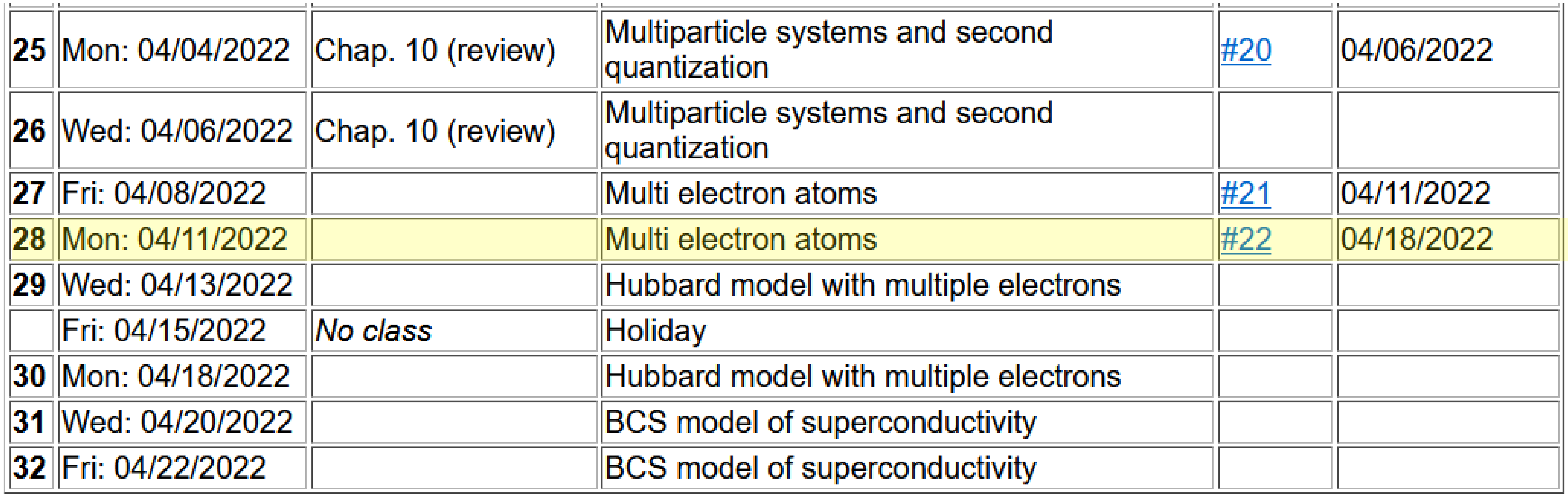
PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Plan for Lecture 28

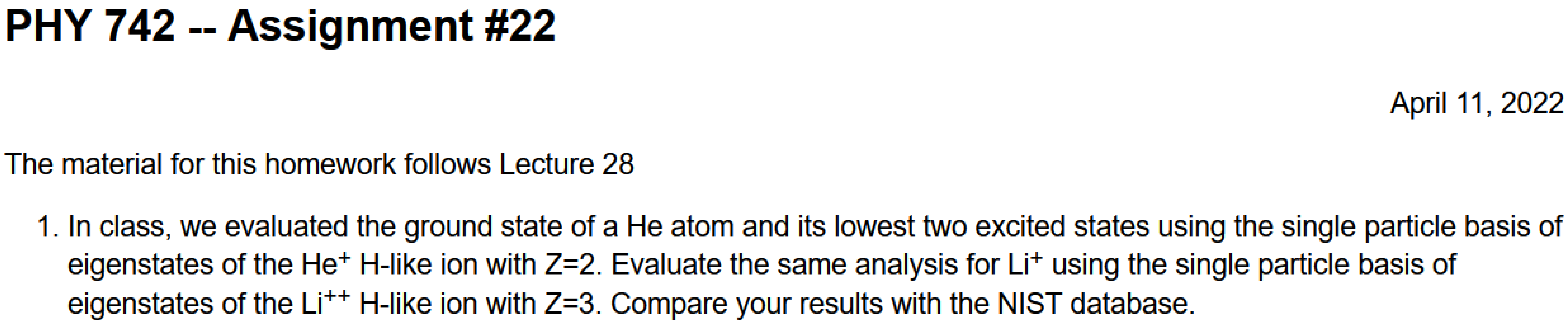
Quantum mechanics of a multi electron atom

Using second quantization formalism together with material from Professor Carlson's textbook: Chapter 10. Multiple particles (Sec. F) and also Chapter 8. Spin and Adding Angular Momentum (Sec. C)

1. Review of what we have learned so far
2. General discussion of atomic term analysis
3. Examples and comparison with NIST atomic database



25	Mon: 04/04/2022	Chap. 10 (review)	Multiparticle systems and second quantization	#20	04/06/2022
26	Wed: 04/06/2022	Chap. 10 (review)	Multiparticle systems and second quantization		
27	Fri: 04/08/2022		Multi electron atoms	#21	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	#22	04/18/2022
29	Wed: 04/13/2022		Hubbard model with multiple electrons		
	Fri: 04/15/2022	*No class*	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons		
31	Wed: 04/20/2022		BCS model of superconductivity		
32	Fri: 04/22/2022		BCS model of superconductivity		



PHY 742 -- Assignment #22

April 11, 2022

The material for this homework follows Lecture 28

1. In class, we evaluated the ground state of a He atom and its lowest two excited states using the single particle basis of eigenstates of the He$^+$ H-like ion with Z=2. Evaluate the same analysis for Li$^+$ using the single particle basis of eigenstates of the Li^{++} H-like ion with Z=3. Compare your results with the NIST database.

