



2nd Spectral Line Shapes in Plasmas Code Comparison Workshop

August 5–9, 2013

Vienna, Austria

Call for Submissions (rev. July 8, 2013)

Introduction

This document is intended to define 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/slsp2/>. 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:

- June 3 — web interface for file uploads opens
- July 13 — **submission deadline (cases 11* and 12*)**
- July 20 — **submission deadline (other cases)**
- July 20 — **hotel booking deadline**
- August 5 — workshop opens
- August 9 — 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. For example, the plasma model in Case 4 is described as “Plasma ions: protons”, meaning the plasma consists of electrons and protons of an equal density.) In addition, some cases are further detailed by specifying extra parameters, such as the magnetic field. Therefore, subcases for each case are defined on a four-dimensional grid.

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. For example, 1.2.3.1.1 identifies H Lyman- α , calculated for $n_e = 10^{18} \text{ cm}^{-3}$ and $T = 100 \text{ eV}$, assuming only electrons as perturbers. Similarly, 8.2.1.1.3 stands for Al XIII Lyman- α in a plasma with $n_e = 10^{22} \text{ cm}^{-3}$ and $T = 500 \text{ eV}$ in the presence of harmonic electric field with an amplitude of 2 GV/cm, calculated neglecting the fine structure.

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. E.g., 3.1.1.0.1 would designate the He II $n = 4 \rightarrow 3$ transition calculated for $n_e = 5 \times 10^{18} \text{ cm}^{-3}$ and $T = 5 \text{ eV}$ including, say, all discrete levels up to $n = \infty$. 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

2.1 Reference cases

These cases are not necessarily realistic, but good for basic comparison and understanding what is wrong/different if there is a significant scatter in the results of more advanced cases below. There are quite a few sub-cases, however the models are simplest: ideal plasma (straight path trajectories and infinite Debye length for MD, or Holtsmark distribution for analytical approaches) and pure linear Stark effect (interactions between states with $\Delta n \neq 0$ ignored and no fine structure). In order to assess influence of electrons and ions (protons), we ask to calculate the broadening assuming e and p acting separately and together, i.e., three variants in total for each pair of n_e and T .

1. Hydrogen Lyman- α in an ideal plasma is a classical ion-dynamics test. This is an identical case from SLSP1. Due to an unexpectedly large scatter of results [1] we decided to repeat it again.
2. Hydrogen Lyman- β . Similarly to the previous case, but now a line with no central component.

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

2.2 n - α transitions

A representative of $n, n' \gg 1, \Delta n \ll n$ class of transitions. Radio-frequency lines which are of great interest for astrophysics belong to it. We do not want to go to really high n , however, due to the computational costs. Nevertheless, we shall deal with the coupling between states with $\Delta n \neq 0$. This set of cases continues the similar work from SLSP1 by adding Paschen- α line and extending number of states included.

3. Hydrogen-like He II $n = 4 \rightarrow n = 3$ (Paschen- α) transition. We ask to calculate this case using four atomic models: (i) no $\Delta n \neq 0$ coupling accounted for, (ii) $n = 3$ and $n = 4$ states couple, (iii) $n = 3, 4$, and 5 states included in the Hamiltonian and allowed to mix, and (iv) also $n = 6$ added.
4. Hydrogen $n = 6 \rightarrow n = 5$ transition. Similar to the above, four atomic models: (i) no $\Delta n \neq 0$ coupling accounted for, (ii) $n = 5$ and $n = 6$ states couple, (iii) $n = 5, 6$, and 7 states couple, and (iv) $n = 5 - 8$.

Table 1: Case definitions.

