Institute of Physics
University of Belgrade

SLSP

IAEA
International Atomic Energy Agency

5th Spectral Line Shapes in Plasmas
Code Comparison Workshop

May 27–31, 2019

Vrdnik, Serbia

Call for Submissions (rev. April 10, 2019)

Introduction

This document defines the particulars of the workshop submissions. In the sections below we define the case problems, the comparison quantities which we require and the detailed format of the data files that we will be expecting.

The webpage of the meeting is at `http://plasma-gate.weizmann.ac.il/slsp5/`. The submission files are to be uploaded to the same server using a web interface with userid and password. Details will be announced separately.

Timeline (2019):

April 06	—	web interface for file uploads opens
April 20	—	hotel booking deadline
May 12	—	submission deadline
May 27	—	workshop opens
May 31	—	workshop adjourns

Contents

1 Statement of cases 2

2 Justification of cases and details 3
- 2.1 Reference cases . . . 3
- 2.2 Quadrupole corrections in H-like . . . 3
- 2.3 Isolated lines . . . 3
- 2.4 External fields . . . 4
  - 2.4.1 B-induced trajectory effects . . . 4
  - 2.4.2 Non-linear B . . . 5
  - 2.4.3 B-field effect in MagLIF . . . 5
- 2.5 MagLIF density diagnostics . . . 5
- 2.6 Ionization potential depression . . . 5

3 Atomic data 5
- 3.1 Hydrogen-like . . . 5
- 3.2 Non-hydrogen . . . 6

4 Submission format 7

Table 1: Case definitions.

ID	Transition(s)	# of subcases	n_e (cm^{-3})	T (eV)	Extra parameters
1	H Balmer-α	$5 \times 2 \times 3 \times 1 = 30$	10^{15}, 10^{16}, 10^{17}, 10^{18}, 10^{19}	1, 10	—
			Model: $\Delta n \neq 0$ dipole interactions ignored (strictly linear Stark effect); no fine structure; straight path trajectories of Debye quasiparticles in **three** variants: only electrons, only protons, and electrons and protons together.		
2	H Balmer-β	$6 \times 2 \times 3 \times 1 = 36$	10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18}, 10^{19}	1, 10	—
			Model: Same as above.		
3	H Balmer-β	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as case 2, but with quadrupole interactions included.		
4	H Balmer-β	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as case 2, but with $\Delta n = 1$ dipole couplings included.		
5	H Balmer-β	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as case 2, but both dipole and quadrupole ($\Delta n \leq 1$) couplings included.		
6	Li I 3s–3p	$1 \times 6 \times 2 \times 1 = 12$	10^{17}	1, 2, 5, 10, 20, 50	—
			Model: $n = 3$ levels included, no fine structure. Only **fixed-energy** electron broadening is included. No Debye screening. Two variants of calculations: only dipole or dipole + quadrupole interactions.		
7	O VI 3s–3p	$1 \times 6 \times 2 \times 1 = 12$	10^{18}	4, 7, 10, 20, 50, 100	—
			Model: Same as above.		
8	H Lyman-α	$1 \times 1 \times 3 \times 3 = 7$	10^{17}	5	$B = 0, 200, 500$ T
			Model: No fine structure. Electron OCP, no ions. For non-zero B, three variants of calculations (see the case description).		
9	H Lyman-α	$1 \times 1 \times 2 \times 4 = 7$	10^{19}	5	$B = 0, 0.5, 2, 5$ kT
			Model: No fine structure. For non-zero B, two variants of calculations (without and with the B^2 term).		
10	H Lyman-β	$1 \times 1 \times 2 \times 4 = 7$	10^{19}	5	$B = 0, 0.5, 2, 5$ kT
			Model: Same as above.		
11	Fe XXVI Lyman-α	$1 \times 3 \times 1 \times 4 = 12$	$10^{23}, 3 \times 10^{23}, 10^{24}$	2000	$B = 0, 5, 10, 20$ kT
			Model: deuterium plasma, fine structure included.		
12	Fe XXV He-β	$1 \times 3 \times 2 \times 1 = 6$	$10^{23}, 3 \times 10^{23}, 10^{24}$	2000	—
			Model: deuterium plasma, fine structure included. Two variants of calculations: only singlet states or singlets and triplets together. Assume LTE populations.		
13	Ar XVII $n = * \to 1$	$3 \times 1 \times 2 \times 1 = 6$	3×10^{22}, 10^{23}, 3×10^{23}	1000	—
			Model: Deuterium plasma, **two** variants: only bound–bound transitions included or both bound–bound and free–bound. Assume LTE populations.		

