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Calculating the simultaneous effect of ion dynamics and oscillating electric fields on Stark profiles

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Abstract

We calculate hydrogen line shapes resulting from the simultaneous Stark effect of the plasma microfield and an oscillating electric field. Like laboratory plasmas, many kinds of space plasmas are affected by oscillating electric fields with a magnitude similar to that of the microfield. Here we focus on conditions where we expect that the effect of ion dynamics and oscillating electric are both significant. The combined effect of their dynamics on the quantum emitter is retained by a computer simulation coupled to a numerical integration of the Schrödinger equation. Our calculations are applied for conditions and transitions where significant changes in the line shape allow for a diagnostic of the plasma and oscillating field.

Keywords: Plasma diagnostic; Stark effect; oscillating electric field; Spectral line shape

1. Introduction

Oscillating electric fields can change the radiative properties of plasmas, with in particular changes in the line shape. In a laboratory, such fields can be generated by an external source, such as a microwave generator or laser radiation, with the aim of diagnosing or heating the plasma. They may also be created inside the plasma, resulting from a non-thermal effect driven by plasma instabilities. This is also the case in space and astrophysical plasmas where clouds or beams of electrons or ions interact with electric and magnetic fields allowing the creation of different plasma waves. Plasma waves are present in the low density plasma of magnetospheres, but also in star atmospheres, and during the interaction of a black hole with matter (Peratt, 1992). In solar physics, the spectral lines emitted in the partially ionized plasma of the photosphere may be affected by magnetized plasma waves (Cranmer and Ballegoijen, 2005). Recent observations connect the generation of solar wind with numerous nanoflares rooted in the photosphere, and able to accelerate a large number of energetic electron beams (Che, 2016). Such beams can generate Langmuir waves and radio bursts which may affect the emitted hydrogen line shapes.

Changes in the line shapes brought by the presence of oscillating electric fields have long been predicted and observed in laboratory hydrogen and helium plasmas. In early works they consist mainly in the appearance of satellite like structures near to multiples of the oscillation frequency assumed to be monochromatic (Baranger and Mozer, 1961; Cohn et al., 1972; Ben-Yosef and Rubin, 1971; Rutgers and de Kluiver, 1974; Ramette and Drawin, 1976). For experimental conditions with magnitudes of the oscillating field larger than the plasma microfield, satellites having about half of the central intensity and symmetrically positioned either side of the line center have been observed on the H β line (Gallagher and Levine, 1971). Such a striking effect is rarely observed in the presence of a Langmuir wave, but is well documented for emitters submitted to microwaves or laser (Lisitsa, 1994; Oks, 1995). Last decades theoretical studies retain the simultaneous effects of the plasma microfield and the oscillating field using a dressed atom picture (Oks, 2000; Alexiou, 2001) or a Floquet formalism (Peyrusse, 2009; Sauvan and Dalimier, 2009; Alexiou, 2021). With the exception of the works of Alexiou, 2001; Alexiou, 2021, these models do not take into account the time dependency of the ion microfield. But this ion dynamics effect is ubiquitous for the first Lyman and Balmer lines across a wide range of conditions. The typical ionic microfield fluctuation frequency can be estimated by $\omega_f = v_i/r_0$, where v_i is the ion thermal velocity, and r_0 the average distance between ions. The expected wave frequencies (e.g. the electron plasma frequency for Langmuir waves) are in many cases of the same order of magnitude as ω_f , indicating that these two dynamic fields are intertwined, and therefore require the simultaneous treatment of their effects on the emitter quantum dynamics. This quantum dynamics is well known for its variety of behaviors: fluctuating electric fields may simply shift the emitters energy levels (adiabatic interaction), or induce a radiationless transition to another energy state (nonadiabatic interaction). In the presence of an oscillating field of frequency Ω , a photon may be emitted after the absorption or emission of one or more

