THEORETICAL ANALYSIS OF SPECTRAL LINES OF ONE- AND TWO-ELECTRON IONS IN
HOT PLASMAS

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Abstract

We discuss the line shapes for the $1s-2p$, $1s-3p$ and $(1s)^2 - 1s2p$, $(1s)^2 - 1s3p$ absorption lines in hot plasmas. In our model calculations the perturbing ions are considered quasi-static and widths due to collisions with electrons are calculated in the impact approximation. The collective effect of the plasma electrons is accounted for by a self-consistent model or by a simple Debye-Hückel screening. These models in general predict different line shapes. We present calculations for the HeII, SiXIV and SiXIII ions.

1. Introduction

In recent years the literature on spectral line analysis in hot plasmas has grown quite large [1]. The theoretical interpretation of shifts, widths and shapes has reached the level of sophistication that it is used for plasma diagnostics despite the fact that discrepancies still exist between theory and experiment and among different theories as well. The purpose of this report is to illustrate some of the differences in theoretically predicted line shapes and to describe a simple algorithm for line shape calculations. We will give special attention to the asymmetry of line shapes in low Z plasmas. In our model calculations we assume that the perturbing ions are quasistatic, coulombic and interact with the radiator but not with each other. For the electronic states of the radiator we use wave functions and energies

predicted by the Debye-Hückel or, alternatively, by a self-consistent radiator-free electron model.

In Section 2 we present the ion-microfield calculation and in Section 3 we outline the line shape calculation, together with discussing our computed data.

2. Microfield Distribution

Let E be the electric field produced by all the perturbing ions at the position of the radiator, then the probability of finding this field between E and $E + dE$ is given by $4\pi W(E) E^2 dE$ [2] where

$$W(E) = \frac{1}{(2\pi)^3} \int \exp \{-i\vec{\zeta} \cdot \vec{E}\} A_N(\zeta) d^3 \zeta. \quad (1)$$

We state that in Eq. (1) the direction of E is of no significance since the perturbing ions are assumed to be quasi-static. The index N stands for the number of ionic perturbers in the macroscopic volume, which is large. In Eq. (1) $A_N(\zeta)$ is the Fourier transform of $W(E)$ which can be calculated in a straightforward way using the principles of Ref. [2]. We obtain

$$A_N(\zeta) = \left\{ 1 - \frac{3}{2Nr_0} (Z_p e \zeta)^{3/2} I(p) \right\}^N \quad (2)$$

where r_0 is the ion sphere radius determined by the matter density. In Eq. (2) Z_p is the perturber charge and p is given by $Z_p Z_i e^2 / kT [Z_p e \zeta]^{1/2}$ where Z_i is the radiator charge, kT is the temperature in energy units and $I(p)$ is an integral given by

$$I(p) = 2 \int_0^\infty \left(1 - \frac{\sin y^2}{y^2} \right) \frac{1}{y^4} e^{-py} dz. \quad (3)$$

The integral $I(p)$ can be very accurately approximated by

$$I(p) = \frac{4}{15} \frac{\sqrt{2\pi}}{(1+p)^q}; \quad q = 1.2876 \quad (4)$$

We show the exact and approximated values of $I(p)$ in Fig. 1. Using Eq. (4) we obtain

$$A_N(z) = \exp \left\{ - \frac{(zE_0)^{3/2}}{(1+p)^q} \right\} \quad (5)$$

and

$$W(E) = \frac{1}{2\pi^2} \int_0^\infty \frac{\sin \zeta E}{E} \zeta \exp \left\{ - \frac{(\zeta E_0)^{3/2}}{(1+p)^q} \right\} d\zeta \quad (6)$$

where E_0 stands for the "normal field" given by

$$E_0 = \frac{Z_D e^2}{r_0} 1.00176.$$

Introducing the quantities

$$\bar{W}(E) = 4\pi E^2 W(E); \quad \beta = \frac{E}{E_0}; \quad x = \zeta E_0$$

Fig. 1 The integral $I(p)$ in Eq. (2). Solid line--exact, dots--approximation by Eq. (4).

we obtain

$$W(E) = \frac{1}{E_0} H^\Gamma(\beta)$$

where

$$H^\Gamma(\beta) = \frac{2}{\pi} \int_0^\infty x \sin \beta x \exp \left\{ - \frac{x^{3/2}}{(1 + \frac{\Gamma}{\sqrt{x}})^q} \right\} dx \quad (7)$$

and Γ stands for the plasma parameter

$$\Gamma = \frac{Z_p Z_i e^2}{kT r_0}.$$

A similar derivation leading to a more complicated form for $H^\Gamma(\beta)$ was done by Margenau and Lewis [3]. We think that our Eq. (7) is easy to handle for computation and is sufficiently accurate. To account somehow for the perturber-perturber interaction we make the substitution in Eq. (7)

$$\Gamma^1 = \Gamma(1 + e^\Gamma) \quad (8)$$

and find good agreement with the numerical calculations of Weisheit and Pollock [4] as shown in Fig. 2. It should be noted that for $\Gamma = 0$, Eq. (7) gives the Holtsmark distribution.

