



6th Spectral Line Shapes in Plasmas Code Comparison Workshop

October 17–21, 2022

Hyères, France

Call for Submissions (rev. September 18, 2022)

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/slsp6/>. 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 (2022):

August 28	—	web interface for file uploads opens
August 31	—	hotel pre-booking deadline
October 02	—	submission deadline
October 17	—	workshop opens
October 21	—	workshop adjourns

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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.

2 Justification of cases and details

The previous five 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 new topics to be pursued at SLSP6 are full Coulomb interactions, penetrating collisions, radiation frequency redistribution, and Feshbach resonances.

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 and Balmer lines were considered. However, some phenomena (including those considered in the cases below) are absent in neutral radiators. Therefore, singly-ionized hydrogenlike He II lines are added this time.

The “ideal” one-component plasma (OCP) model, extensively used for many cases in the previous workshops, turned out [5] to be potentially problematic for computer simulations. To avoid this issue, in SLSP5 a pseudo-ideal OCP (PIOCP) model was introduced assuming a set of *non-interacting* Debye pseudo particles with a *prescribed* effective screening length $\bar{\lambda}$. For this workshop, this approach will also be used. **Specifically, one should assume 100 particles of each type in an effective Debye sphere, i.e.,**

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

1. Hydrogen Balmer- α in an ideal plasma is a classical ion-dynamics test.
2. Hydrogen Balmer- β . Similarly to the previous case, but now a line with no central component.
3. H-like helium Paschen- α .
4. H-like helium Paschen- β .

2.2 Full Coulomb interaction

Interest to non-dipole contributions to the Stark broadening has recently resurfaced [6], indicating an importance of these type of corrections, with the quadrupole interactions investigated for hydrogen at SLSP5. More generally, calculations entirely avoiding the “standard” multipole expansion were introduced long ago [7], with a few studies published this year [8, 9].

5. H Balmer- β . Quite an obvious choice.
6. He II Paschen- α . The line was analyzed in depth at SLSP3, but the discrepancy between the theory and experiment was not resolved [10].

The plasma model remains the same as in the “reference” cases, with the parameters as a strict subset.