Focusing on multielectron systems --

$$H(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)=\sum_{i=1}^{N}h(\mathbf{r}_i)+V(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)$$

$$\text{where: } V(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)=\sum_{i=1\ (i>j)}^{N}\sum_{j=1}^{N}v(\mathbf{r}_i-\mathbf{r}_j)$$

Single particle basis: $h(\mathbf{r})\varphi_k(\mathbf{r})=\varepsilon_k\varphi_k(\mathbf{r})$

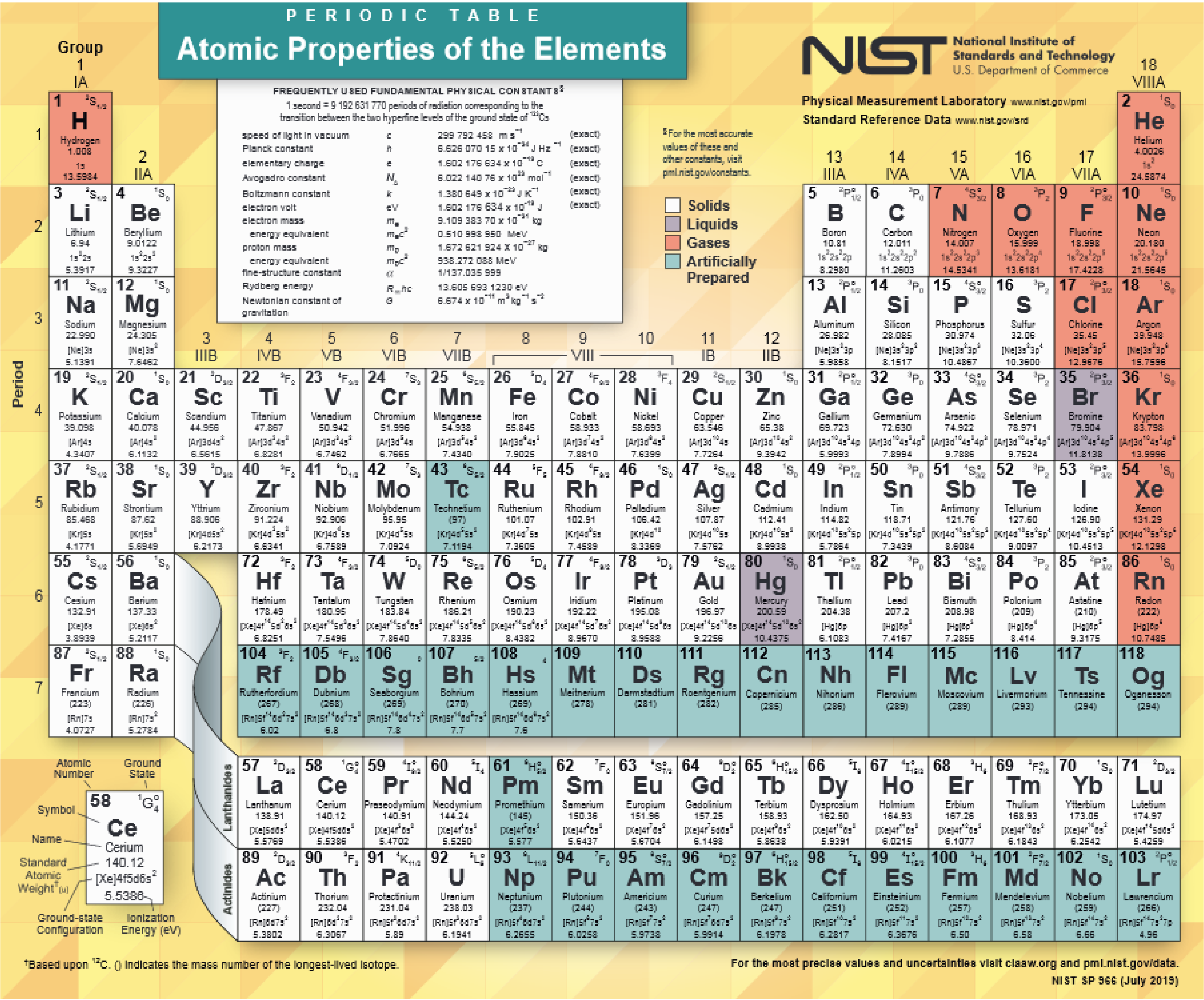
In this basis and using second quantization formalism --

$$\left|\varphi_k(\mathbf{r})\right\rangle \Rightarrow f_k^\dagger f_k\ \left|0\right\rangle$$

Second quantized Hamiltonian: $H=\sum_i \varepsilon_i f_i^\dagger f_i+\sum_{ijkl}v_{ijkl}f_i^\dagger f_j^\dagger f_l f_k$

$$\text{where } v_{ijkl}\equiv\left\langle\varphi_i(\mathbf{r}_1)\varphi_j(\mathbf{r}_2)\middle|v(\mathbf{r}_1-\mathbf{r}_2)\middle|\varphi_k(\mathbf{r}_1)\varphi_l(\mathbf{r}_2)\right\rangle$$

https://www.nist.gov/system/files/documents/2019/12/10/nist_periodictable_july2019_crop.pdf



PERIODIC TABLE

Atomic Properties of the Elements

National Institute of Standards and Technology
U.S. Department of Commerce

Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS§

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.626 070 15 x 10^{-34} J Hz^{-1}	(exact)
elementary charge	e	1.602 176 634 x 10^{-19} C	(exact)
Avogadro constant	N_A	6.022 140 76 x 10^{23} mol^{-1}	(exact)
Boltzmann constant	k	1.380 649 x 10^{-23} J K^{-1}	(exact)
electron volt	eV	1.602 176 634 x 10^{-19} J	(exact)
electron mass	m_e	9.109 383 70 x 10^{-31} kg	
energy equivalent	m_ec^2	0.510 998 950 MeV	
proton mass	m_p	1.672 621 924 x 10^{-27} kg	
energy equivalent	m_pc^2	938.272 088 MeV	
fine-structure constant	α	1/137.035 999	
Rydberg energy	$R_\infty hc$	13.605 693 1230 eV	
Newtonian constant of gravitation	G	6.674 x 10^{-11} m^3 kg^{-1} s^{-2}	