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energy quantum $\hbar\Omega$. This leads to the appearance of Blokhintsev satellites, which had been predicted since the beginning of quantum mechanics (Trautenberg et al., 1932; Blokhintsev, 1933). We study in the following the fate of such satellites in the presence of a time dependent ionic microfield. An accurate calculation for this problem is provided by a numerical integration of the Schrödinger equation for a hydrogen emitter under the simultaneous interaction of a simulated ion and electrons dynamic field, and an oscillating field $\vec{E}_w(t)\cos(\Omega t + \varphi)$, where φ is a phase. We have calculated Lyman and Balmer lines for conditions of laboratory, fusion and space plasmas, taking into account an oscillating electric field up to one order of magnitude larger than the mean plasma microfield. Line shapes presented in the following do not include Doppler effect, a broadening mechanism which can be significant for some of the spectra reported, and thus should be added with a convolution for comparing to experimental measures. Since we use a dipole interaction potential and neglect fine structure, the line shapes shown are symmetric about the line center, and we plot only the blue side of the lines.

2. Computer simulation of the line shape

The quantum formalism of line broadening in plasmas has been developed in the sixties in the frame of dipolar radiation of the emitter (Griem, 1964). A usual starting point is the emitter dipole autocorrelation function $C(t)$ expressed as a trace over the atomic states, and an average (denoted by the brackets $\{\dots\}$) over all the electric field configurations (Griem, 1997):

$$C(t) = Tr\{\vec{d}U^+(t)\vec{d}U(t)\rho\} \quad (1)$$

where \vec{d} and $U(t)$ are the dipole and evolution operator of the emitter, and ρ is the density matrix. We assume in the following that the initial levels of a transition are equally populated and in statistical equilibrium. In presence of an electric field the emitter evolution operator $U(t)$ follows the Schrödinger equation:

$$i\hbar \frac{dU(t)}{dt} = [H_0 - \vec{d} \cdot \vec{E}(t)]U(t) \quad (2)$$

where H_0 is the unperturbed emitter Hamiltonian, and $\vec{E}(t)$ is the sum of the plasma microfield and wave electric field:

$$\vec{E}(t) = \vec{E}_e(t) + \vec{E}_i(t) + \vec{E}_w(t) \cos(\Omega t + \varphi) \quad (3)$$

The plasma microfield is the sum of the electronic $\vec{E}_e(t)$ and ionic $\vec{E}_i(t)$ components, and the wave field is assumed to be a monochromatic longitudinal oscillation at the angular frequency Ω . The phase φ accounts the fact that every emitter on the line of sight is submitted to a different phase. We thus make an average over a set of random phases, and possibly over a random direction and a probability density function for the magnitude of the oscillating field. We use a computer simulation of the plasma microfield which consists in calculating for each time step the electric field at the center of a cubic box containing hundreds of charged particles with random initial conditions.

We retain screening effects between the charged particles by using a Debye potential (Stamm et al., 1984). For plasma particles with a kinetic energy large compared to the Coulomb potential energy, straight lines trajectories provide a good approximation to the actual trajectories, and a realistic time dependent electric field. The simulation of both ionic and electronic components is possible, but we found that a simple impact approximation for the electron did not significantly change the line shape. The electron field frequency fluctuations are higher by a factor of about 40 than that of the ionic field for a hydrogen plasma, and these fluctuations act on the emitter as a sequence of short binary collisions which can be modelled by a constant impact operator (Griem, 1997). In our computer simulation, we numerically solve the Schrödinger equation for each history of the electric field up to a time until the dipole is completely decorrelated.

Obtaining the dipole autocorrelation function $C(t)$ requires an average over a set of several thousand histories which explore a large number of electric field configurations. Such a number of histories is chosen to ensure that the statistical noise remains weak. An alternative approach allowing a more efficient reduction of this noise has been recently proposed (Rosato et al., 2020) but is not used here. The line shape is finally obtained by a Fourier transform of $C(t)$:

$$I(\omega) = \frac{1}{\pi} \text{Re} \int_0^{\infty} C(t) \exp(i\omega t) dt. \quad (4)$$

