Shifts of one-electron ions lines from $\Delta n = 0$ interactions 
with electrons in hot and dense plasma

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Abstract. This paper is concerned with lineshifts of hydrogen-like ions due to electron collisions in dense and hot plasmas. These collisions are treated by including all effects due to monopole, dipole, and quadrupole interactions between radiator and electron perturbers. The latter follow exact hyperbolic trajectories with a possible penetrating part inside atomic orbits. A simple closed form for the line shift has been derived. Comparison between our semi-classical results and the quantum mechanical ones shows good agreement for a large range of high electron densities and temperatures.

PACS. 32.70.Jz Line shapes, widths, and shifts – 32.70.n Intensities and shapes of atomic spectral lines

1 Introduction

Stark-broadened spectral lines emitted or absorbed by dense and hot plasmas are currently used in density and temperature diagnostics, and radiative transfer measurements, especially for X-ray Laser research.

Spectral lines emitted by hydrogenic ions have been reported to be shifted when they are excited in dense plasma [1–5]. Since the standard Stark-broadening theories [6] when applied to hydrogen-like ions do not predict line shifts, the observed effect was first related to the formation of a time-averaged negative charge which overlaps the bound electron orbits, and produces shifts of energy levels. This “plasma polarization shift” has been considered in several theoretical advances. There are two equivalent methods of calculation: the first one is based on the ensemble average of atomic properties, such as the Debye-Hückel theory, average atom method [7] and the self-consistent-field for confined atom model [8]; the second one corresponds to the time average of these properties using quantum mechanical impact theory [8–10].

The purpose of this paper is to use the semi-classical approximation for treating the effect of electronic collisions in the shift of hydrogenic lines. In particular, the penetrating collisions in the atomic orbitals, which were analyzed by the quantum mechanical theory in the literature as mentioned previously, are treated here by the semi-classical approximation. The monopole, dipole and quadrupole terms are used in the ion-electron interaction and the hyperbolic trajectory effects of electron collision are included. Accordingly, a simple analytical formula will be established to evaluate the electronic shift. The results deduced from this method for electronic shift are in agreement with those obtained from the quantum mechanical impact theory in the Coulomb-Born-Oppenheimer (CBO) approximation [8].

2 Method of calculation

In the framework of impact theory [6,11], the electron width $w$ and shift $d$ of a spectral line, are given by:

$$w + id = \int d\gamma \langle i, f | 1 - S_i \otimes S_f^\dagger | i, f \rangle.$$  (1)

Here, $\int d\gamma$ denotes the thermal average and the subscripts $i$ and $f$ of the $S$-matrix allow the specification of the initial and final states of the optical transition. $S = T^{(+\infty, -\infty)}$ is deduced from the time dependent Schrödinger equation:

$$i\hbar \frac{d}{dt} T(t, 0) = V(t) T(t, 0) \quad \text{and} \quad T(0, 0) = 1$$  (2)

where, $T(t, 0)$ is the time development operator and $V(t)$ is the binary electron-radiator interaction which intervene in the line broadening. In equation (2), transitions between states with different principal quantum number $n$ are neglected (non-quenching approximation), $T(t)$ and $V(t)$ correspond to one level $i$ or $f$. The symbols $\mathbf{r}$ and $\mathbf{R}(t)$ denote the operator position of bound electron and vector position of perturbing electron respectively. In the semi-classical description, the potential $V(t)$ and the hyperbolic trajectory are deduced from the total interaction...
\[ V_{\text{tot}}(t) \] by the following relations:

\[
V_{\text{tot}}(t) = -\frac{Ze^2}{r} + \frac{Ze^2}{R(t)} + e^2 \left[ \frac{\rho}{|\mathbf{R}(t) - \mathbf{r}|} - \frac{1}{R(t)} \right].
\]

The potential \( V(t) \) is given by,

\[
V(t) = e^2 \left[ \frac{1}{|\mathbf{R}(t) - \mathbf{r}|} - \frac{1}{R(t)} \right] = V^{(0)} + \sum_{p=1}^{\infty} V^{(p)}(t)
\]

\[
V^{(0)}(t) = -e^2 \left[ \frac{1}{R(t)} - \frac{1}{|\mathbf{r}|} \right] E(R(t) < r)
\]

\[
V^{(p)}(t) = e^2 \frac{P_p(\cos \alpha)}{R^2} \left[ \frac{r^p}{R^{p+1}} E(R(t) > r) + \frac{R^{p+2}}{r^{p+1}} E(R(t) < r) \right] \text{ for } p \geq 1; \alpha = \langle R, \mathbf{R}(t) \rangle
\]

where, \( V^{(0)}, V^{(p)} \) and \( P_p \) are the monopolar, the \( 2^p \)-polar potential and the Legendre polynomial of degree \( p \), respectively. To separate the penetrating interactions \( (R(t) < r) \) and the external interactions \( (R(t) > r) \) one uses the Heaviside function \( E(...) \).

