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RESEARCH ARTICLE

IONIC BROADENING WITH DYNAMICAL EFFECTS IN PLASMAS: PATH INTEGRAL POINT OF VIEW

M. DIFALLAH[1,2], M.T. MEFTAH[3], N. BEDIDA[3], D. BOLAND[1] AND R. STAMM[1]

[1]PIIM, Aix-Marseille Université et CNRS, Centre Saint Jérôme, Case 232, 13397 Marseille, France.

[2]VTRS, Centre Universitaire d'El Oued 39000, Algérie

[3]Laboratoire LENREZA, Université de Ouargla 30000, Algérie

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Abstract: Using a path integral formalism, ion dynamics effects are taken into account for the broadening of spectral lines in a plasma. A compact expression of the dipole autocorrelation function is derived for the Lyman alpha line of hydrogen. The static and the impact regime for the ions may be recovered by our approach. For a regime intermediate between the static and impact case we compare our approach to a profile obtained by a numerical simulation.

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1. INTRODUCTION

The spectral line shapes of radiative atoms and ions in the plasma provide valuable diagnostic tools for a number of physical quantities, such as the density and temperature of charged particles, the transported radiative energy, and possibly the determination of electric fields [1]. The shape of lines in a plasma results from the interactions between the radiator and all constituents (neutrals, electrons and ions) of the plasma. With variable contributions depending on plasma conditions, causes of broadening are the Doppler effect, which is produced by the movement of the radiator, natural broadening, due to the finite lifetime of the atomic excited state, and what will be the focus of this paper, the Stark broadening which is due to the interaction between the radiator and the electric field of the two kind of perturbers (ions-electrons) [2]. This problem has been widely studied using the standard Hamiltonian approach of quantum mechanics. It started with the work of Baranger [3], and Kolb and Griem [4]. In these classic papers on Stark broadening, the electrons are treated within the impact theory, and the ions in the quasi-static approximation. Both kind of particles having a Coulomb interaction with the radiator, the difference between ions and electrons is merely due to their velocity difference. For many plasma conditions, ions are slow enough to justify the use of a quasi-static approximation. But for hydrogen plasmas with rather low density, and/or high temperature, this static approximation may however no longer be valid. In our investigation, we introduce an alternative method able to take into account the effect of ion dynamics. This method is based on the Feynman path integral formalism [5] which deals with electrons and ions on the same physical basis. The general frame for this formalism has been previously developed [6], but has then only be applied to the static ion case. Using this formalism, one can treat time-independent and time-dependent problems on the same footing, which is a real advantage over the standard Hamiltonian approach when solving time-dependent problems. For the purpose of comparing our results to a simulation for a simple line, we apply our formalism to the Lyman alpha line of hydrogen or hydrogen-like ions.

Our paper is organized as follows: in part two, we derive the time dipolar autocorrelation function (TDAF) taking into account the dynamical effects of ions, which are represented by the time microfield autocorrelation function (TMAF), and discuss in part 3 the behaviour of our result in the static and impact limits for ions. In part 4, we apply our model to a case intermediate between the static and impact limits, and compare the obtained

line shape to a reference profile obtained with a computer simulation technique.

2. THE TIME DIPOLAR AUTOCORRELATION FUNCTION

We start here by deriving a path integral expression for the time dipolar autocorrelation function (TDAF) of the radiator from which the spectral line shapes are generally deduced. The emitter is perturbed by ions and electrons treated as charged particles moving on classical paths. For a description of the radiator-perturber interaction, it is usually sufficient to keep only the first term in the multipole expansion, using the so-called dipolar approximation. As quoted before, the effect of the electrons is usually treated with the impact theory by a collision operator. Our path integral approach could be applied to both electrons and ions, but we shall also use an impact approximation for the electrons in our numerical calculations. The electric microfield appearing in our formalism could thus be created by the electrons, the ions or both kind of particles.