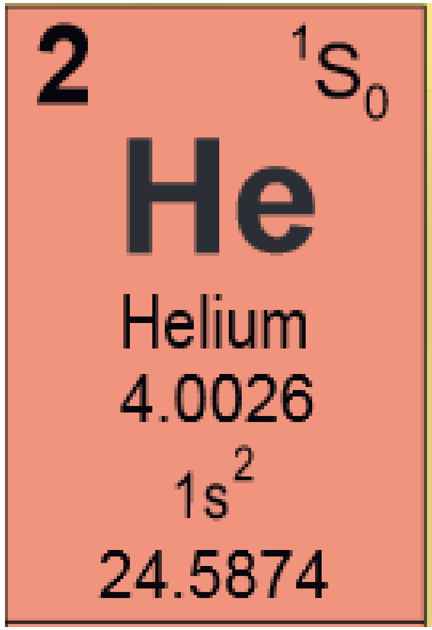
§ For the most accurate values of these and other constants, visit pml.nist.gov/constants.

- ☐ Solids
- ▨ Liquids
- 🟥 Gases
- 🟩 Artificially Prepared

†Based upon ^{12}C. () indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciaaw.org and pml.nist.gov/data.

NIST SP 966 (July 2019)



2 $^1S_0$

He

Helium

4.0026

$1s^2$

24.5874

The Hamiltonian for an He atom (Z=2): (cgs Gaussian units)

$$H(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - 2e^2\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$= \underbrace{-\frac{\hbar^2\nabla_1^2}{2m}-\frac{2e^2}{r_1}}_{} \underbrace{-\frac{\hbar^2\nabla_2^2}{2m}-\frac{2e^2}{r_2}}_{} + \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$= \qquad h(\mathbf{r}_1) \quad + \quad h(\mathbf{r}_2) \quad + v(\mathbf{r}_1,\mathbf{r}_2)$$

Single particle basis:

$$h(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) \equiv h(\mathbf{r}_1)\varphi_{nlmm_s}(\mathbf{r}_1) = \varepsilon_n\varphi_{nlmm_s}(\mathbf{r}_1)$$

Second quantized version of the He atom Hamiltonian

$$H(\mathbf{r}_1,\mathbf{r}_2) \Rightarrow \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

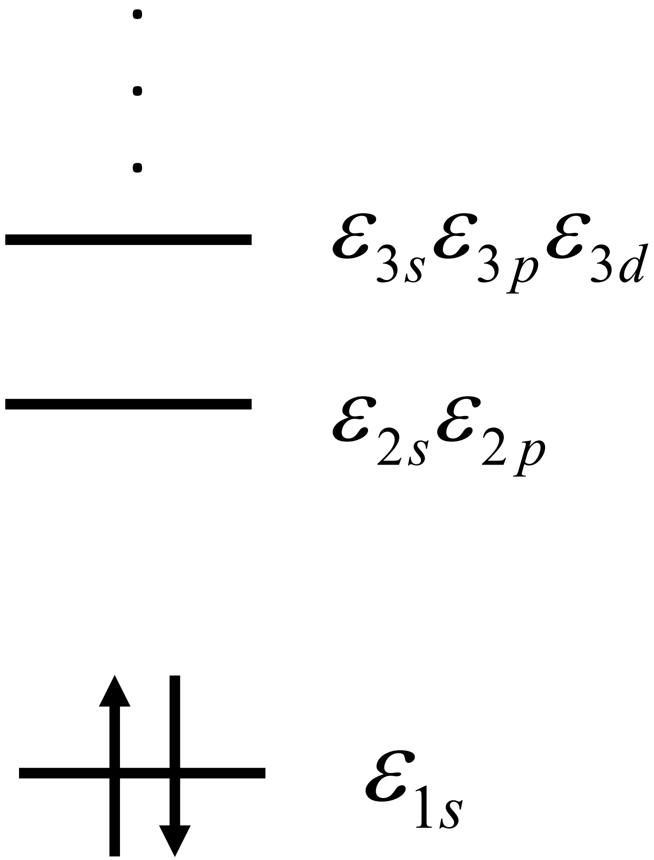
Here v_{ijkl} denotes matrix elements such as

$$v_{ijkl} = \left\langle \varphi_i(\mathbf{r}_1)\varphi_j(\mathbf{r}_2) \middle| v(\mathbf{r}_1 - \mathbf{r}_2) \middle| \varphi_k(\mathbf{r}_1)\varphi_l(\mathbf{r}_2) \right\rangle$$

The matrix element $i \equiv nlmm_s$

In general, we will use $nl \Rightarrow n\{spdf..\}$ for $n\{0123..\}$

Ground state configuration for He atom



$\varepsilon_{3s}\varepsilon_{3p}\varepsilon_{3d}$

$\varepsilon_{2s}\varepsilon_{2p}$

ε_{1s}

$$\psi = f^{\dagger}_{1s\alpha} f^{\dagger}_{1s\beta} \left|0\right\rangle$$

Summary of results

$$H = \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

Need to evaluate $\langle \psi | H | \psi \rangle$ for $\psi = f_{1s\alpha}^\dagger f_{1s\beta}^\dagger |0\rangle$

$$\langle \psi | H | \psi \rangle = 2\varepsilon_{1s} + v_{ijij}$$

Note that in coordinate and spin representation,

$$\psi = \frac{1}{\sqrt{2}} \varphi_{1s}(\mathbf{r}_1)\varphi_{1s}(\mathbf{r}_2)\left(\alpha_1\beta_2 - \alpha_2\beta_1\right)$$