1 Statement of cases

We have selected a number of transitions to consider, given in Table 1. For each transition we are requesting results on a grid of electron densities (n_e) and temperatures ($T = T_e = T_i$). For each case, the atomic and plasma models are specified, and for some cases, there are more than one atomic or plasma model suggested. Unless specified otherwise, plasma is assumed quasi-neutral, consisting of electrons and a single type of ions.

Each calculation will be referenced by its subcase name. The subcase name is of the form Case_ID.N.T.M.F, where Case_ID is from the first column of Table 1, and the N, T, M, and F correspond, respectively, to the n_e, T, model, and external-field indices, each counting from 1.

The models suggested are limited – some by design, others by necessity, to make them manageable without too much computational resources and human time spent. If you feel that the best suggested model for a particular case is still too far from reality, you are encouraged to submit a separate result using an alternative model you see fit best, using "0" as the model index. Submissions of all such results should include an adequate description of the model used in the <comments> field of the file (see Sec. 4).

2 Justification of cases and details

The previous SLSP workshops ([1, 2, 3, 4] and references therein) have been a great success. We have covered a lot of interesting and physically sound spectral lines in a variety of plasma conditions.

The spread of results for some of the cases of SLSP1&2 demanded a deeper investigation, which was a focus at SLSP3. This detailed "debugging" followed at SLSP4 and will be continued now. The new topics, first introduced at SLSP4 (the quadrupole effects and influence of the magnetic field on the trajectories of plasma particles) will further be pursued.

2.1 Reference cases

The so called "reference" cases, involving simple atomic systems with many simplifying assumptions about the plasma environment, are the baseline of code comparisons. At the previous workshops, various H Lyman lines were considered. To introduce some novelty, this time the lines are hydrogen Balmer-α and Balmer-β. The "ideal" one-component plasma (OCP) model, extensively prescribed for many cases in the previous workshops, turned out [5] to be potentially problematic for computer simulations, as confirmed by specially crafted cases at SLSP3, due to a formally infinite Debye length. To avoid this issue, for this workhop an effective screening will be prescribed. This pseudo-ideal OCP (PIOCP) model assumes a set of *non-interacting* Debye pseudo particles with a fixed effective screening length $\bar{\lambda}$ to avoid the problem of very slow convergence of the impact width with the number of particles. Specifically, one should assume 100 particles in an effective Debye sphere, i.e.,

$$\frac{4\pi}{3} n \bar{\lambda}^3 = 100. \tag{1}$$

1. Hydrogen Balmer-α in an ideal plasma is a classical ion-dynamics test. We hope to observe convergence between simulations and analytical models...

2. Hydrogen Balmer-β. Similarly to the previous case, but now a line with no central component.

Compared to the previous workshops, we extended the density range from three to five orders of magnitude but reduced the temperature grid to two values to keep the total number of calculations similar.

2.2 Quadrupole corrections in H-like

Interest to quadrupole (in general, higher-than-dipole multipole) contributions to the Stark broadening has recently resurfaced [6], indicating an importance of these type of corrections. We focus on the non-linear Stark effects of hydrogen Balmer-β [7]. Furthermore, the plasma model remains the same as in the "reference" cases, with the parameters as a strict subset:
$n_e = 10^{18}$ & $10^{19}\,\mathrm{cm}^{-3}$, $T = 1$ & $10\,\mathrm{eV}$.

3. Balmer-β with dipole and quadrupole effects ($\Delta n = 0$).

The quadrupole and quadratic effects are believed to often be comparable. Thus, the following case, includes these corrections. For simplicity, we restrict the expansion of the basis sets to states with $n = 4$.