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	$5 \times 2 \times 3 \times 1 = 30$	$10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18}$	1, 10	—
					Model: Same as above.
3	He II Paschen- α	$3 \times 2 \times 3 \times 1 = 18$	$10^{17}, 10^{18}, 10^{19}$	1, 10	—
					Model: $\Delta n \neq 0$ dipole interactions ignored (strictly linear Stark effect); no fine structure; plasma model in three variants: only electrons, only ions (singly-ionized He), and electrons and ions together.
4	He II Paschen- β	$3 \times 2 \times 3 \times 1 = 18$	$10^{16}, 10^{17}, 10^{18}$	1, 10	—
					Model: Same as above.
5	H Balmer- β	$2 \times 2 \times 4 \times 1 = 16$	$10^{17}, 10^{18}$	1, 10	—
					Model: no $\Delta n \neq 0$ interactions, no fine structure. Four variants: “standard” dipole approximation, “standard” dipole and quadrupole, dipole with penetration effects, and full interaction. Plasma as in the 3rd variant of case 1.
6	He II Paschen- α	$2 \times 2 \times 4 \times 1 = 16$	$10^{18}, 10^{19}$	1, 10	—
					Model: Same as above.
7	H Lyman- α	$1 \times 1 \times 1 \times 6 = 6$	10^{14}	1	$B = 0, 2$ T; detuning = $0, 0.5, 1$ cm ⁻¹
					Model: no $\Delta n \neq 0$ interactions, no fine structure.
8	H Balmer- α	$1 \times 1 \times 1 \times 6 = 6$	10^{17}	1	$B = 0, 100$ T; detuning = $0, 50, 100$ cm ⁻¹
					Model: Same as above.
9	H Lyman- α	$2 \times 2 \times 1 \times 4 = 16$	$10^{16}, 10^{17}$	1, 10	$F = 0, F_0, 3F_0, 10F_0$
					Model: Same as above.
10	H Lyman- β	$2 \times 2 \times 1 \times 4 = 16$	$10^{16}, 10^{17}$	1, 10	$F = 0, F_0, 3F_0, 10F_0$
					Model: Same as above.
11	H Balmer- α	$2 \times 2 \times 1 \times 4 = 16$	$10^{16}, 10^{17}$	1, 10	$F = 0, F_0, 3F_0, 10F_0$
					Model: Same as above.
12	H Balmer- β	$2 \times 2 \times 1 \times 4 = 16$	$10^{16}, 10^{17}$	1, 10	$F = 0, F_0, 3F_0, 10F_0$
					Model: Same as above.
13	Li I 2s-2p	$1 \times 3 \times 2 \times 1 = 6$	10^{17}	5, 15, 50	—
					Model: 2s and 2p levels included, no fine structure. Only electron broadening included. Two variants: “standard” dipole approximation and that with the penetrating collisions included.
14	B III 2s-2p	$1 \times 3 \times 3 \times 1 = 9$	10^{18}	5, 15, 50	—
					Model: Same as above plus the variant with the Feshbach resonances accounted for.
15	N V 2s-2p	$1 \times 3 \times 3 \times 1 = 9$	10^{19}	5, 15, 50	—
					Model: Same as above.
16a	Kr XXXV He- β	$3 \times 1 \times 1 \times 1 = 3$	$10^{24}, 3 \times 10^{24}, 10^{25}$	3000	—
					Model: plasma ions are deuterons. Atomic model: all (singlet and triplet) $n = 3$ states.
16b	Kr XXXIV He- β^* $n = 2$	$3 \times 1 \times 1 \times 1 = 3$	$10^{24}, 3 \times 10^{24}, 10^{25}$	3000	—
16c	Kr XXXIV He- β^* $n = 3$	$3 \times 1 \times 1 \times 1 = 3$	$10^{24}, 3 \times 10^{24}, 10^{25}$	3000	—
16d	Kr XXXIV He- β^* $n = 4$	$3 \times 1 \times 1 \times 1 = 3$	$10^{24}, 3 \times 10^{24}, 10^{25}$	3000	—
					Plasma model: Same as above.
17	H Balmer series	1	*	*	*
					Model: Do your best!

2.3 Radiation redistribution

Radiation scattering in plasma is described by the redistribution function $R(\omega, \vec{n}, \omega', \vec{n}')$ (e.g., see [11] and references therein). However, for consistency with the submission format of other cases, only the resulting re-emitted spectra will be analyzed, with the incoming radiation (and, as always, plasma parameters) prescribed.

7. Lyman- α in a magnetic-fusion divertor plasma;
8. Balmer- α in a white-dwarf atmosphere.

Each line is calculated without magnetic field and for a given (in Table 1) B -field value. With the detuning from the line center assuming three possible values, there are six variants in total for each case. Assume the magnetic field and the polarization vector of the incoming photon to be along the z and x axis, respectively.

2.4 Periodic electric fields

We investigate a simultaneous effect of the plasma microfields and an external harmonic field in the form of $\vec{F} \cos(\omega t + \phi)$, where the phase ϕ is assumed random for different radiators (but not changing within the light train formation time for a given radiator) (e.g., see [12]). \vec{F} should be assumed to lie in the z direction, while F , in units of the Holtsmark field F_0 , is given in Table 1. Assume $\omega = \omega_{pe}$ in each case.

9. Lyman- α
10. Lyman- β
11. Balmer- α
12. Balmer- β

2.5 Isolated lines

$\Delta n = 0$ transitions in Li-like species present a puzzle by disagreement between experimental and different theoretical calculations [13]. In the second SLSP meeting, the 2s–2p resonance lines of the Li-like sequence were considered. We continue investigating these lines, this time adding to the consideration penetration effects and Feshbach resonances.

Each of the three species (below) is asked to be calculated for a single representative density and three values of the temperature. Both widths (FWHM) **and** shifts are requested.

13. Li I – the first, neutral, species in the sequence;
14. B III – one that ignited a long discussion some time ago;
15. N V – with higher yet Z to check the Z -dependence.