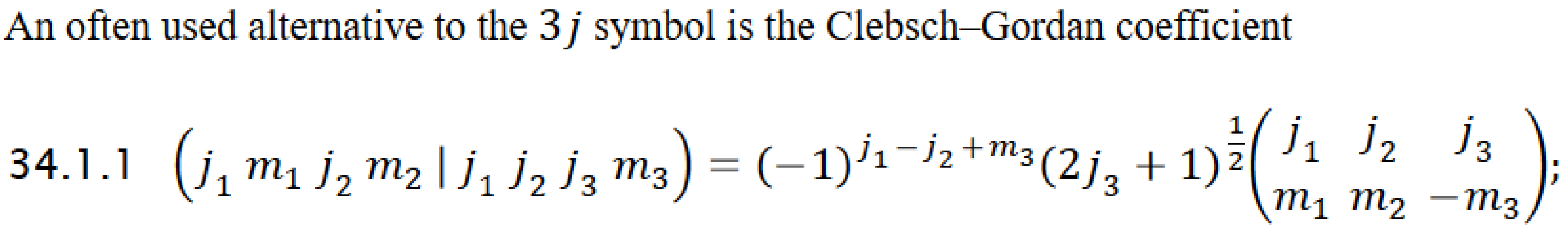
While the ground state of the He atom is a very simple case, it illustrates the general properties of many electron atoms in a spherical environments. Because of the spherical symmetry, total angular moment of the system is conserved. If we assume that spin-orbit interactions are negligible, then total spin angular momentum and total orbital angular momentum are each separately conserved. Please review Chapter 8 of your textbook to know how to "add" angular momentum using Clebsch-Gordan coefficients.

$$\left|jm\right\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \left|j_1 j_2; m_1 m_2\right\rangle \left\langle j_1 j_2; m_1 m_2 \middle| jm\right\rangle \qquad (8.12a)$$

$$\left|j_1 j_2; m_1 m_2\right\rangle = \sum_{j=\left|j_1-j_2\right|}^{j_1+j_2} \sum_{m=-j}^{j} \left|jm\right\rangle \left\langle jm \middle| j_1 j_2; m_1 m_2\right\rangle \qquad (8.12b)$$

Here $\left|jm\right\rangle$ describes the total angular moment quantum numbers, while $\left|j_1 j_2; m_1 m_2\right\rangle$ describes the product of two angular momenta $\left|j_1 j_2; m_1 m_2\right\rangle \equiv \left|j_1 m_1\right\rangle \left|j_2 m_2\right\rangle$. "$j$" can represent orbital or spin angular momentum.

Note, for practical calculations of Clebsch-Gordan coefficients, a good source is NIST's DLMF -- https://dlmf.nist.gov/34.1



An often used alternative to the $3j$ symbol is the Clebsch–Gordan coefficient

34.1.1 $$\left(j_1\, m_1\, j_2\, m_2 \,|\, j_1\, j_2\, j_3\, m_3\right) = (-1)^{j_1-j_2+m_3}(2j_3+1)^{\frac{1}{2}}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix};$$

Professor Carlson also has a working maple script on his website.

For the spherical atom without spin-orbit coupling, the total spin angular momentum *S* and the total orbital angular momentum *L* are both conserved. The atomic term notation is

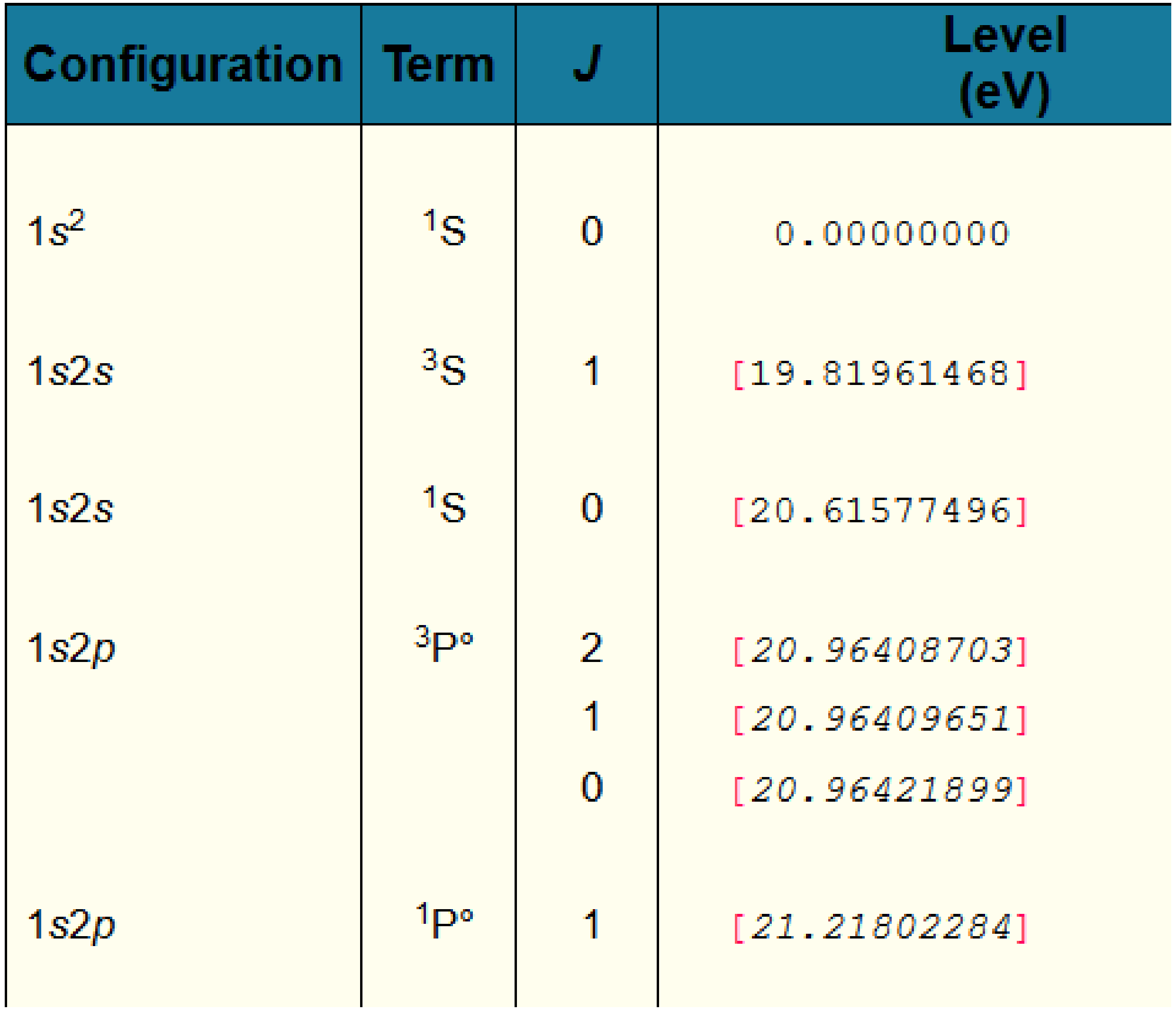
$$^{2S+1}L \qquad \text{Examples:} \quad {}^1S, {}^3S, {}^1P, {}^1D, {}^4G....$$