3. Convolution compared to full simulation

We have done our first calculations for the case of Langmuir waves in non-thermal plasma conditions. We consider in Section 3 and Section 4 random excitations of a large number of waves having random directions

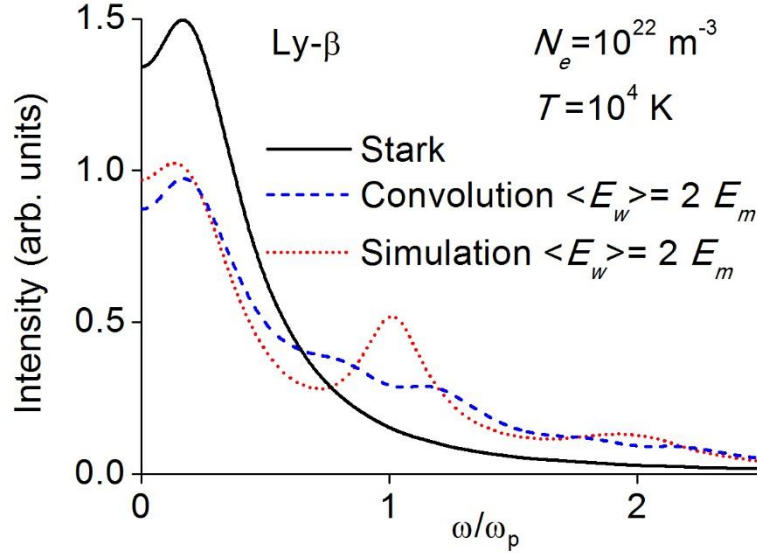


Fig. 1. Ly- β line shapes without oscillating field (Stark), and for $\langle E_w \rangle = 2 E_m$, using a convolution (dashed line) and a full simulation (dotted line).

and phases (Baranger and Mozer, 1961). Another consequence of non-thermal conditions is that we have to sample the magnitudes E_w of Langmuir waves. For conditions of plasma turbulence, Gaussian probability density function (PDF) have been predicted (Robinson and Newman, 1990) and measured (Levron et al., 1987). We propose to sample the oscillating field magnitude with a half-normal PDF:

$$P(F) = \frac{2}{\pi \langle E_w \rangle} \exp\left(-\frac{F^2}{\pi \langle E_w \rangle^2}\right). \quad (5)$$

where $\langle E_w \rangle$ is the mean magnitude of the wave. We will compare $\langle E_w \rangle$ to the mean magnitude of the microfield, a quantity which is equal to $E_m = 3.4 E_0$ in a weakly coupled plasma, with E_0 the microfield at mean interparticle distance r_0 (Griem, 1974). A simple model consists in calculating separately the dipole autocorrelation function (DAF) for the Stark effect including ion dynamics, and the DAF for the wave effect. We assume a monochromatic oscillation at the plasma angular frequency $\omega_p = \sqrt{N_e e^2 / m_e \epsilon_0}$, where m_e and e are the electron mass and charge, N_e the electron density, and ϵ_0 the permittivity of free space.

For our calculations, we average over a set of several thousand histories. A convolution line shape is obtained by a Fourier transform of the product of Stark and wave DAF. We have plotted in Fig.1 the hydrogen Lyman β line (Ly- β) for a density $N_e = 10^{22} \text{ m}^{-3}$ and a temperature $T = 10^4 \text{ K}$. The Stark profile (solid line) retains ion dynamics and electron broadening with an impact operator (Griem, 1964). For $\langle E_w \rangle = 2 E_m$, both the convolution calculation (dashed line) and the simultaneous simulation of wave and microfield (dotted line) exhibit remarkable structures near multiples of the plasma frequency. Both calculations also almost agree in predicting that a significant fraction of the intensity in the central part of the Stark profile is transferred to the satellites in presence of the wave. A clear difference is that the convolution acts as a translation by a frequency ω_p of the central part of Ly- β , leading to a dip around ω_p . The dip is barely visible in Fig.1, but clearly seen on

Fig.2, where the calculation is made with a static ions approximation. As it can be seen in Fig.1 and Fig.2 simultaneous calculation of the effect of microfield and wave fields leads to satellites with a single peak located