As mentioned above, the main quantity in the study of spectral line shapes is the TDAF defined, for Lyman alpha without the fine structure by the following formula:

$$C(s) = \exp\left(-ise_b/\hbar\right) \sum_{\alpha\alpha'\beta} \vec{d}_{\alpha\beta} \left\{\langle\alpha|T_\alpha(s,0)|\alpha'\rangle\right\} \vec{d}^{\,*}_{\alpha'\beta}, \quad \ldots (1)$$

where d is the dipole operator, T is the evolution operator considered here to possess matrix elements only between substates α. The summation runs over all the upper states α, α', and the subscript av means that we must take a statistical average over the perturbers. The energy of the lower unperturbed level is noted ε_β. As we are interested in the Lyman alpha line, we shall sum in (1) only over the states α, since the lower state is unperturbed, and we neglect the interaction between levels with different principal quantum numbers. Using the Wigner-Eckart theorem, we obtain in the $|n, l, m>$ representation:

$$C(s) = (1/3)\ \exp\left(-is\varepsilon_\beta/\hbar\right) \left|\left\langle 21\left\|\vec{d}\right\|10\right\rangle\right|^2 \left(\left\{\langle 210|T|210\rangle\right\}_{av} + 2\left\{\langle 211|T|211\rangle\right\}_{av}\right) \quad \ldots (2)$$

A reduced dipole matrix element appears in this expression, as well as two terms of the evolution operator. Let us compute first the matrix element $\left\{\langle 211|T|211\rangle\right\}_{av}$ which can be written as:

$$\left\{\langle 211|T|211\rangle\right\}_{av} = \iint dy dy' \varphi_{211}(y)\, \varphi^*_{211}(y') \left\{K(y, s; y', 0)\right\}_{av}, \quad \ldots (3)$$

where $K(y, s; y', 0)$ is the Feynman propagator given by:

$$K(y, s; y', 0) = \int_{y(0)=y'}^{y(s)=y} D\left[\vec{y}(s)\right] \exp\left\{\frac{i}{\hbar}\int_0^s \left(\frac{m_e}{2}\dot{\vec{y}}^2 + \frac{Ze^2}{|\vec{y}|} + e\vec{y}\vec{E}(\tau)\right) d\tau\right\} \quad \ldots (4)$$

In this expression, $\vec{E}(\tau)$ is the electric field due to all components of plasma acting on the radiator, e and m_e denote the electron charge and mass, and Z is the charge number of the radiator nucleus. Knowing the initial propagator relative to the unperturbed hydrogen-like ion,

$$K_0(y, s; y', 0) = \int_{y(0)=y'}^{y(s)=y} D\left[\vec{y}(s)\right] \exp\left\{\frac{i}{\hbar}\int_0^s \left(\frac{m_e}{2}\dot{\vec{y}}^2 + \frac{Ze^2}{|\vec{y}|}\right) d\tau\right\}, \quad \ldots (5)$$

it is possible to develop the propagator $K(y, s; y', 0)$ as a series:

$$K(y, s; y', 0) = \sum_{k=0}^{\infty} \left(\frac{i}{\hbar}\right)^k \frac{1}{k!} \int_0^s d\tau_1 \ldots \int_0^s d\tau_k \int d\vec{y}_1 \ldots \int d\vec{y}_k \left(e\vec{E}_1\vec{y}_1\right) \ldots \left(e\vec{E}_k\vec{y}_k\right) \prod_{j=0}^{k} K_0\left(\vec{y}_{j+1}, \tau_{j+1}; \vec{y}_j, \tau_j\right), \quad \ldots (6)$$

with $\vec{y}_{k+1} = \vec{y}$, $\vec{y}_0 = \vec{y}'$. The expression for K_0 is known [7], and involves the hydrogen wavefunctions:

$$K_0\left(y_{j+1}, \tau_{j+1}; y_j, \tau_j\right) = \sum_n \varphi_n^*\left(y_{j+1}\right)\varphi_n\left(y_j\right) \exp\left[-i\varepsilon_n\left(\tau_{j+1} - \tau_j\right)\right] \quad \ldots (7)$$

