High Energy Density Physics 9 (2013) 528–534

Contents lists available at SciVerse ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Review of the 1st Spectral Line Shapes in Plasmas code comparison workshop

Evgeny Stambulchik

Faculty of Physics, Weizmann Institute of Science, Rehovot 76100, Israel

ARTICLE INFO

Article history:
Received 2 May 2013
Accepted 2 May 2013
Available online 11 May 2013

Keywords:
Spectral line shapes
Stark broadening
Zeeman effect
Numerical methods
Computer simulations

ABSTRACT

A review is given of the first workshop dedicated to the detailed comparison of various approaches to the calculation of spectral line shapes in plasmas. A standardized set of case problems was specified in advance, together with the prescribed atomic data and assumptions to be used. In this brief review, motivations for the case problems chosen are outlined, followed by a discussion of selected results. Plans for the next workshop are discussed in the conclusion.

1. Introduction

Line-shape analysis is one of the most important tools for diagnostics of both laboratory and space plasmas [1]. Its reliable implementation requires sufficiently accurate calculations. In the formation of a line shape Stark broadening is the most computationally challenging contribution, with other factors, such as the Zeeman and Doppler effects, further complicating the calculations. Therefore, except for limiting cases, line-shape calculations imply the use of computer codes of varying complexity and requirements of computational resources. There exist several such codes and, necessarily, limits of applicability, accuracy, and in the end, results, differ from one to another. However, studies comparing different computational and analytical methods are almost nonexistent. The 1st Spectral Line Shapes in Plasma (SLSP) code comparison workshop [2] was organized to fill this gap. The organization of the meeting was modeled after the very successful series of NLTE workshops running from the mid 1990's [3] until now [4]. The NLTE workshops were inspired by the Opacity Workshops, initiated in the late 1980's [5], where a detailed comparison of results for a preselected set of standardized case problems was carried out and analyzed.

A general review of the SLSP workshop is presented, focusing on motivation for the case problems chosen, and followed by discussion of selected results.

2. Cases

A number of transitions were selected and are presented in Table 1. For each transition results on a grid of electron densities (n_e) and temperatures were requested – assuming one temperature for the ions and electrons, i.e., $T = T_e = T_i$. For each case, the atomic and plasma models are specified, and for some cases, there are more than one atomic or plasma model suggested. Here unless specified otherwise, the plasma is assumed to be quasi-neutral, consisting of electrons and a single type of ions. In addition, some cases are further detailed by specifying extra parameters, such as the magnetic field. In total, 184 subcases were defined.

In order to exclude the influence of variance of atomic data on the results, the case definitions also included exact atomic models to be used. That is, provided were a list of the levels to be accounted for, level energies, and matrix elements between them.

2.1. Reference cases

1. Hydrogen Lyman-α in an ideal plasma is a classical ion-dynamics test.
2. A relatively high-n line for hydrogen. For the plasma parameters selected, this is a test of the transition for electrons from dynamic to almost static regime.

These cases are not necessarily realistic, but are good for basic comparison and understanding what is wrong/different if there is a significant scatter in the results from the more advanced cases below. There are quite a few sub-cases of these reference cases; however, the

---

E-mail address: Evgeny.Stambulchik@weizmann.ac.il.

1574-1818/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.hedp.2013.05.003

Table 1
Case definitions.