Example from NIST

NIST Atomic Spectra Database Levels Data

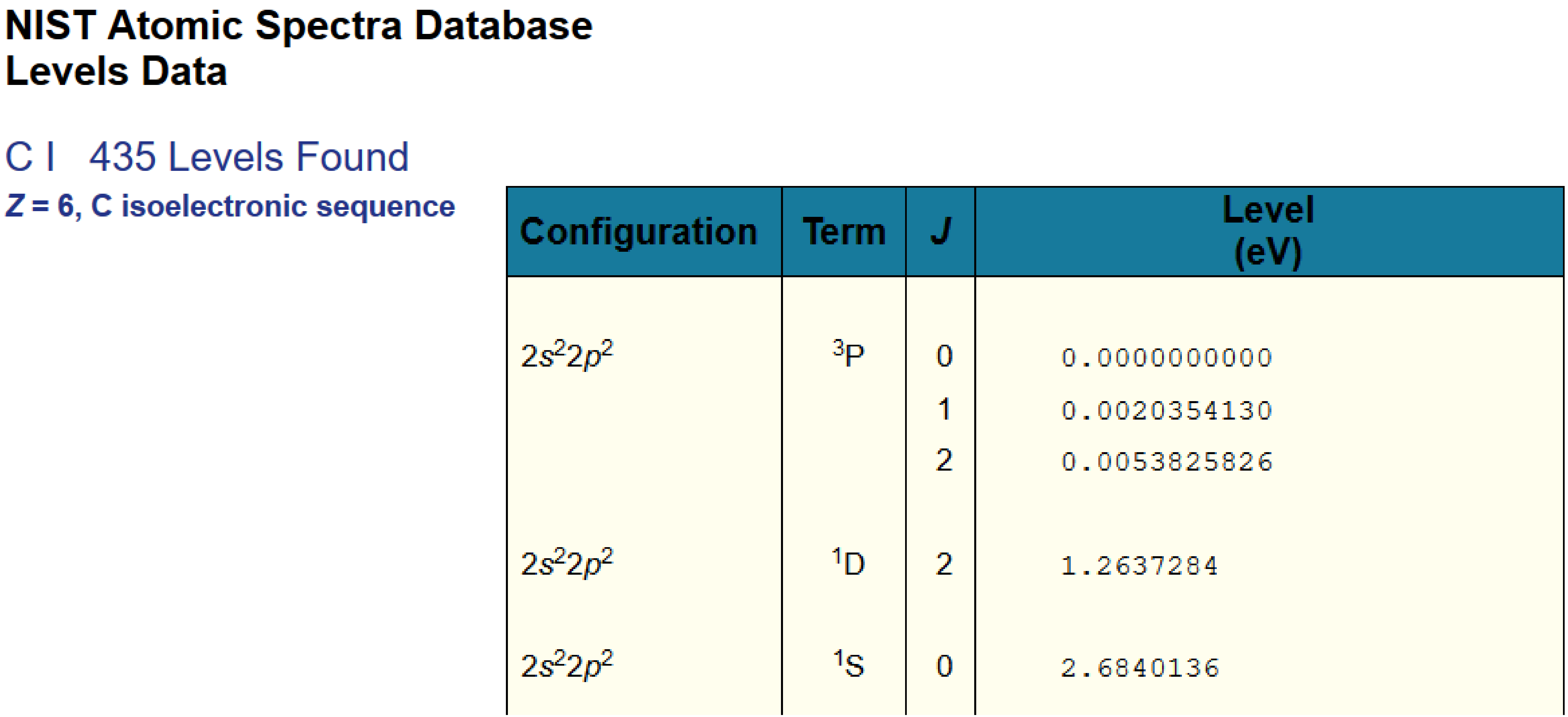
He I 198 Levels Found

$Z = 2$, He isoelectronic sequence



Configuration	Term	J	Level (eV)
$1s^2$	^1S	0	0.00000000
$1s2s$	^3S	1	[19.81961468]
$1s2s$	^1S	0	[20.61577496]
$1s2p$	$^3P^\circ$	2	[20.96408703]
		1	[20.96409651]
		0	[20.96421899]
$1s2p$	$^1P^\circ$	1	[21.21802284]