ID	Transition(s)	# of subcases	n_e (cm ⁻³)	T (eV)	Extra parameters
1	H Lyman- α	$3 \times 3 \times 3 \times 1 = 27$	$10^{17}, 10^{18}, 10^{19}$	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- β	$3 \times 3 \times 3 \times 1 = 27$	$10^{17}, 10^{18}, 10^{19}$	1, 10, 100	—
			Model: Same as above.		
3	He II $n = 4 \rightarrow 3$	$1 \times 2 \times 4 \times 1 = 8$	5×10^{18}	5, 20	—
			Model: $\Delta n \neq 0$ interactions included in four approximations: none, only $n = 3$ and 4 levels interact, all from $n = 3$ to $n = 5$, and all from $n = 3$ to $n = 6$. Plasma ions: He ⁺ for $T = 5$ eV and He ²⁺ for $T = 20$ eV.		
4	H $n = 6 \rightarrow 5$	$1 \times 2 \times 4 \times 1 = 8$	2×10^{16}	1, 10	—
			Model: $\Delta n \neq 0$ interactions included in four approximations: none, only $n = 5$ and 6 levels interact, all from $n = 5$ to $n = 7$, and all from $n = 5$ to $n = 8$. Plasma ions: protons.		
5	Li I 2s-2p	$1 \times 3 \times 1 \times 1 = 3$	10^{17}	5, 15, 50	—
			Model: 2s and 2p levels included, no fine structure. Only electron broadening included.		
6	B III 2s-2p	$1 \times 3 \times 2 \times 1 = 6$	10^{18}	5, 15, 50	—
			Model: Same as above, but in two variants: without and with Coulomb interactions between the radiator and electrons.		
7	N V 2s-2p	$1 \times 3 \times 2 \times 1 = 6$	10^{19}	5, 15, 50	—
			Model: Same as above.		
8	Al XIII Lyman- α	$2 \times 1 \times 2 \times 3 = 12$	$10^{21}, 10^{22}$	500	$\omega = 10^{15}$ rad/s, $F = 0, 1, 2$ GV/cm
			Model: $n = 1$ and 2 levels in two variants: without and with fine structure. Plasma ions are Al XIII.		
9	He II Lyman- α	$2 \times 2 \times 3 \times 1 = 12$	$10^{18}, 10^{19}$	1, 10	—
			Model: linear Stark, OCP consisting of protons (no electrons). Three plasma field models: usual and “vibrational” and “rotational” components.		
10	He II Lyman- β	$2 \times 2 \times 3 \times 1 = 12$	$10^{18}, 10^{19}$	1, 10	—
			Model: Same as above.		
11	C II 723 nm	$1 \times 2 \times 1 \times 2 = 4$	10^{17}	2, 4	$B = 0, 4$ T
			Model: Fine structure included, carbon plasma under LTE.		
11a	C II 723 nm	1	*	*	*
			Model: Do your best!		
12	Li I 460 nm	$2 \times 2 \times 1 \times 1 = 4$	$3 \times 10^{16}, 10^{17}$	0.5, 2	—
			Model: Fine structure neglected, lithium plasma under LTE.		
12a	Li I 460 nm	1	*	*	*
12b	Li I 460 nm	1	*	*	*
12c	Li I 460 nm	1	*	*	*
12d	Li I 460 nm	1	*	*	*
			Model: Do your best!		

2.3 Isolated lines

$\Delta n = 0$ transitions in Li-like species present a puzzle by disagreement between experimental and different theoretical calculations [2]. For the first SLSP meeting, the Li-like 3s–3p isoelectronic sequence was considered. Now we continue with the 2s–2p resonance lines of the same sequence. 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. The plasma model for these cases consists only of electrons, and we ask to assume either no interactions between the radiator and the electrons (i.e., straight path trajectories) or the more realistic model where such interactions are taken into account (resulting in hyperbolic-like trajectories due to the Coulomb interaction with the radiator). Evidently, this does not affect the neutral-radiator case (Li I).

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

2.4 External fields

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

8. 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 shapes. Two variants of the atomic model: with and without fine structure taken into account.