ID	Transition(s)	n_e (cm^{-3})	T (eV)	Extra parameters
1	H Lyman-α	10^{17}, 10^{18}, 10^{19}	1, 10, 100	–
	Model: $\Delta n \neq 0$ interactions ignored (strictly linear Stark effect); no fine structure; ideal plasma (straight path trajectories and infinite Debye length for MD or Holtsmark distribution for analytical models) in three variants: only electrons, only protons, and electrons and protons together.			
2	H Lyman-δ	10^{16}, 10^{17}, 10^{18}	1, 10, 100	–
	Model: same as above.			
3	H $n = 6 \to 5$	5×10^{15}, 2×10^{6}	1, 10	–
	Model: $\Delta n \neq 0$ interactions included in three approximations: none, only $n = 5$ and 6 levels interact, and all from $n = 5$ to $n = 7$. Plasma ions: protons.			
4	Be II 3s–3p	10^{17}	5, 15, 50	–
	Model: 3s, 3p, and 3d levels included, no fine structure. Only electron broadening included, in two approximations: straight paths and hyperbolic trajectories.			
5	N V 3s–3p	10^{18}	5, 15, 50	–
	Model: same as above.			
6	Ne VIII 3s–3p	10^{19}	5, 15, 50	–
	Model: same as above.			
7	Al III 4s–4p	10^{18}	2, 4, 8	–
	Model: 4s, 4p, and 4d levels included, no fine structure. Plasma perturbations in two approximations: only electrons and both electrons and ions (Al III).			
8	Si XIII $n = 3 \to 1$	10^{21}, 10^{22}, 10^{23}	300	–
	Model: $n = 1$ and 3 singlet levels only, ignoring $\Delta n \neq 0$ interactions. Plasma ions are protons.			
9	Al XIII Lyman-α	10^{21}, 10^{22}	500	$\omega = 10^{15}$ rad/s, $F = 0$, 1, 2 GV/cm
	Model: $n = 1$ and 2 levels in two variants: with and without fine structure. Plasma ions are Al XIII, no electrons.			
10	D Balmer-α	2×10^{14}, 10^{15}	1, 5	$B = 0$, 5, 10 T
	Model: with/without fine structure for the lower/higher density, respectively; ideal plasma in two variants: ions are either deuterons or infinitely massive particles.			
11	D Balmer-β	2×10^{14}, 10^{15}	1, 5	$B = 0$, 5, 10 T
	Model: same as above.			
12	D $n = {}^{*} \to 2$	10^{15}, 10^{16}, 10^{17}	1	–
	Model: fully ionized D plasma, LTE, two variants: only bound–bound transitions included or both bound–bound and free–bound.			
13	H Balmer-α	10^{18}	1	–
	Model: linear Stark, plasma in two variants: ideal and interacting. Plasma ions: protons.			
14	H Balmer-β	10^{18}	1	–
	Model: same as above.			
15a	Ar XVII He-β	5×10^{23}, 10^{24}, 2×10^{24}	1000	–
	Model: plasma ions are deuterons with 0.1% of Ar XVII.			
15b	Ar XVI He-β^{*} $n = 2$	5×10^{23}, 10^{24}, 2×10^{24}	1000	–
15c	Ar XVI He-β^{*} $n = 3$	5×10^{23}, 10^{24}, 2×10^{24}	1000	–
15d	Ar XVI He-β^{*} $n = 4$	5×10^{23}, 10^{24}, 2×10^{24}	1000	–
	Atomic model: with and without the interference term in the electron broadening; plasma model: as above.			

corresponding models are purposefully made simple: 1) we assume an ideal plasma which for the line broadening calculations will mean straight path trajectories and infinite Debye length for molecular dynamics (MD) simulations, or a Holtsmark distribution for analytical approaches and 2) pure linear Stark effect so that interactions between states with $\Delta n \neq 0$ are ignored and no fine structure is included. In order to assess the influence of electrons and ions, which are protons for the reference cases, the broadening was calculated assuming the electrons and protons act separately and together, so that there are three variants in total for each pair of n_e and T.

2.2. High-n $\Delta n = 1$ transitions

3. Hydrogen $n = 6 \to n = 5$ transition. This case was calculated using three atomic models: (i) no $\Delta n \neq 0$ coupling accounted for, (ii) $n = 5$ and $n = 6$ states couple, and (iii) $n = 5$, 6, and 7 states included in the Hamiltonian and allowed to mix.

This line is a representative of $n, n' \gg 1, \Delta n \ll n$ class of transitions that includes the radio-frequency lines, which are of great interest for astrophysics. However, due to the computational costs, an n was chosen that is not sufficiently high to be categorized as a radio-frequency transition. Nevertheless, the couplings between states with $\Delta n \neq 0$ were important.

2.3. Isolated lines

First, three species from the Li-like 3s–3p sequence were chosen, for which the divergence between quantum mechanical (QM) calculations and experiments grows with Z [6]:

4. Be II is the first non-neutral species of the sequence.
5. N V – an intermediate Z.
6. Ne VIII is about the highest Z for which the 3s–3p broadening can be reliably measured.

The plasma model for these cases included only electrons, and it was assumed that they move either along straight path trajectories or the more realistic quasi-classical hyperbolic trajectories (due to the Coulomb interaction with the radiator) in order to investigate this effect.

In addition, another isolated line was considered for which quantum effects are not expected to be so significant (i.e., larger matrix elements and cross-sections):

7. Al III 4s–4p. In addition to the width, values of the line shift were compared.

2.4. Intermediate case between isolated and degenerate regimes

8. He-like Si XIII 3 → 1 transitions without inter-combination lines. At the lower density, only 1s–3p (He-β proper) is seen, then 1s–3d and 1s–3s appear as well, approaching Lyman-β-like shape at the highest density. Plasma ions are protons.

2.5. External fields

9. Al XIII Lyman-α under external harmonic perturbation, e.g., a laser. The functional dependence of the electric field is $F\cos(\omega t)$, with ω and F given in Table 1. The two plasma densities correspond to laser-dominated and plasma-dominated line