Example from NIST



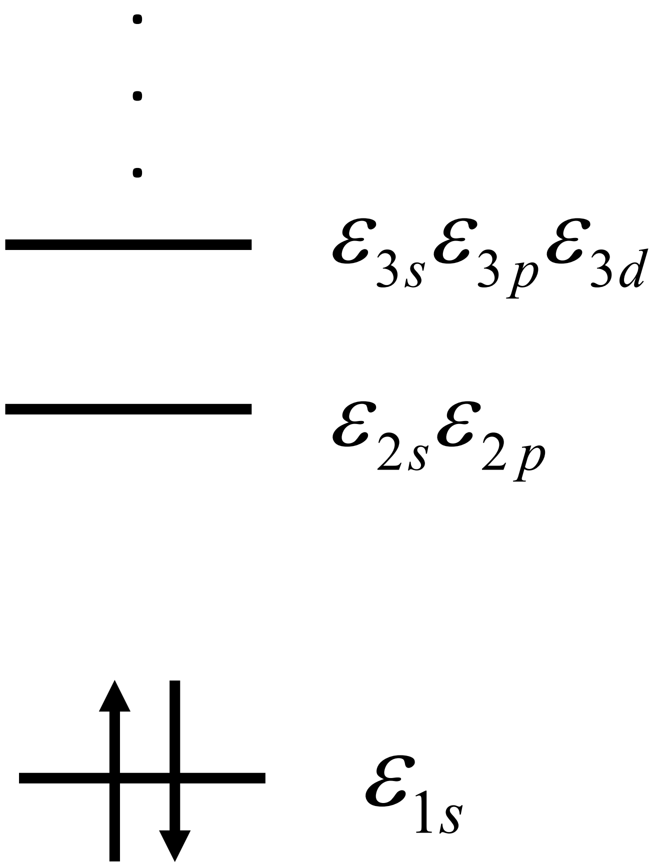
NIST Atomic Spectra Database
Levels Data

C I   435 Levels Found

Z = 6, C isoelectronic sequence

Configuration	Term	*J*	Level (eV)
$2s^2 2p^2$	^{3}P	0	0.0000000000
		1	0.0020354130
		2	0.0053825826
$2s^2 2p^2$	^{1}D	2	1.2637284
$2s^2 2p^2$	^{1}S	0	2.6840136

Back to the discussion of He



Ground state:

$$\psi = f^{\dagger}_{1s\alpha} f^{\dagger}_{1s\beta} \left|0\right\rangle$$

$$\psi = \frac{1}{\sqrt{2}} \varphi_{1s}(\mathbf{r}_1)\varphi_{1s}(\mathbf{r}_2)\left(\alpha_1\beta_2 - \alpha_2\beta_1\right)$$

$$S = 0 \qquad\qquad L = 0$$

Atomic term: ^{1}S

Energy estimate: $\left\langle \psi \middle| H \middle| \psi \right\rangle = 2\varepsilon_{1s} + v_{1s1s1s1s}$

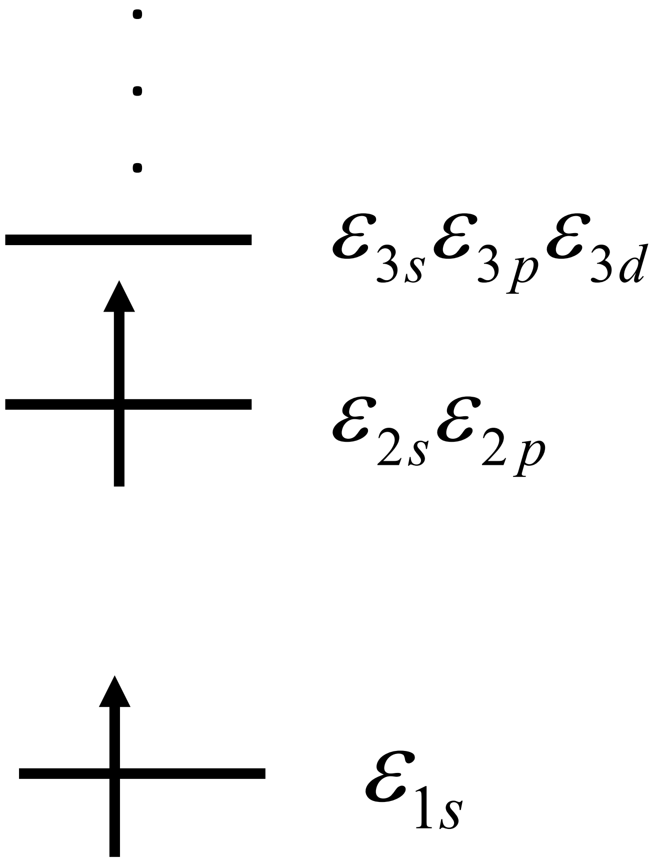
Digression -- How do we know that the total spin of this state is *S*=0?

$$\frac{1}{\sqrt{2}}\left(\alpha_1\beta_2-\alpha_2\beta_1\right)$$

Clearly M_S=0 -- but do we really know that *S*=0?

1. **We don't know**
2. **We know because ??**

Back to the discussion of He



A possible excited state:

$$\psi = f^{\dagger}_{1s\alpha} f^{\dagger}_{2s\alpha} \left|0\right\rangle$$

$$\psi = \frac{1}{\sqrt{2}}\left(\varphi_{1s}(\mathbf{r}_1)\varphi_{2s}(\mathbf{r}_2)-\varphi_{1s}(\mathbf{r}_2)\varphi_{2s}(\mathbf{r}_1)\right)\alpha_1\alpha_2$$

$$S = 1 \qquad L = 0$$

Atomic term: ^3S

Energy estimate of the ^3S excited state of He

$$\psi = f^\dagger_{1s\alpha} f^\dagger_{2s\alpha} \left|0\right\rangle$$

$$H = \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

Evaluation of $\langle\psi|H|\psi\rangle$ for $\psi = f_k^\dagger f_l^\dagger |0\rangle$ $(k \neq l)$