2.5 Influence of micro-field directionality on line shapes

Here we want to *separately* analyze how changing the direction and magnitude of the micro-field $\vec{F}(t)$ influence the line shape. Let us define “rotational” and “vibrational” micro-fields as

$$\vec{F}_{\text{rot}}(t) = F_0 \frac{\vec{F}(t)}{F(t)} \quad (1)$$

and

$$\vec{F}_{\text{vib}}(t) = \vec{n}_z F(t), \quad (2)$$

respectively. Here, F_0 is the Holtsmark field.

9. He II Lyman- α in a OCP consisting of protons only (no electrons). The line shapes will be calculated as affected by either full $\vec{F}(t)$ or “vibrational” and “rotational” components of the micro-fields separately.
10. Same for He II Lyman- β .

2.6 Modeling experimental data

A “real life” type of calculations, not present among the SLSP1 cases. The objective of these cases is to discuss in detail how different researchers approach analysis of experimental spectra. To have a better understanding of why different approaches might end up with different best-fit plasma parameters, we also ask to calculate the relevant line shapes on a small predefined grid of parameters. **For these calculations (on the predefined grid), please submit only the Stark-broadened profiles, i.e., no Doppler broadening etc, while in the “best-fit” subcases (11a, 12a-d), include any relevant effects.** Please note that the experimental data are unpublished, and are provided solely for the purpose of this workshop. For any other use, please contact the authors (see below) directly.

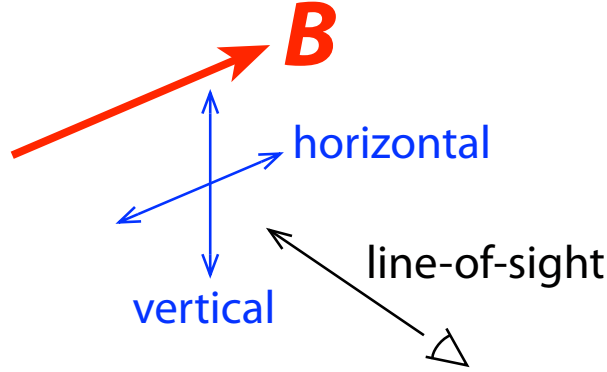


Figure 1: Arrangement of observations for the experimental spectra in case 11a.

11. C II 723-nm $3p(^2P) - 3d(^2D)$ transition in the presence of a magnetic field in the Large Helical Device. The experiment is described in Ref. [3]. The data were kindly provided by M. Goto and his colleagues. Please note that the data contain two spectra, measured at the line of sight that is (nearly) perpendicular to the magnetic field, with the polarizer rotated either (nearly) parallel to the field (“horizontal”) or (nearly) perpendicular to the magnetic field (“vertical”). Please see Fig. 1 for the arrangement. The extinction ratio of the polarizer was $\sim 10^{-4}$. The spectra should be analyzed assuming for the instrumental function a Gaussian with an 0.01-nm FWHM. The wavelengths are not absolutely calibrated.

Experimental spectra (case 11a): [exp_723nm.dat](#)

12. Li I 460.3-nm $2p - 4d$ line and its forbidden components. The experimental setup, data processing, and plasma diagnostic techniques are given in Ref. [4]. The data were kindly provided by M. Cvejić and his colleagues. The spectra should be analyzed assuming for the instrumental function a Gaussian with an 0.093-nm FWHM. The wavelengths are not absolutely calibrated.

Experimental spectrum 1 (case 12a): [exp_460nm_1.dat](#)

Experimental spectrum 2 (case 12b): [exp_460nm_2.dat](#)

Experimental spectrum 3 (case 12c): [exp_460nm_3.dat](#)

Experimental spectrum 4 (case 12d): [exp_460nm_4.dat](#)

Although we do not specify atomic data for the “best-fit” cases like this one, it should be noted that $\Delta E_{4d,4f} \approx 6.8 \text{ cm}^{-1}$ as inferred from the NIST database [5] is likely wrong; we suggest $\Delta E_{4d,4f} \approx 5.0 \text{ cm}^{-1}$ instead [6].