The term \( \frac{(Z-1)e^2}{R(t)} \) in (3a) gives the equation-trajectory of the perturber, which is in the form,

\[
R(t) = \frac{\rho \sqrt{\epsilon^2 - 1}}{1 + \epsilon \cos \theta(t)}, \quad \epsilon = \left( 1 + \frac{\rho^2}{\rho_0} \right)^{1/2};
\]

\[
\rho_0 = \frac{(Z-1)e^2}{mv^2} \quad \text{and} \quad R^2 \frac{d\theta}{dt} = \rho v\]

(4)

where the symbols \( \rho, v, \theta \) and \( Z \) denote the impact parameter, the velocity, the polar angle of perturber and nuclear charge of radiator, respectively.

The diffusion-matrix \( S \) is given by,

\[
S = T(+\infty, -\infty) = \Theta \exp (-i\Phi)
\]

where \( \Phi = \frac{1}{\hbar} \int_{-\infty}^{+\infty} V(t) dt \).

Since \( V(t) \), restricted to level \( i \) or \( f \), does not commute with itself at different instants generally, the \( S \)-matrix must be expressed with the ordering-time operator \( \Theta \). However, the electronic lineshift depends essentially on the monopole. Indeed, this spherical operator commutes with itself at different instants.

In order to prove the aforesaid statement, we study high and low temperature regimes.

### 2.1 Case of high temperatures

At the limit of high temperatures, the phase-shift \( \Phi \) nearly vanishes. Therefore, the corresponding \( S \)-matrix can be studied within the second order perturbation theory. Accordingly, we have

\[
S = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} V(t) dt - \frac{1}{\hbar^2} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} V(t)V(t') dt'.
\]

(6)

The lineshift which is given by the imaginary part of the electron broadening operator expressed in equation (1), becomes,

\[
\hbar d = \int d\gamma \int_{-\infty}^{+\infty} dt (V_i(t) - V_f(t)).
\]

(7)

The angular average of the integrand in (7) contributes only for monopole. The effects of dipole and multipole terms vanishes. Therefore, the lineshift depends only on the monopolar potential and becomes,

\[
\hbar d = \left\langle \int_{-\infty}^{+\infty} dt (V_i^{(0)}(t) - V_f^{(0)}(t)) \right\rangle_{av}
\]

(8)

where, the symbol \( \langle \cdots \rangle_{av} \) indicates the average over the impact-parameter and the velocity of the perturber.

### 2.2 Case of low temperatures

In this region, we show that the interactions inside the atomic orbital, that are the first causes of lineshift, contribute essentially via the monopole term. In fact, we show in the appendix, that the matrix-elements of multipoles are modified by a factor namely the “reduction factor”, which truncates the multipolar effects inside the atomic orbital. This factor is given by,

\[
\langle nlm|V^{(p)}(R)|nl'm' \rangle = \frac{e^2}{R^{p+1}} \langle nlm|\rho P_p(\cos \alpha)nl'm' \rangle \Delta_p(X)
\]

(9)

where,

\[
\Delta_0(X) \approx \begin{cases} 1 - \frac{X}{X_{nl}} = 1 - \frac{R}{r_{nl}} & \text{for } R < r_{nl} \\ 0 & \text{for } R > r_{nl} \end{cases}
\]

(10)

\[
\Delta_p(X) \approx \begin{cases} 0 & \text{for } R < R_p^{(1)} \\ A_p(X - X_p^{(0)}) + B_p & \text{for } R_p^{(1)} < R < R_p^{(2)} \\ 1 & \text{for } R > R_p^{(2)} \end{cases}
\]

(11)

\( X = ZR/a_0, r_{nl} \) is in the order of the atomic rayon, which will be determined later. The quantities expressed in (11) are given in the appendix.

The analytical forms of “reduction factors” shows that the internal orbital interactions contributes essentially by the monopole.