Replacing the propagator K_0 by its expression, integrating over y and y', and using the orthogonality of the wave functions we get for $\left\{\langle 211|T|211\rangle\right\}_{av}$:

$$\left\{\langle 211|T|211\rangle\right\}_{av} = \sum_{k=0}^{\infty}\sum_{\alpha_2,\ldots\alpha_k}\left(\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_0^s d\tau_1 \ldots d\tau_k \int d\vec{y}_1 \ldots \int d\vec{y}_k \exp\left[\frac{is}{\hbar}\varepsilon_{211}\right]\left\{\left(e\vec{E}_1\vec{y}_1\right)\ldots\left(e\vec{E}_k\vec{y}_k\right)\right\}_{av}\varphi_{211}\left(\vec{y}_k\right) \varphi_{\alpha_k}^*\left(\vec{y}_k\right)\ldots\varphi_{\alpha_2}^*\left(\vec{y}_1\right)\varphi_{211}^*\left(\vec{y}_1\right) \quad \ldots (8)$$

Let us examine the structure of the first terms in this expansion. Calling U^k the successive terms in the sum over k in Eq. 8, we can write the first four terms as:

- term $k = 0$: $U^{k=0} = 1$
- term $k = 1$: $U^{k=1}$

$$= \frac{ie}{\hbar}\left\{\int_0^s d\tau_1\, \vec{E}\left(\tau_1\right)\left[\int d\vec{y}_1\, \varphi_{211}\left(\vec{y}_1\right)\cdot \vec{y}_1\, \varphi_{211}^*\left(\vec{y}_1\right)\right]\right\}_{av} = 0 \quad \ldots (9)$$

where we have used the selection rule for the orbital moment l.

- term $k = 2$

$$U^{k=2} = \frac{1}{2!}\left(\frac{ie}{\hbar}\right)^2 \int_0^s d\tau_1 \int_0^s d\tau_2 \left\{\sum_{\alpha_2}\left[\vec{E}\left(\tau_2\right)\int d\vec{y}_2\, \varphi_{211}\left(\vec{y}_2\right)\cdot\vec{y}_2\, \varphi_{\alpha_2}^*\left(\vec{y}_2\right)\right]\cdot \left[\vec{E}\left(\tau_1\right)\int d\vec{y}_1\, \varphi_{\alpha_2}\left(\vec{y}_1\right)\cdot\vec{y}_1\, \varphi_{211}^*\left(\vec{y}_1\right)\right]\right\}_{av} \quad \ldots (10)$$

only the state $\alpha_2 = 200$ contributes in the summation. We can thus write:

$$U^{k=2} = \frac{1}{2!}\left(\frac{ie}{\hbar}\right)^2 \left\{\left[\int_0^s d\tau\, \vec{E}\left(\tau\right)\int d\vec{y}\varphi_{200}\left(\vec{y}\right)\cdot\vec{y}\varphi_{211}^*\left(\vec{y}\right)\right]^2\right\}_{av} \quad \ldots (11)$$

- term $k = 3$:

$$U^{k=3} = \frac{1}{3!}\left(\frac{ie}{\hbar}\right)^3 \int_0^s d\tau_1 \int_0^s d\tau_2 \int_0^s d\tau_3 \sum_{\alpha_3}\left\{\begin{array}{l}\left[\vec{E}\left(\tau_3\right)\int d\vec{y}_3\, \varphi_{211}\left(\vec{y}_3\right)\cdot\vec{y}_3\, \varphi_{\alpha_3}^*\left(\vec{y}_3\right)\right]\cdot \\ \left[\vec{E}\left(\tau_2\right)\int d\vec{y}_2\, \varphi_{\alpha_3}\left(\vec{y}_2\right)\cdot\vec{y}_2\, \varphi_{\alpha_2}^*\left(\vec{y}_2\right)\right]\times \\ \vec{E}\left(\tau_1\right)\int d\vec{y}_1\, \varphi_{\alpha_2}\left(\vec{y}_1\right)\cdot\vec{y}_1\, \varphi_{211}^*\left(\vec{y}_1\right)\end{array}\right\} \quad \ldots (12)$$

Applying the selection rule imposes that $\alpha_2 = \alpha_3 = 200$ only contribute in Eq. 12, which means that $U^{k=3} = 0$.