4. Balmer-β dipole Stark both linear and quadratic ($\Delta n \leq 1$).

Finally, the quadrupole and quadratic effects are calculated together.

5. Balmer-β with dipole and quadrupole effects ($\Delta n \leq 1$).

Please note that all cases below do NOT assume an ideal plasma, unless explicitly said so.

2.3 Isolated lines

$\Delta n = 0$ transitions in Li-like species present a puzzle by disagreement between experimental and different theoretical calculations [8]. For the first SLSP meeting, the Li-like 3s–3p isoelectronic sequence was considered, while for the second one, the 2s–2p resonance lines of the same sequence were calculated. At SLSP3&4, the study was continued with a deeper analysis of the 2s–2p series, asking to provide partial elastic and inelastic cross-sections [9]. We continue with the Li-like 3s–3p isoelectronic sequence [10], adding 3d states to the consideration. The quadrupole corrections, that were found to differ quite significantly between the codes, should be more pronounced with this addition.

For semiclassical models and simulations, these are to be calculated in the following way: The Lth partial wave contribution to the inelastic cross-section of transition from level i to level f ($i \neq f$) is, for a given energy E,

$$\sigma_{if}^{(L)}(E) = \frac{2\pi}{g_i} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho \sum_{m_i,m_f} |\langle J_i m_i | T(\rho, E) | J_f m_f \rangle|^2, \tag{2}$$

where g_i is the initial level degeneracy. T may be the S-matrix since the states are different and a square is taken. Different choices of R_{max} and R_{min} are discussed in [11]. A simple one that we adopt here is

$$R_{min}^{(L)} = L \frac{\hbar}{mv}, \tag{3}$$

$$R_{max}^{(L)} = (L+1) \frac{\hbar}{mv}, \tag{4}$$

where $v = \sqrt{2E/m}$. Now, we add calculation of the elastic contribution in the form of pseudo "cross-section" $\tilde{\sigma}$, defined as

$$\tilde{\sigma}_{if}^{(L)}(E) = \frac{2\pi}{g_i g_f} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho \sum_{m_i,m_f} |\langle J_i m_i | T(\rho, E) | J_i m_i \rangle - \langle J_f m_f | T(\rho, E) | J_f m_f \rangle|^2. \tag{5}$$

Furthermore, we are looking separately for contributions of so called "weak" and "strong" collisions. The relative "strongness" of a collision is defined based on breaking the perturbative unitarity,

$$\delta_{if}(\rho, E) = \frac{1}{g_i g_f} \left| \sum_{m_i,m_f} \left[\langle J_i m_i | S(\rho, E) | J_i m_i \rangle \langle J_f m_f | S(\rho, E) | J_f m_f \rangle - 1 \right] \right| \tag{6}$$

(e.g., see the unnumbered expression above Eq. (4-46) and arguments in [12]). To make correspondence to $\sigma_{if}^{(L)}(E)$, one should average Eq. (6) over the partial wave "rings", i.e.,

$$\delta_{if}^{(L)}(E) = \frac{2}{\left[R_{max}^{(L)}\right]^2 - \left[R_{min}^{(L)}\right]^2} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho \, \delta_{if}(\rho, E). \tag{7}$$

These $\sigma_{if}^{(L)}(E)$, $\tilde{\sigma}_{if}^{(L)}(E)$, and $\delta_{if}^{(L)}(E)$ should be provided at least for L's from 0 through 10 (please go up to 100, if possible). Each of the two species (below) is asked to be calculated for a single representative density. The plasma model for these cases consists only of electrons. Contrary to all other cases, here the electrons should be assumed to have a fixed energy (i.e., **not** a Maxwellian distribution). The width and shift (which are required, too) should also be calculated for the same fixed energy of the electrons. The energy values are listed in the "T" column of Table 1. Please also ignore the Debye screening, but if this is problematic for your calculations, assume screening corresponding to $T_e = E$.

6. Li I– the first, neutral, species in the sequence;

7. O VI

Each calculation will be done in two variants—only dipoles (as usual), or dipoles and quadrupoles together.

2.4 External fields

The external macro fields (both electric and magnetic) are always assumed to be parallel to the z axis.