3. Outline of Line-Shape Calculations

We diagonalize the radiator electronic states in the presence of the ion-dipole and ion-quadrupole fields. The dipole field strength is E_0 with distribution $H^\Gamma(\beta)$ and for the quadrupole field we take the relationship which is valid in the nearest neighbor approximation

$$E_q = E_d^{3/2} [Z_p e]^{-1/2} \quad (9)$$

In the case of many perturbors the relationship between the dipole and

quadrupole fields is not so obvious and Eq. (9) is valid for high β values only. This is discussed briefly in Ref. [4]. When diagonalizing the radiator states we use jj coupling wave functions and energies so the spin orbit separation is accounted for. The ion quadrupole-field removes the hydrogenic degeneracy which leads to asymmetric profiles. This was recognized some time ago by Sholin [5] and is also discussed briefly by Pittman and Kelleher [6]. The screening by the plasma electrons also removes the hydrogenic degeneracy of the radiator states, thus the reasons of asymmetry are the combined effects of the ion-quadrupole field and that of the plasma electrons. This was pointed out some time ago by Weisheit and Rozsnyai [7]. We compute the electronic states of the radiator by using the Debye-Hückel model or a temperature-density dependent self-consistent model [8]. After having obtained the Stark-profile we convolute it with a Lorentzian and Doppler profile to obtain physically meaningful line shapes. The widths of the Lorentzian parts are due to electron impact and are calculated as described in a report by Rozsnyai [9].

Our results are summarized in Figs. 3-8. We present photoabsorption cross sections, whereas experimental data are usually emissions. The connection between the two is simple. For the HeII Ly α and Ly β lines the differences predicted by a self-consistent and Debye-Hückel models are clearly visible as shown in Figs. 3 and 4. The Debye-Hückel model predicts a larger red shift and in the case of the Ly β line the asymmetries predicted by the two models are opposites. None of our calculations show blue shifts as reported by Neiger and Griem [10], unless those blue shifts are associated with the asymmetry of the lines. However, the line shapes in Figs. 3 and 4 obtained by using the self-consistent electronic states of Ref. [8] seem to be in general agreement with those of Ref. [10].

For higher Z ions the difference between the two chosen models is not visible and the line shape is modified to a large extent by the increased spin-orbit splitting as shown in Fig. 5. This increased spin orbit splitting seems to be the reason for the apparent reversal in the asymmetry of the Ly β line which becomes less pronounced as the

density increases, as shown in Fig. 6. The helium-like transitions for the SiXIII ion are shown in Figs. 7 and 8. There, again is a reversal in the asymmetry in the $(1S)^2 - 1S3p$ line as the density increases. Our Fig. 8 (c) agrees fairly well with the results of Lee, Bromage and Richards [11] who calculated this line under the same physical conditions.

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References

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Fig. 2 Calculated microfield distributions for $\Gamma = .2, 2$, and 5 (a, b, c). Solid line --Eq. (7) and (8), circles--Weisheit and Pollock, Ref. [4].

Fig. 3 Photoabsorption cross section versus incident photon energy for the HeII Ly α line at $kT = 4$ eV. The densities are 10^{-5} , 10^{-4} and 10^{-3} g/cc (a, b, c) corresponding to 1.510^{18} , 1.510^{19} and 1.510^{20} cm $^{-3}$ electron densities. Solid line--using the self-consistent electronic states of Ref. [8], dashed line--using Debye-Hückel electronic states.

Fig. 4 Same as Fig. 3 for the Ly β line.

Fig. 5 Photoabsorption cross section for the SiXIV Ly α line at $kT = 800$ eV. (a) $.002 \text{ g/cc}$ ($n = 5.61020 \text{ cm}^{-3}$), (b) $.020 \text{ g/cc}$, (c) $.2 \text{ g/cc}$.

Fig. 6 Same as Fig. 5 for the $\text{Ly}\beta$ line.

Fig. 7 Photoabsorption cross section of the $(1s)^2 - 1s2p$ line for Si XIII at the same temperature and densities as in Fig. 6.

Fig. 8 Same as Fig. 7 for the $(1s)^2 - 1s 3p$ line.