Each line is calculated in three variants: the “standard” dipole (no advanced effects), with the penetration effects included, and with the Feshbach accounted for (except for the neutral Li I, of course). There is no need to included the two effects together, as these are believed to be largely additive.

2.6 Satellite broadening

Satellites from the previous charge state with a spectator electron. A similar case was present in SLSP1 (Ar XVII He- β). He- β lines continue to be used as the density diagnostics in ICF experiments, shifting to higher- Z species as the densities go up. For example, see a recent study [14].

16. Kr XXXV He- β and its Li-like satellites.

Case 16a corresponds to Kr XXXV He- β proper, and 16b,c,d to its Kr XXXIV $n = 2$, $n = 3$, and $n = 4$ spectator satellites, respectively.

- 16a — Kr XXXV He- β . Upper configurations: $1s3s$, $1s3p$, and $1s3d$; lower configurations: $1s^2$.
- 16b — Kr XXXIV satellite transitions with spectator electron in $n = 2$. Upper configurations: $1s2s3s$, $1s2s3p$, $1s2s3d$, $1s2p3s$, $1s2p3p$, and $1s2p3d$; lower configurations: $1s^22s$, and $1s^22p$.

- 16c — Kr XXXIV satellite transitions with spectator electron in $n = 3$. Upper configurations: $1s3s^2$, $1s3s3p$, $1s3s3d$, $1s3p^2$, $1s3p3d$, and $1s3d^2$; lower configurations: $1s^23s$, $1s^23p$, and $1s^23d$.
- 16d — Kr XXXIV satellite transitions with spectator electron in $n = 4$. Upper configurations: $1s3s4s$, $1s3p4s$, $1s3d4s$, $1s3s4p$, $1s3p4p$, $1s3d4p$, $1s3s4d$, $1s3p4d$, $1s3d4d$, $1s3s4f$, $1s3p4f$, and $1s3d4f$; lower configurations: $1s^24s$, $1s^24p$, $1s^24d$ and $1s^24f$.

Assume an equilibrium (i.e., LTE) distribution of population within the initial (upper) energy levels of the transitions within a given line shape.

2.7 Modeling experimental data

A bit unusual this time, we consider astrophysical “experimental” data. Specifically, hydrogen spectra from white dwarfs with a significant magnetic field. The challenge, thus, is to model the combined Stark+Zeeman effect and infer the plasma density and temperature as well as the magnetic field magnitude.

17. Hydrogen Balmer series. Spectrum of the white dwarf SDSS J124851.31-022924.73.

Original data, in units of Å and \propto W/cm²/Å: [SDSS-J124851.31-022924.73.csv](#)

Same in units of cm⁻¹ and \propto W/cm²/cm⁻¹: [SDSS-J124851.31-022924.73.dat](#)

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

$$\langle \alpha j m | r_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 1 & j' \\ -m & q & m' \end{pmatrix} \langle \alpha j | r | \alpha' j' \rangle, q = 0, \pm 1. \quad (2)$$

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

$$\langle \alpha j m | Q_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 2 & j' \\ -m & q & m' \end{pmatrix} \langle \alpha j | Q | \alpha' j' \rangle, q = 0, \pm 1, \pm 2. \quad (3)$$

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 hartree ≈ 27.211 eV, corresponding to $\approx 2.1947 \times 10^5$ cm⁻¹)

$$E_n^0 = -\frac{Z^2}{2n^2}. \quad (4)$$

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

$$E_{nj} = E_n^0 - \frac{\alpha^2 Z^4}{2n^3} \left(\frac{1}{j+1/2} - \frac{3}{4n} \right), \quad (5)$$

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

Reduced matrix elements of radius-vector are

$$(n\ell | r | n'\ell') = (-1)^{\ell+\ell'} \sqrt{\ell_{>}} R_{n\ell}^{n'\ell'}, \quad (6)$$