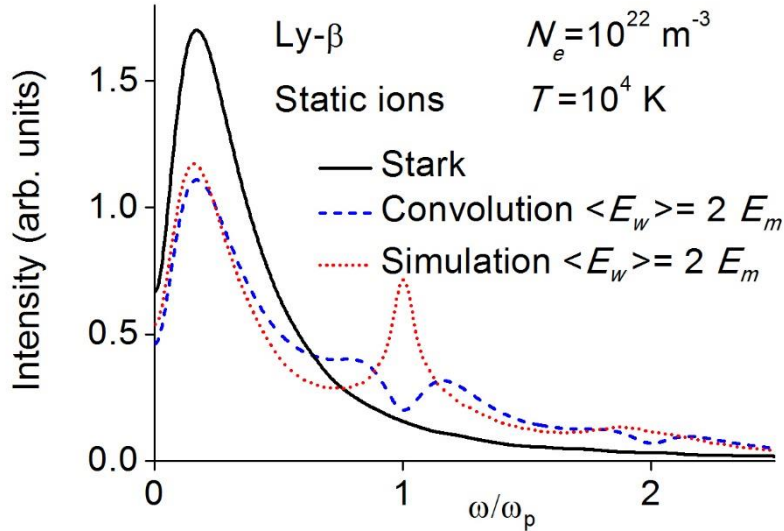


Fig. 2. Same as Fig.1 for static ions.

near to multiples of the plasma angular frequency. Similar to what can be seen on a pure Stark profile, ion dynamics smears out the structures on the line shape, increasing the width of the satellite by more than a factor 2, and leaving its intensity reach about half of the central peaks intensity. Considering that Stark and wave broadening are independent, as is done by the convolution, misses the synergetic effect of the two broadening mechanisms, emphasizing the need for a simultaneous calculation of the wave and microfield effects.

4. Photosphere conditions

We consider here Langmuir waves resulting from the presence of electron beams accelerated by nanoflares close to the surface of the sun (Che, 2016). There is a growing interest for the studies of nanoflares since they may be involved in the generation of solar wind. Here we are interested by the presence of Langmuir waves generated by well described kinetic instabilities in presence of energetic electron beams (Che, 2016). Balmer line shapes are commonly used for the spectroscopic diagnostic of plasma since they are broad lines in the visible spectra. We consider the emission of Balmer beta ($H\beta$) in the photosphere assuming the presence of Langmuir waves with electric field magnitudes of the order or a few times larger than the average plasma microfield, and study the detectability of such waves on the line shape. We retain the upper and lower broadening, thus increasing the possibilities of resonance effects between the wave frequency and the level splitting. In Fig.3 we calculate the $H\beta$ line for a density $N_e = 5 \times 10^{19} \text{ m}^{-3}$ and a temperature $T = 6000 \text{ K}$, conditions that can be found in the solar photosphere. A fraction of the central intensity of $H\beta$ is gradually transferred to satellites as $\langle E_w \rangle$ is increased from one to three E_m . For $\langle E_w \rangle = 3 E_m$, the maximum intensity of the first satellite is one third of the central peak intensity, and its width is about half that of the central peak. For $\langle E_w \rangle = E_m$, the maximum intensity of the first satellite is under 10 per cent of that of the central intensity. For values of $\langle E_w \rangle$ smaller than E_m , random ion dynamics gradually dominates the line shape and all the effects of the wave disappear. We show in Fig.4 the $H\beta$ line shape calculated for a fixed value of the magnitude $E_w = 3 E_m$ (dotted line). Compared to a Stark profile without wave (solid line), our calculation predicts a reduction of the central peak intensity similar to that observed with sampled values (dashed line). However the calculation with a fixed value of E_w leads to a first satellite with an intensity 30 percent larger, and a second satellite with

an intensity two times smaller. Sampling E_w thus slightly decreases the visibility of the first satellite but favours the appearance of more satellites.