Following then step by step all the terms, we can show that all the odd terms vanish, and only even terms in Eq. 8 contribute to the TDAF. For obtaining a tractable solution, we propose at this stage the use of a pair approximation for the electric fields. We thus neglect all correlations of higher than second order, and assume the correlations of second order to be small. It is then possible to sum all the terms, and the result for the element $\left\{\langle 211|T|211\rangle\right\}_{av}$ may be written as:

$$\left\{\langle 211|T|211\rangle\right\}_{av} = \left[1 + \frac{1}{3}\sum_{p=1}^{\infty}\left(\frac{i}{\hbar}\right)^{2p} \frac{\left[d_0^2\int_0^s d\tau\int_0^s d\tau'\left\{\vec{E}\left(\tau\right)\vec{E}\left(\tau'\right)\right\}\right]^p}{(2p)!}\right]$$

$$\exp\left[\frac{is}{\hbar}\varepsilon_2\right], \quad \text{... (13)}$$

where we have used the square of the reduced matrix element $D_0^2 = \left|\langle 21\|e\vec{r}\|10\rangle\right|^2$.

If we proceed similarly for $\left\{\langle 210|T|210\rangle\right\}_{av}$ we obtain:

$$\left\{\langle 210|T|210\rangle\right\}_{av} = \left[1+\frac{1}{3}\sum_{p=1}^{\infty}\left(\frac{i}{\hbar}\right)^{2p}\frac{\left[D_0^2\int_0^s d\tau\int_0^s dt'\left\{\vec{E}(\tau)\vec{E}(\tau')\right\}_{av}\right]^p}{(2p)!}\right]$$

$$\exp\left[\frac{is}{\hbar}\varepsilon_2\right] \quad \text{... (14)}$$

By combining the terms $\left\{\langle 211|T|211\rangle\right\}_{av}$ and $\left\{\langle 210|T|210\rangle\right\}_{av}$, and noting $\Delta\varepsilon = \varepsilon_1 - \varepsilon_2$, we get the final TDAF [8, 9]:

$$C(s) = (1/3)\left|\left\langle 21\|\vec{d}\|10\right\rangle\right|^2 \exp\left(\frac{is\,\Delta\varepsilon}{\hbar}\right)\left[2+\cos\frac{D_0}{\hbar}\sqrt{\int_0^s d\tau\int_0^s d\tau'\left\{\vec{E}(\tau)\vec{E}(\tau')\right\}_{av}}\right] \quad \text{... (15)}$$

We can express $C(s)$ in terms of the time microfield auto-correlation function (TMAF) $C_{EE}(\tau)$. Performing the integral over τ', we obtain:

$$C(s) = (1/3)\left|\left\langle 21\|\vec{d}\|10\right\rangle\right|^2 \exp\left(\frac{is\,\Delta\varepsilon}{\hbar}\right)\left[2+\cos\frac{D_0}{\hbar\omega_p}\sqrt{2s\left\langle E^2\right\rangle\int_0^s d\tau\left(1-\frac{\tau}{s}\right)C_{EE}(\tau)}\right] \quad \text{... (16)}$$

In this equation, the time is expressed in units of the inverse of the electronic plasma frequency $\omega_p = (4\pi N_e e^2/m_e)^{1/2}$. The quantity $C_{EE}(\tau)$ contains in our approach the dynamical effect of the microfield on the emitters radiative properties.

Equation 16 gives the TDAF regardless of the nature of charged particles. We can apply it according to our interests, either to ions or to electrons. In the following we limit our attention to derive the TDAF for ions in different regimes.