$$\langle\psi|H|\psi\rangle = \varepsilon_k + \varepsilon_l + v_{klkl} - v_{kllk}$$

$$= \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} - v_{1s2s2s1s}$$

Excited state energies -- continued

$$\langle \psi | H | \psi \rangle = \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} - v_{1s2s2s1s}$$

$$v_{ijkl} \equiv \left\langle \varphi_i(\mathbf{r}_1)\varphi_j(\mathbf{r}_2) \middle| v(\mathbf{r}_1 - \mathbf{r}_2) \middle| \varphi_k(\mathbf{r}_1)\varphi_l(\mathbf{r}_2) \right\rangle$$

$$v_{1s2s1s2s} = \int d^3r_1 d^3r_2 \left|\varphi_{1s}(\mathbf{r}_1)\right|^2 \left|\varphi_{2s}(\mathbf{r}_2)\right|^2 v(\mathbf{r}_1 - \mathbf{r}_2)$$

$$v_{1s2s2s1s} = \int d^3r_1 d^3r_2 \left(\varphi_{1s}(\mathbf{r}_1)\varphi_{2s}(\mathbf{r}_1)\right)\left(\varphi_{1s}(\mathbf{r}_2)\varphi_{2s}(\mathbf{r}_2)\right) v(\mathbf{r}_1 - \mathbf{r}_2)$$

Specific basis states for He atom $Z = 2$ in terms of a_0 (Bohr radius)

$$\varphi_{1s}(\mathbf{r}) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

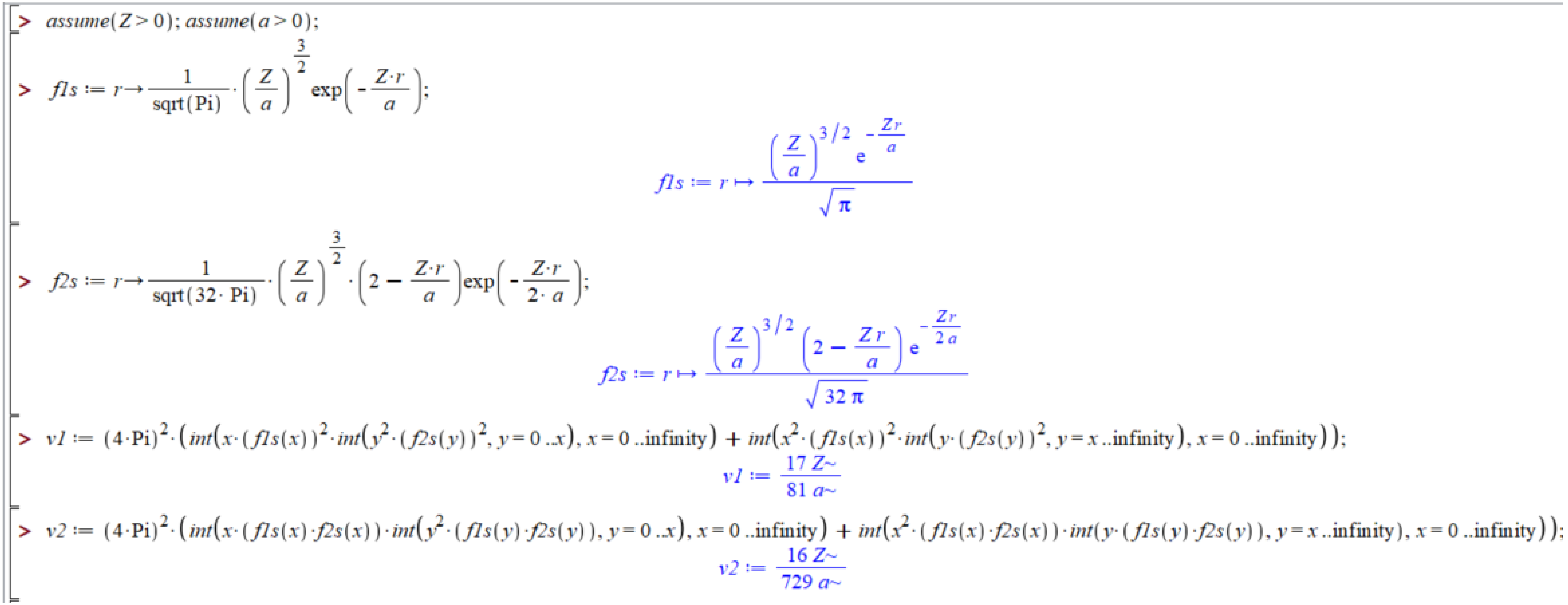
$$\varphi_{2s}(\mathbf{r}) = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/(2a_0)}$$

In this spherically symmetric case, the integrals can be evaluated:

$$v_{1s2s1s2s} = (4\pi)^2\int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \left(\varphi_{1s}(r_1)\right)^2 \left(\varphi_{2s}(r_2)\right)^2 \frac{1}{r_>} = \frac{Ze^2}{a_0}\frac{17}{81}$$

$$v_{1s2s2s1s} = (4\pi)^2\int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \left(\varphi_{1s}(r_1)\varphi_{2s}(r_1)\right)\left(\varphi_{1s}(r_2)\varphi_{2s}(r_2)\right)\frac{1}{r_>} = \frac{Ze^2}{a_0}\frac{16}{729}$$

Maple script for evaluating integrals --



> $assume(Z > 0); assume(a > 0);$

> $$f1s := r \rightarrow \frac{1}{\mathrm{sqrt}(\mathrm{Pi})} \cdot \left(\frac{Z}{a}\right)^{\frac{3}{2}} \exp\left(-\frac{Z \cdot r}{a}\right);$$

$$f1s := r \mapsto \frac{\left(\frac{Z}{a}\right)^{3/2} \mathrm{e}^{-\frac{Z r}{a}}}{\sqrt{\pi}}$$