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

$$\langle \alpha j m | r_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 1 & j' \\ -m & q & m' \end{pmatrix} \langle \alpha j | r | \alpha' j' \rangle. \quad (3)$$

Table 2: Hydrogen reduced matrix elements up to $n = 5$.

	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

The reduced radius-vector matrix elements $(\alpha j|r|\alpha' j')$, relevant for the cases considered, are given below.

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 $E_H \approx 27.211$ 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

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

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

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

for diagonal terms (e.g., Eq. (63.5) in [7]) and

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

for off-diagonal ones (Eq. (63.2) in [7]). 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.

3.2 Non-hydrogen

The data are taken from the NIST on-line compilation [5]. 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

$$|(n\ell|r|n'\ell')| = \sqrt{\frac{3f(2\ell+1)}{2(E_{n\ell} - E_{n'\ell'})}}, \quad (9)$$

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

Table 4: Oscillator strengths for isolated 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 (cases 11* and 12*)**. 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 (5 – 7)**, we ask to provide entire line shapes on a reasonably dense grid, typically ~ 1000 points (see Table 5). When the spectral range is

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 >
```


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:

$$\hbar\omega_0 = \frac{\sum_i g_i E_i}{\sum_i g_i} - \frac{\sum_f g_f E_f}{\sum_f g_f}. \quad (10)$$

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 (cases 8 and 11), 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

$$I_{\text{tot}}(\omega) = I_{\pi}(\omega) + 2I_{\sigma}(\omega). \quad (11)$$

In the case of fitting measured polarized spectra (case 11a), the two columns should contain spectra corresponding to the observation arrangement (see Fig. 1). In all cases, no normalization condition is imposed, i.e., you can use peak- or area-normalized profiles.

<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 5 – 7)**. In units of cm^{-1} .

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

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] 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.
- [3] M. Goto, S. Morita, and M. Koubiti. Spectroscopic study of a carbon pellet ablation cloud. *J. Phys. B: At. Mol. Opt. Phys.*, 43(14):144023, 2010. doi:10.1088/0953-4075/43/14/144023.
- [4] M. Cvejić, M.R. Gavrilović, S. Jovićević, and N. Konjević. Stark broadening of Mg I and Mg II spectral lines and Debye shielding effect in laser induced plasma. *Spectrochim. Acta Part B*, 85:20–33, 2013. doi:10.1016/j.sab.2013.03.011.

Table 5: Recommended spectral grids.

Subcase	Spectral range (cm ⁻¹)	Step (cm ⁻¹)
1.1.*.*.*	± 200	0.2
1.2.*.*.*	± 1,000	1
1.3.*.*.*	± 5,000	5
2.1.*.*.*	± 1,000	2
2.2.*.*.*	± 5,000	20
2.3.*.*.*	± 25,000	100
3.1.*.*.*	± 4000	20
4.1.*.*.*	± 400	2
8.*.*.*.*	±5 × 10 ⁴	50
9.1.*.*.*	± 1,000	2
9.2.*.*.*	± 5,000	20
10.1.*.*.*	± 5,000	20
10.2.*.*.*	± 20,000	100
11.*.*.*.*	± 40	0.1
12.*.*.*.*	± 400	2

- [5] NIST Atomic Spectra Database. <http://www.nist.gov/pml/data/asd.cfm>. URL: <http://www.nist.gov/pml/data/asd.cfm>.
- [6] M. S. Safronova, C. Froese Fischer, and Yu. Ralchenko. Relativistic all-order and multiconfiguration Hartree-Fock calculations of the 4d-4f energy separation in Li I. *Phys. Rev. A*, 76:054502, 2007. doi:10.1103/PhysRevA.76.054502.
- [7] Hans A. Bethe and Edwin E. Salpeter. *Quantum Mechanics of One- and Two-Electron Atoms*. Plenum, New York, 1977.