, account of penetration gives I = -113, i.e. the contribution of the collision in question is *underestimated* by more than 4 orders of magnitude if penetration is not accounted for.

It should be stressed that these results are in *sharp contrast* to the case of isolated lines, i.e. lines where the energy difference between each participating level and the levels perturbing them via collisions is much larger than the typical inverse collision duration, discussed some time ago [4-6]: There, penetration resulted a decrease in



Fig. 1. C_1 vs. u for different channels for $\epsilon = 1.008$ and $\xi = 60$.

(11)

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