2.4.1 B-induced trajectory effects

There are claims [13] about strong influence on Zeeman patterns through modifications of the electron trajectories ("spiraling") due to the magnetic field. We are going to test this phenomenon.

One-component electron plasma will be assumed for these cases. For non-zero magnetic field, three variants of its inclusion will be calculated: (i) the "standard" one, V_B is included in the radiator Hamiltonian, but no influence on the electron trajectories, (ii) only trajectories are affected, but no direct effect on the radiator, and (iii) "full" calculations. We repeat the case from SLSP4, hoping for more contributions this time. The magnetic field range is also extended to make the effect more prominent.

8. Lyman-α. Typical "white dwarf atmosphere" conditions: $n_e = 10^{17}\,\mathrm{cm}^{-3}$, $T = 5\,\mathrm{eV}$, $B = 0, 200, 500\,\mathrm{T}$.

2.4.2 Non-linear B

Check importance of the $\sim B^2$ term in the Hamiltonian.

The field goes to really high values here. To make the Stark broadening not negligible, the density is also increased. These conditions are also relevant for the WD atmospheres, perhaps to deeper/denser layers than in cases 8. We test the effect for Lyman-α and Lyman-β.

9. Lyman-α.
10. Lyman-β.

2.4.3 B-field effect in MagLIF

Typical MagLIF conditions: $n_e = 10^{23} - 10^{24}\,\mathrm{cm}^{-3}$, $T = 2\,\mathrm{keV}$, $B = 0, 5, 10, 20\,\mathrm{kT}$; deuterium plasma.

11. Fe XXVI Lyman-α.

2.5 MagLIF density diagnostics

Typical MagLIF conditions: $n_e = 10^{23} - 10^{24}\,\mathrm{cm}^{-3}$, $T = 2\,\mathrm{keV}$; deuterium plasma. Contrary to the Ar He-β considered at the first SLSP [14], we do not consider here Li-like satellites, restricting the complexity to the He-like ion.

12. Fe XXV He-β.

2.6 Ionization potential depression

Spectroscopy-wise, discrete transitions start to overlap between themselves and the free–bound continuum. The topic of discrete line merging and continuum lowering is of broad interest; it is also another area where applicability of the linear-Stark-effect approximation may be questioned; different approaches to this problem were considered at SLSP4 [15]. We now switch form the relatively low density and temperature cases to those typical for inertial fusion setups.

13. He-like Ar at $T = 1\,\mathrm{keV}$ and three densities from 3×10^{22} to $3 \times 10^{23}\,\mathrm{cm}^{-3}$. Assume deuterium plasma, LTE level populations, but please do **not** include the trivial $\exp(-\hbar\omega/T)$ factor in the spectrum output (this corresponds to the equal bound-state populations). The suggested spectral range (see Table 6) for this case covers transitions from He-β to continuum.

3 Atomic data

In all cases, we assume the dipole approximation both for the radiation ($E1$) and the perturbation due to the plasma micro-fields. The relevant matrix elements are

$$\langle \alpha j m | r_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 1 & j' \\ -m & q & m' \end{pmatrix} (\alpha j | r | \alpha' j')\,, q = 0, \pm 1\,. \tag{8}$$

The reduced radius-vector matrix elements $(\alpha j | r | \alpha' j')$, relevant for the cases considered, are given below. For some cases, quadrupole interaction is also considered. Then similarly, the quadrupole matrix elements are

$$\langle \alpha j m | Q_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 2 & j' \\ -m & q & m' \end{pmatrix} (\alpha j | Q | \alpha' j')\,, q = 0, \pm 1, \pm 2\,. \tag{9}$$

3.1 Hydrogen-like

For hydrogen ($Z = 1$) and hydrogen-like cases, the data are to be calculated analytically. For cases where the fine structure is neglected, the binding energies to be assumed are (in atomic units, $1\,\mathrm{hartree} \approx 27.211\,\mathrm{eV}$, corresponding to $\approx 2.1947 \times 10^5\,\mathrm{cm}^{-1}$)

$$E_n^0 = -\frac{Z^2}{2n^2}\,. \tag{10}$$

Table 2: Hydrogen reduced matrix elements up to $n = 5$. Note that in the SLSP4 version, the $\Delta n \neq 0$ signs were flipped!