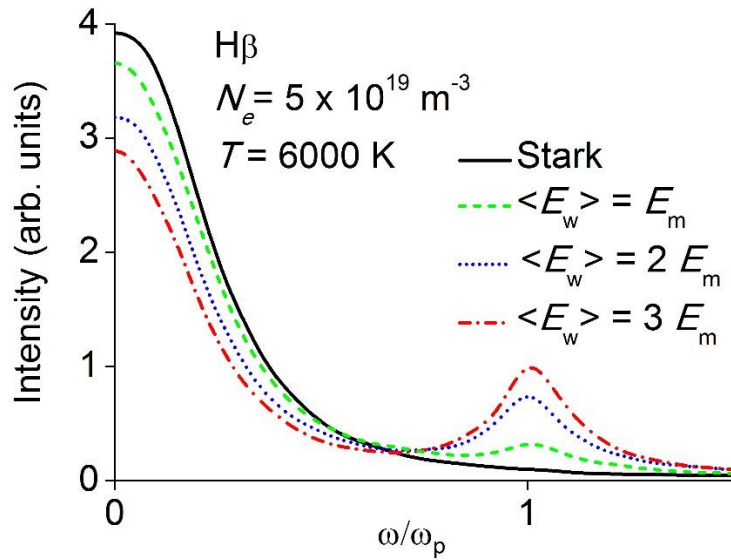


Fig. 3. H β line shapes without oscillating field (Stark), and for three values of $\langle E_w \rangle$.

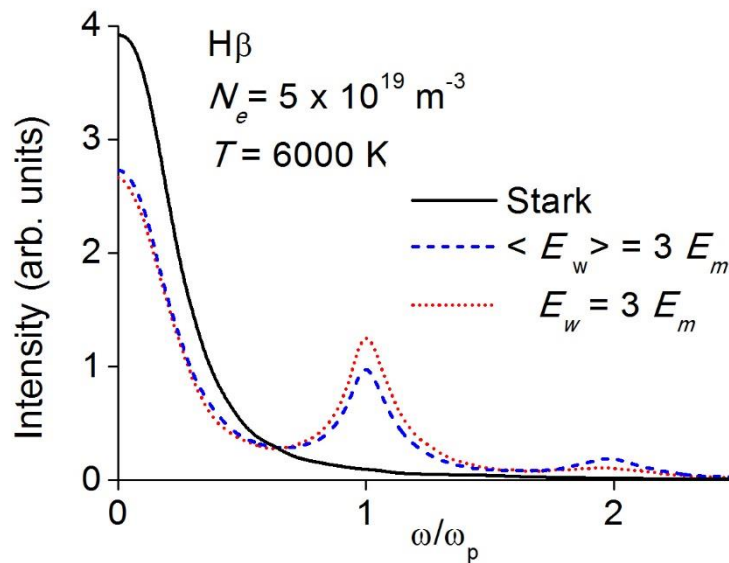


Fig. 4. H β line shapes without oscillating field (Stark), for sampled E_w magnitudes with $\langle E_w \rangle = 3 E_m$ and for a fixed value of $E_w = 3 E_m$.