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

$$R_{n\ell}^{n'\ell-1} = -\frac{3}{2Z} n \sqrt{n^2 - \ell^2} \quad (7)$$

for diagonal terms (e.g., Eq. (63.5) in [15], but notice the wrong sign there!) and

$$\left\{ F_{21}^{n'\ell-1} = Z^{-1} \frac{(-1)^{n'-\ell}}{4(2\ell-1)!} \sqrt{\frac{(n+\ell)!(n'+\ell-1)!}{(n-\ell-1)!(n'-\ell)!}} \frac{(4nn')^{\ell+1} (n-n')^{n+n'-2\ell-2}}{(n+n')^{n+n'}} \times \right. \\ \left. \left\{ F_{21} \left(-n_r, -n'_r, 2\ell, -\frac{4nn'}{(n-n')^2} \right) - \left(\frac{n-n'}{n+n'} \right)^2 F_{21} \left(-n_r - 2, -n'_r, 2\ell, -\frac{4nn'}{(n-n')^2} \right) \right\} \right\} \quad (8)$$

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

for off-diagonal ones (Eq. (63.2) in [15]). 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

$$(n\ell|Q|n'\ell') = (-1)^\ell \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} ({}^2)R_{n\ell}^{n'\ell'}. \quad (9)$$

For $n = n'$, $({}^2)R_{n\ell}^{n\ell'}$ can be derived using recurrent relations [16]:

$$({}^2)R_{n\ell}^{n\ell} = \frac{n^2}{2Z^2} [5n^2 + 1 - 3\ell(\ell+1)] \quad (10)$$

and

$$({}^2)R_{n,\ell\pm 2}^{n\ell} = \frac{5n^2}{2Z^2} \sqrt{(n^2 - \ell_{>}^2) [n^2 - (\ell_{>} - 1)^2]}. \quad (11)$$

3.2 Isolated lines

The data are taken from the NIST on-line compilation [17]. 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

$$|(n\ell|r|n'\ell')| = \sqrt{\frac{3f(2\ell'+1)}{2(E_{n\ell} - E_{n'\ell'})}}, \quad (12)$$

and sign as in respective H-like from Eqs. (6) – (8). The data are summarized in Table 4.

Table 3: Atomic level energies for isolated lines.

Species	Level	Energy (cm ⁻¹)
Li I	2s	0.00
	2p	14903.89
B III	2s	0.00
	2p	48381.07
N V	2s	0.00
	2p	80635.67

3.3 Data for case 16

The data for cases 16a–d, calculated with the cFAC code [18], can be downloaded from [this link](#).

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>
```

Table 4: Oscillator strengths for non-hydrogenic lines.

Species	Transition	f
Li I	2s — 2p	7.472e-1
B III	2s — 2p	3.629e-01
N V	2s — 2p	2.34e-01

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>
```

`<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 (13 – 15)**, we ask to provide entire line shapes on a reasonably dense grid, typically ~ 1000 points (see Table 5). 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:

$$\hbar\omega_0 = \frac{\sum_i g_i E_i}{\sum_i g_i} - \frac{\sum_f g_f E_f}{\sum_f g_f}. \quad (13)$$

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

$$I_{\text{tot}}(\omega) = I_{\pi}(\omega) + 2I_{\sigma}(\omega). \quad (14)$$

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 Holtmark 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 13, 14, and 15). In units of cm^{-1} .

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

References

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Table 5: 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
3.1.*.*	±100	0.1
3.2.*.*	±500	0.5
3.3.*.*	±2000	2
4.1.*.*	±250	0.25
4.2.*.*	±1000	1
4.3.*.*	±5000	5
5.1.*.*	±2000	2
5.2.*.*	±10000	10
6.1.*.*	±500	0.5
6.2.*.*	±2000	2
7.1.*.*	±5	0.005
8.1.*.*	±100	0.1
9.1.*.*	±100	0.1
9.2.*.*	±300	0.3
10.1.*.*	±200	0.2
10.2.*.*	±1000	1
11.1.*.*	±100	0.1
11.2.*.*	±300	0.3
12.1.*.*	±300	0.3
12.2.*.*	±2000	2
16.1.*.*	±1e6	5000
16.2.*.*	±1.5e6	1e4
16.3.*.*	±3e6	2e4
17.1.*.*	14000–26000	10

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