	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f
2p	1.29	-5.20												
3s			-0.938											
3p	0.517	3.06		-12.7										
3d			6.71		-14.2									
4s			-0.382		-2.44									
4p	0.305	1.28		5.47		-1.84	-23.2							
4d			2.418		10.7			-29.4						
4f						17.7			-27.5					
5s			-0.228		-0.970			-4.60						
5p	0.209	0.774		2.26		-0.683	8.52		-4.31		-36.7			
5d			1.38		4.20			15.6		-2.88		-48.6		
5f						5.75			24.4				-52.0	
5g										35.4				-45.0

When the fine structure is asked to be accounted for, the energies are

$$E_{nj} = E_n^0 - \frac{\alpha^2 Z^4}{2n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right), \tag{11}$$

where $\alpha \approx 7.2974 \times 10^{-3}$ is the fine-structure constant.

Reduced matrix elements of radius-vector are

$$(n\ell|r|n'\ell') = (-1)^{\ell+\ell_>}\sqrt{\ell_>}R_{n\ell}^{n'\ell'}, \tag{12}$$

where $\ell_> = \max(\ell, \ell')$ and

$$R_{n\ell}^{n\ell-1} = -\frac{3}{2Z}n\sqrt{n^2-\ell^2} \tag{13}$$

for diagonal terms (e.g., Eq. (63.5) in [16], but notice the wrong sign there!) and

$$R_{n\ell}^{n'\ell-1} = Z^{-1}\frac{(-1)^{n'-\ell}}{4(2\ell-1)!}\sqrt{\frac{(n+\ell)!(n'+\ell-1)!}{(n-\ell-1)!(n'-\ell)!}}\frac{(4nn')^{\ell+1}(n-n')^{n+n'-2\ell-2}}{(n+n')^{n+n'}} \times$$
$$\left\{F_{21}\left(-n_r, -n_r', 2\ell, -\frac{4nn'}{(n-n')^2}\right) - \left(\frac{n-n'}{n+n'}\right)^2 F_{21}\left(-n_r-2, -n_r', 2\ell, -\frac{4nn'}{(n-n')^2}\right)\right\} \tag{14}$$

for off-diagonal ones (Eq. (63.2) in [16]). Here, F_{21} is the Gauss hypergeometric function and $n_r = n - \ell - 1$, $n_r' = n' - \ell$ are the radial quantum numbers of the two states. For convenience, the reduced matrix elements up to $n = 5$ are given in Table 2.

The reduced matrix elements of the quadrupole operator are

$$(n\ell|Q|n'\ell') = (-1)^\ell\sqrt{(2\ell+1)(2\ell'+1)}\begin{pmatrix}\ell & 2 & \ell' \\ 0 & 0 & 0\end{pmatrix}{}^{(2)}R_{n\ell}^{n'\ell'}. \tag{15}$$

For $n = n'$, ${}^{(2)}R_{n\ell}^{n\ell'}$ can be derived using recurrent relations [17]:

$${}^{(2)}R_{n\ell}^{n\ell} = \frac{n^2}{2Z^2}\left[5n^2 + 1 - 3\ell(\ell+1)\right] \tag{16}$$

and

$${}^{(2)}R_{n,\ell\pm2}^{n\ell} = \frac{5n^2}{2Z^2}\sqrt{(n^2-\ell_>^2)\left[n^2-(\ell_>-1)^2\right]}. \tag{17}$$

3.2 Non-hydrogen

The data are taken from the NIST on-line compilation [18]. The level energies, averaged over the fine-structure components for $\ell > 0$, are given in Table 3. The absolute values of the matrix elements are obtained from the respective multiplet-averaged absorption oscillator strengths f according to

$$|(n\ell|r|n'\ell')| = \sqrt{\frac{3f(2\ell'+1)}{2(E_{n\ell} - E_{n'\ell'})}}, \tag{18}$$

Table 3: Atomic level energies for non-hydrogenic lines.