3. IMPACT AND STATIC APPROXIMATION FOR IONIC PERTURBERS

3.1 Impact Approximation

The impact approximation is valid when the mean duration of a collision τ_c is much smaller than the interval Δs between two successive collisions. The duration Δs is of the order of the inverse of the collisional line width expressed in angular frequency units. This criterion is equivalent to say that the average collision is weak, i.e. the product of the interaction by the collision time must be small compared to $\hbar$; this ensures that the collisions can be treated by perturbation theory and do not produce a large perturbation on the emitter. The argument of the cosine in Eq. 16 represents a cumulated phase change of the radiation between time 0 and s. If we are looking for conditions where the impact approximation is valid, we may thus assume that this phase change is small, and expand the cosine up to the second order term. Noting that $2+\cos(X) \cong 3\left(1-X^2/6\right)$ we can write Eq. 16 as:

$$C(s) = \left|\left\langle 21\|\vec{d}\|10\right\rangle\right|^2 \exp\left(\frac{is\Delta\varepsilon}{\hbar}\right)\left[1-3\left(\frac{D_0}{\hbar\omega_p}\right)^2 s\left\langle E^2\right\rangle\int_0^s d\tau\left(1-\frac{\tau}{s}\right)C_{EE}(\tau)\right] \quad \text{... (17)}$$

Since the mean duration of a collision is very small compared to the time between two successive collisions we extend the boundary of the integral in the last equation from (0, s) to (0, ∞):

$$\int_0^s d\tau\left(1-\frac{\tau}{s}\right)C_{EE}(\tau) \to \int_0^{\infty} d\tau C_{EE}(\tau) \quad \text{... (18)}$$

Using an impact operator Φ_i for the ions, the TDAF may be written:

$$C(s) = \left|\left\langle 21\left\|\vec{d}\right\|10\right\rangle\right|^2 \exp\left(\frac{is\Delta\varepsilon}{\hbar}\right)\exp\left[s\phi_i\right] \quad \text{... (19)}$$

Comparing with Eq. 17, we obtain for our model an impact operator in the weak collision limit:

$$\phi_i = -\frac{1}{3}\left(\frac{D_0^2}{\hbar\omega_p}\right)\left\langle E^2\right\rangle \int_0^\infty d\tau C_{EE}(\tau) \quad \text{... (20)}$$

This expression is similar to those of impact operators for hydrogen emitters found in the literature [1], when a second order approximation in the interaction potential is assumed.

3.2 Static Approximation

In the static case, the microfield is considered to be slowly varying in time, so that $\vec{E}(\tau) \cong \vec{E}(0)$. The TMAF may then be taken constant $C_{EE}(\tau) = C_{EE}(0) = 1$, allowing to write for the TDAF in the static limit as:

$$C(s) = (1/3)\left|\left\langle 21\left\|\vec{d}\right\|10\right\rangle\right|^2 \exp\left(\frac{i\Delta\varepsilon}{\hbar}\right)s \left[2 + \cos\frac{D_0 s}{\hbar\omega_p}\sqrt{\left\langle E^2\right\rangle}\right] \quad \text{... (21)}$$

We can compare this expression to previously published calculations for the Lyman alpha line in the static case [10]. In that limit, our TDAF $C(s)$ for an average field has the same structure as the previous result (see Eq. 3.2 of reference 10).