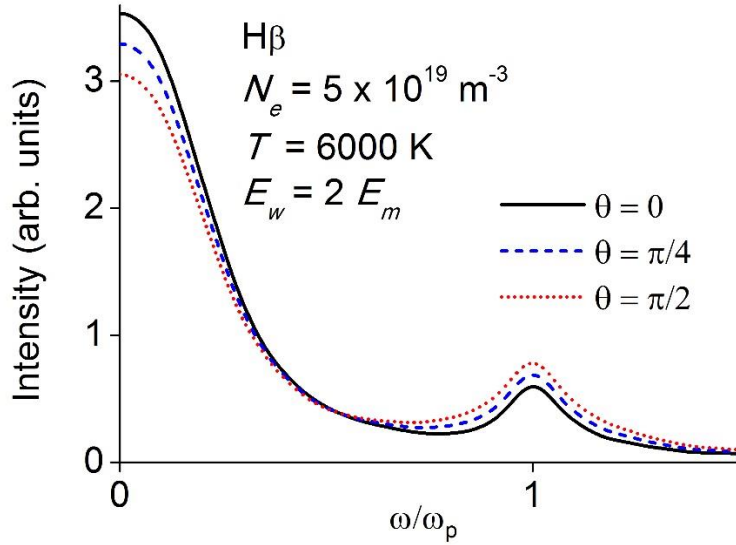


Fig. 5. H β line shapes for an oscillating field with a fixed magnitude $E_w = 2 E_m$, and observed at angles $\theta=0, \pi/4$ and $\pi/2$ with a fixed oscillation direction.

5. Partial polarization of H β

We now consider that the oscillating electric field has a fixed magnitude $E_w = 2 E_m$, and a fixed direction assumed to be along the z axis. If this field were alone, the dipolar radiation emitted would be permanently separated in π ($\Delta m = 0$) components with emitted electric field oscillating parallel to z , and σ ($\Delta m = \pm 1$) components with emitted electric field perpendicular to z . In such a situation the emitted radiation is polarized, with an intensity I_{\parallel} observed parallel to z , and I_{\perp} observed perpendicular to z . For an arbitrary angle θ between the line of sight and the z axis, the θ dependent line shape can be written (Peyrusse, 2009):

$$I(\omega, \theta) = I_{\parallel}(\omega) \cos^2 \theta + I_{\perp}(\omega) \sin^2 \theta \quad (6)$$

where the parallel and perpendicular line shapes can be expressed in terms of the σ and π components of the line shape (Peyrusse, 2009). In our calculation we add electron broadening and the ion dynamics field. During the time of interest, which is also the correlation time of the dipole, the emitter is submitted to ion microfield changes in magnitude and direction. The changes in magnitude of the field modify the level splitting and thus the frequency of emission, while the change in direction submits the atomic dipole to a torque which tends to force the dipole in the field direction. Early studies of these effects (Voslamber and Stamm, 1981) have shown that the dipole follows only imperfectly the electric field rotation. Here also nonadiabatic effects are acting, and prevent the dipole from rotating in phase with the electric field. The simultaneous effects of ion dynamics and fixed direction oscillating field thus leaves only a partial polarization observable. We show in Fig.5 H β profiles for the same plasma conditions as in Fig. 4, and a fixed direction oscillating field. The angle dependent line shapes exhibit intensity changes of about 15 percent as θ varies from 0 to $\pi/2$, with the largest intensity transfer to the first satellite for a $\theta = \pi/2$ line of sight.

6. Conclusion

For conditions where ion dynamics and an oscillating electric field simultaneously act on a radiating atom, there is no analytical approach that accounts for the complexity of the emitter quantum dynamics. We have proposed here a computer based approach that combines a simulation of the microfield resulting from the motion of a large number of charged particles with the effect of an oscillating electric field, and solves numerically the Schrödinger equation for the quantum emitter evolution. For a temperature of 10^4 K and densities between 5×10^{19} and 10^{22} m^{-3} , our calculations of H β and Ly- β predict the appearance of one or more satellites near to multiples of the plasma frequency.

A transfer of the central intensity to one or more satellites is visible as the magnitude of the oscillating field E_w is of the order of the mean plasma microfield, and this effect increases with E_w . We have shown the need for

an integration of the Schrödinger equation retaining the simultaneous action of the microfield and wave field by comparing to a convolution calculation. The use of a fixed or half Gaussian sampled magnitude does not significantly change the intensity transfers in the line shape. Our calculations of H β made for condition of the sun photosphere assuming there are Langmuir waves with magnitudes up to three times the average plasma microfield leaves open the possibility to observe satellite structures and may be a partial polarization effect of the line shape if the oscillating electric field has a preferred direction. Our model can be easily applied for non hydrogenic emitters, and can be enhanced to include the effect of a magnetic field. The simplified plasma particle simulation used here for low density plasmas can be replaced by a molecular dynamics simulation if coupled plasma are considered.

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