Species	Level	Energy (cm^{-1})
Li I	3s	27206.12
	3p	30925.38
	3d	31283.10
O VI	3s	640039.80
	3p	666217.60
	3d	674656.36

Table 4: Oscillator strengths for non-hydrogenic lines.

Species	Transition	f
Li I	3s — 3p	1.21e+00
	3p — 3d	7.41e-02
O VI	3s — 3p	3.35e-01
	3p — 3d	4.87e-02

and sign as in respective H-like from Eqs. (12 – 14). The data are summarized in Table 4.

The quadrupole reduced matrix elements, needed for cases 6.*.*.2.1 and 7.*.*.2.1 are given in Table 5. These data were calculated with the R. D. Cowan's code [19].

Table 5: Quadrupole reduced radial matrix elements for non-hydrogenic species.

Species	Transition	$(\|Q\|)$
Li I	3p — 3p	-188
	3s — 3d	$+120$
	3d — 3d	-151
O VI	3p — 3p	-5.26
	3s — 3d	$+3.87$
	3d — 3d	-4.18

4 Submission format

We use an XML-based format for submissions, with an example shown schematically in Listing 1.

Everything is included between the <slsp> and </slsp> tags. The meaning of other tags is described below:

<case> The subcase identification in the Case_ID.N.T.M.F format, see Sec. 1.

<contributor> The person who submits these results.

<affiliation> His/her affiliation.

<code> Name of the code/approach.

<version> Version of the code (optional).

<date> Date/time when the calculations were made.

<comments> Any comments you may like to make. The comments are optional, **except for advanced models (M=0 in the subcase id) and fitting experimental data)**. In the later cases, please describe the model employed with sufficient details. If the comments must contain "<" or "&" characters, enclose the entire text with "<![CDATA[" and "]]>":

```
<comments><![CDATA[
  Some bizarre & < > comments.
]]></comments>
```

Listing 1: An example of submission.

```
<?xml version="1.0"?>
<slsp>
  <case>1.1.1.3.1</case>
  <contributor>E. Stambulchik</contributor>
  <affiliation>WIS</affiliation>
  <code>simu</code>
  <version>1.9.0/1.4.0</version>
  <date>2011-12-13 18:34:39</date>

  <comments>
     These are my comments on this calculation.
   </comments>

  <time1>6.826e-11</time1>
  <nruns>400</nruns>

  <accuracy>-10 +5</accuracy>

  <field_distribution unit="128196">
    0.000000 0.000000
    0.025000 0.000421
    0.075000 0.002919
     ...
     ...
    29.875000 0.000333
    29.925000 0.000324
    29.975000 0.000316
   </field_distribution>

  <spectrum unit="1">
    -200.0 0.000741852
    -199.8 0.000751194
    -199.6 0.000747932
     ...
     ...
    199.6 0.000738701
    199.8 0.000752916
    200.0 0.000735306
   </spectrum>
</slsp>
```

<time1> Physical time (not CPU!), in seconds, the evolution of the atomic system is calculated for in a single run. (This and the following entry are specific for MD simulations. When irrelevant, skip or set to zero.)

<nruns> Number of runs used for averaging.

<accuracy> The estimated accuracy (in %) of the calculations, say of the FWHM. Only uncertainties introduced by the calculations should be included (in particular, not those due to an idealized/simplified plasma or atomic models suggested for this specific case). If the error bars are asymmetric, list two numbers with proper signs.

<spectrum> For all cases **except those concerned with isolated lines (6 – 7)**, we ask to provide entire line shapes on a reasonably dense grid, typically ~ 1000 points (see Table 6). When the spectral range is symmetric ($\pm$ something), it means relative to the unperturbed position ω_0, calculated as a difference between the weighted-average energies of the initial and final levels:

$$\hbar\omega_0 = \frac{\sum_i g_i E_i}{\sum_i g_i} - \frac{\sum_f g_f E_f}{\sum_f g_f}\,. \tag{19}$$