4. THE ION DYNAMICS REGIME

For hydrogen line with low principal quantum number, ion dynamics may affect the line shape for the densities found in laboratory plasmas, and in the edge of magnetic fusion devices. Such conditions usually correspond to weakly coupled plasmas. To study the dynamic properties, we use for the ions a theoretical expression for the time microfield autocorrelation function (TMAF) which is derived from the work of Rosenbluth and Rostoker in weakly coupled plasmas [11]:

$$C_{EE}(\tau) = \frac{3}{\sqrt{\pi}}\frac{r_0}{\lambda_D}\frac{1}{\tau}\left[1 + \tau^2 - \sqrt{\pi}\,\tau\left(\tau^2 + \frac{3}{2}\right)\exp\left(-\tau^2\right)erfc(\tau)\right], \quad \text{... (22)}$$

where τ is the time expressed in units of the plasma frequency, and λ_D the electronic Debye length. To obtain the line shape, we must first insert this expression for $C_{EE}(\tau)$ in the TDAF. The line shape in the atom's rest frame at a frequency ω is given by the Fourier transform of the TDAF:

$$I(\omega) = \frac{1}{\pi} Re \int_0^\infty ds\, C(s)\exp(i\omega s) \quad \text{... (23)}$$

We now compare our approach to an ab initio technique which consists in a numerical simulation of the motion of a large number of charged particles, followed a numerical solution of the Schrödinger equation for the emitter evolution operator. This procedure is repeated a large number of times in order to perform a statistical average. Such computer simulations have been used many times by several groups in the last three decades, allowing to establish benchmark profiles for a comparison to models and experiments [12, 13, 14, 15]. For the weakly coupled plasma conditions studied here, we simulate a set of ions moving on straight lines in a cube with periodic boundary conditions [15]. On Fig. 1 we present a first calculation of a line shape obtained with our path integral model, compared to the numerical simulation. For a density of $N_e = 10^{15}$ cm^{-3} and a temperature of 10^5 K, the profile obtained by our model is broader by about 15% than the simulation profile. This difference may be related to the approximation consisting in a factorization of the expressions containing a large number of fields in a product of averages containing only pair of fields. Note that for such conditions a static ion approximation would predict a line shape narrower by more than an order of magnitude. We can conclude that our approach thus captures most of the effect of ion dynamics.

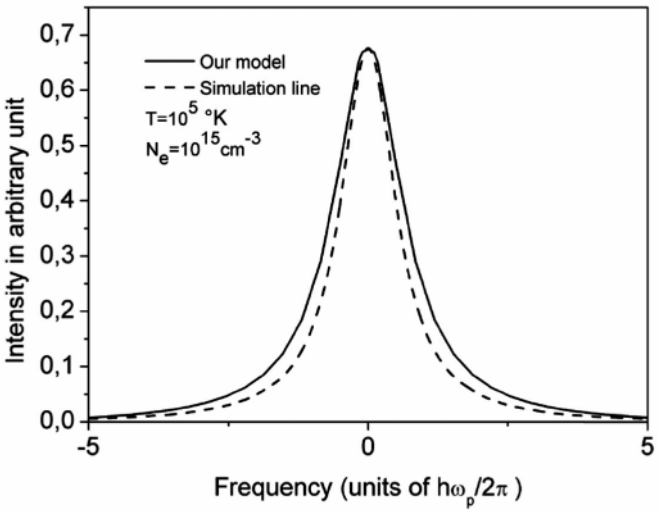

Fig. 1: Profile of lyman alpha for $N_e = 10^{15}$ cm^{-3}, a temperature of 10^5 K. Our path integral model (solid line) is compared to a computer simulation (dashed line)

5. CONCLUSIONS

Using a path integral point of view, we derive an expression for the Lyman alpha line shape retaining the effect of ion dynamics. We show how it is possible to recover the usual impact and static approximation for the ionic component. Our main approximation is a reduction to pair correlation functions of a cluster expansion in the electric microfield. This allows to sum all the terms appearing in the standard perturbative solution for the path integral point of view, and to express the TDAF in a compact expression involving the electric field autocorrelation function. A fairly good agreement between our model and a simulation calculation is found for our first calculation, and is a motivation for further developments with this approach. In particular, we would like to use the ability of the path integral point of view for the description of a full quantum emitter-perturber interaction. Interesting applications of a full quantum approach exist in high temperature plasmas such as found in fusion devices, for a modelling of the emission of multicharged emitters perturbed by electrons.

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