The spectral windows and distances between the consecutive abscissas defined are recommended values. The relatively wide spectral windows are defined on purpose, to investigate far wings of the spectral lines. You can use denser and/or wider grids as you see fit. It is suggested to use equidistant grids. The units are cm^{-1}. The optional `unit` attribute allows for scaling the abscissas, e.g., by using `unit="8065.5"` one can output spectra in eV's. Where the spectra are requested and external fields specified the π ($\Delta M = 0$) and σ ($\Delta M = \pm 1$) polarizations will be needed separately (to be provided as the second and third columns, respectively):

```
...
...
<spectrum>
  w_1  I_pi(w_1)  I_sigma(w_1)
  w_2  I_pi(w_2)  I_sigma(w_2)
   ...
   ...
  w_N  I_pi(w_N)  I_sigma(w_N)
</spectrum>
...
...
```

It is assumed that

$$I_{\mathrm{tot}}(\omega) = I_\pi(\omega) + 2I_\sigma(\omega)\,. \tag{20}$$

In all cases, no normalization condition is imposed, but do preserve correct ratio between I_π and I_σ.

<field_distribution> Quasi-static field distribution (normalized) used for the calculation (due to all plasma particles, but excluding external fields, if any). The fields are in V/cm. The optional `unit` attribute allows for scaling the field strength values conveniently, e.g., by setting it to the Holtsmark normal field strength F_0 one obtains the distribution of the reduced field strengths. The distributions should be calculated on an equidistant grid covering at least $0 - 10$ with a step not exceeding 0.1 (in units of F_0).

<width> FWHM, **for isolated lines only (cases 6 and 7)**. In units of cm^{-1}.

<shift> Shift, for the same cases. In units of cm^{-1}.

<partial_xs> Partial cross-sections; these are also specific to the 6 and 7 cases. The format is

```
...
...
<partial_xs>
  L_1  sigma_e(L_1)  sigma_d(L_1)  sigma_el(L_1)  delta(L_1)
  L_2  sigma_e(L_2)  sigma_d(L_2)  sigma_el(L_2)  delta(L_2)
   ...
   ...
  L_N  sigma_e(L_N)  sigma_d(L_N)  sigma_el(L_N)  delta(L_N)
</partial_xs>
...
...
```

Table 6: Recommended spectral grids.

Subcase	Spectral range (cm^{-1})	Step (cm^{-1})
1.1.*.*.*	± 20	0.02
1.2.*.*.*	± 100	0.1
1.3.*.*.*	± 500	0.5
1.4.*.*.*	± 2000	2
1.5.*.*.*	± 10000	10
2.1.*.*.*	± 20	0.02
2.2.*.*.*	± 100	0.1
2.3.*.*.*	± 500	0.5
2.4.*.*.*	± 2000	2
2.5.*.*.*	± 10000	10
2.6.*.*.*	± 50000	50
3.1.*.*.*	± 10000	10
3.2.*.*.*	± 50000	50
4.1.*.*.*	± 10000	10
4.2.*.*.*	± 50000	50
5.1.*.*.*	± 10000	10
5.2.*.*.*	± 50000	50
6.*.*.*.*	± 200	0.5
7.*.*.*.*	± 50	0.1
8.*.*.*.*	± 300	0.2
9.*.*.*.*	± 5000	10
10.*.*.*.*	± 10000	100
11.*.*.*.*	$\pm 2.5 \times 10^5$	250
12.1.*.*.*	$\pm 2 \times 10^5$	1000
12.2.*.*.*	$\pm 5 \times 10^5$	2500
12.3.*.*.*	$\pm 10^6$	5000
13.*.*.*.*	$(2.5 - 3.5) \times 10^7$	2000

For each L, partial excitation and de-excitation (for the same *incident* energy) cross-sections should be listed in the second and third columns, respectively [see Eq. (2) for semiclassical calculations and simulations]. The fourth column is the elastic "cross-section", Eq. (5). The units are cm^2. Finally, the last column is the measure indicating how "strong" collisions of the given partial wave are, Eq. (7).

References

[1] E. Stambulchik. Review of the 1st Spectral Line Shapes in Plasmas code comparison workshop. *High Energy Density Phys.*, 9(3):528–534, 2013. doi:10.1016/j.hedp.2013.05.003.

[2] E. Stambulchik, A. Calisti, H.-K. Chung, and M. Á González. Special issue on Spectral Line Shapes in Plasmas. *Atoms*, 2(3):378–381, August 2014. doi:10.3390/atoms2030378.

[3] J. Rosato. Report on the third SLSP code comparison workshop. *High Energy Density Phys.*, 22:60–63, March 2017. doi:10.1016/j.hedp.2017.02.011.

[4] E. Stambulchik, A. Calisti, H.-K. Chung, and M. Á. González. Spectral Line Shapes in Plasmas II. *Atoms*, 7(1):20, February 2019. doi:10.3390/atoms7010020.

[5] J. Rosato, H. Capes, and R. Stamm. Ideal Coulomb plasma approximation in line shape models: Problematic issues. *Atoms*, 2(2):253–258, 2014. doi:10.3390/atoms2020253.

[6] A. V. Demura. Beyond the linear Stark effect: A retrospective. *Atoms*, 6(2):33, June 2018. doi:10.3390/atoms6020033.

[7] T. A. Gomez, T. Nagayama, D. P. Kilcrease, M. H. Montgomery, and D. E. Winget. Effect of higher-order multipole moments on the Stark line shape. *Phys. Rev. A*, 94(2):022501, 2016. doi:10.1103/PhysRevA.94.022501.

[8] H. R. Griem and Yu. V. Ralchenko. Electron collisional broadening of isolated lines from multiply-ionized atoms. *J. Quant. Spectr. Rad. Transfer*, 65(1-3):287–296, 2000. doi:10.1016/S0022-4073(99)00074-6.

[9] S. Sahal-Bréchot, E. Stambulchik, M. S. Dimitrijević, S. Alexiou, B. Duan, and N. Bonifaci. The Third and Fourth Workshops on Spectral Line Shapes in Plasma Code Comparison: Isolated lines. *Atoms*, 6(2):30, May 2018. doi:10.3390/atoms6020030.

[10] Yu. V. Ralchenko, H. R. Griem, and I. Bray. Electron-impact broadening of the 3s-3p lines in low-Z Li-like ions. *J. Quant. Spectrosc. Radiat. Transfer*, 81:371–384, 2003. doi:10.1016/S0022-4073(03)00088-8.

[11] S. Alexiou, R. W. Lee, S. H. Glenzer, and J. I. Castor. Analysis of discrepancies between quantal and semiclassical calculations of electron impact broadening in plasmas. *J. Quant. Spectrosc. Radiat. Transfer*, 65(1–3):15–22, 2000. doi:10.1016/S0022-4073(99)00051-5.

[12] H. R. Griem. *Plasma spectroscopy*. McGraw-Hill Book Company, New York, 1964.

[13] E. Oks. Influence of magnetic-field-caused modifications of trajectories of plasma electrons on spectral line shapes: Applications to magnetic fusion and white dwarfs. *J. Quant. Spectrosc. Radiat. Transfer*, 171:15–27, 2016. doi:10.1016/j.jqsrt.2015.10.026.

[14] R. C. Mancini, C. A. Iglesias, S. Ferri, A. Calisti, and R. Florido. The effect of improved satellite line shapes on the argon Heβ spectral feature. *High Energy Density Phys.*, 9(4):731–736, 2013. doi:http://dx.doi.org/10.1016/j.hedp.2013.08.002.

[15] S. Alexiou, E. Stambulchik, T. Gomez, and M. Koubiti. The Fourth Workshop on Lineshape Code Comparison: Line merging. *Atoms*, 6(2):13, March 2018. doi:10.3390/atoms6020013.

[16] H. A. Bethe and E. E. Salpeter. *Quantum Mechanics of One- and Two-Electron Atoms*. Plenum, New York, 1977.

[17] J. D. Hey. On the determination of radial matrix elements for high-n transitions in hydrogenic atoms and ions. *J. Phys. B: At. Mol. Opt. Phys.*, 39(12):2641, 2006. doi:10.1088/0953-4075/39/12/003.

[18] NIST Atomic Spectra Database. http://www.nist.gov/pml/data/asd.cfm. URL: http://www.nist.gov/pml/data/asd.cfm.

[19] R. D. Cowan. *The Theory of Atomic Structure and Spectra*. University of California Press, Berkeley – Los Angeles – London, 1981.