> $$f2s := r \rightarrow \frac{1}{\mathrm{sqrt}(32 \cdot \mathrm{Pi})} \cdot \left(\frac{Z}{a}\right)^{\frac{3}{2}} \cdot \left(2 - \frac{Z \cdot r}{a}\right) \exp\left(-\frac{Z \cdot r}{2 \cdot a}\right);$$

$$f2s := r \mapsto \frac{\left(\frac{Z}{a}\right)^{3/2} \left(2 - \frac{Z r}{a}\right) \mathrm{e}^{-\frac{Z r}{2 a}}}{\sqrt{32 \pi}}$$

> $$v1 := (4 \cdot \mathrm{Pi})^2 \cdot \left(int\left(x \cdot (f1s(x))^2 \cdot int\left(y^2 \cdot (f2s(y))^2, y = 0 ..x\right), x = 0 ..\mathrm{infinity}\right) + int\left(x^2 \cdot (f1s(x))^2 \cdot int\left(y \cdot (f2s(y))^2, y = x ..\mathrm{infinity}\right), x = 0 ..\mathrm{infinity}\right)\right);$$

$$v1 := \frac{17\, Z\sim}{81\, a\sim}$$

> $$v2 := (4 \cdot \mathrm{Pi})^2 \cdot \left(int\left(x \cdot (f1s(x) \cdot f2s(x)) \cdot int\left(y^2 \cdot (f1s(y) \cdot f2s(y)), y = 0 ..x\right), x = 0 ..\mathrm{infinity}\right) + int\left(x^2 \cdot (f1s(x) \cdot f2s(x)) \cdot int(y \cdot (f1s(y) \cdot f2s(y)), y = x ..\mathrm{infinity}), x = 0 ..\mathrm{infinity}\right)\right);$$

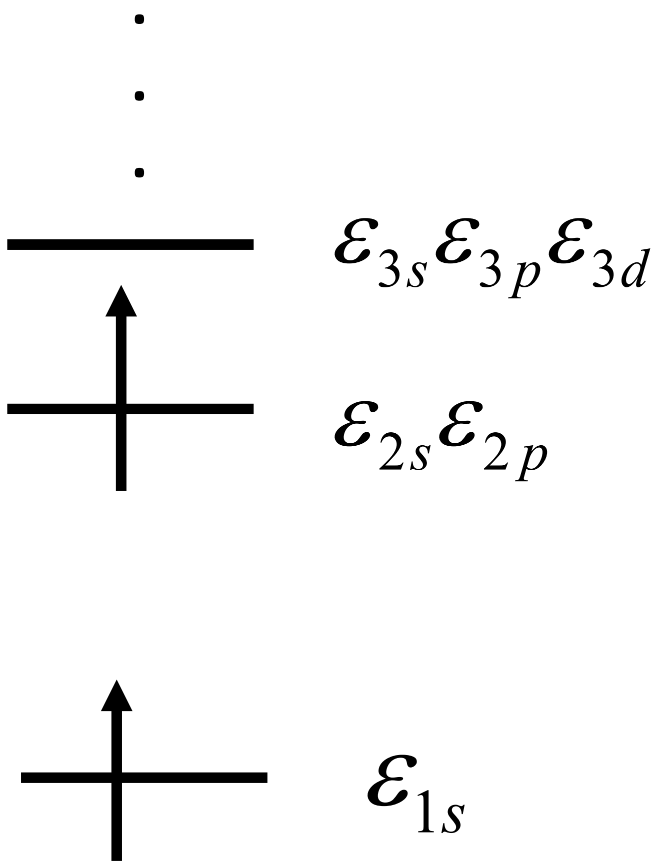
$$v2 := \frac{16\, Z\sim}{729\, a\sim}$$

Summary of results for excited state:

$$\psi = f^{\dagger}_{1s\alpha} f^{\dagger}_{2s\alpha} \left|0\right\rangle$$

$$S = 1 \qquad\qquad L = 0$$

Atomic term: ^{3}S



$$\left\langle\psi\right|H\left|\psi\right\rangle = \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} - v_{1s2s2s1s}$$

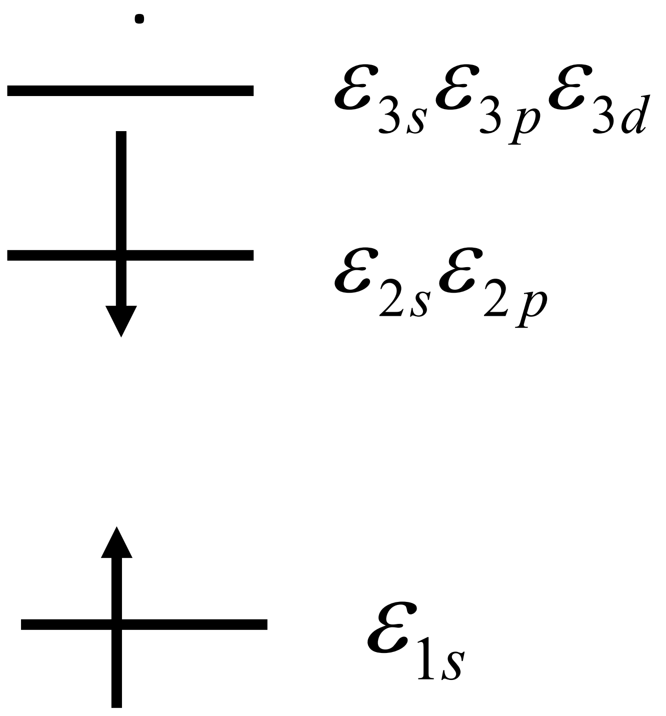
$$= \frac{e^{2}}{2a_{0}}\left(-4 - \frac{4}{4} + \frac{68}{81} - \frac{64}{729}\right)$$

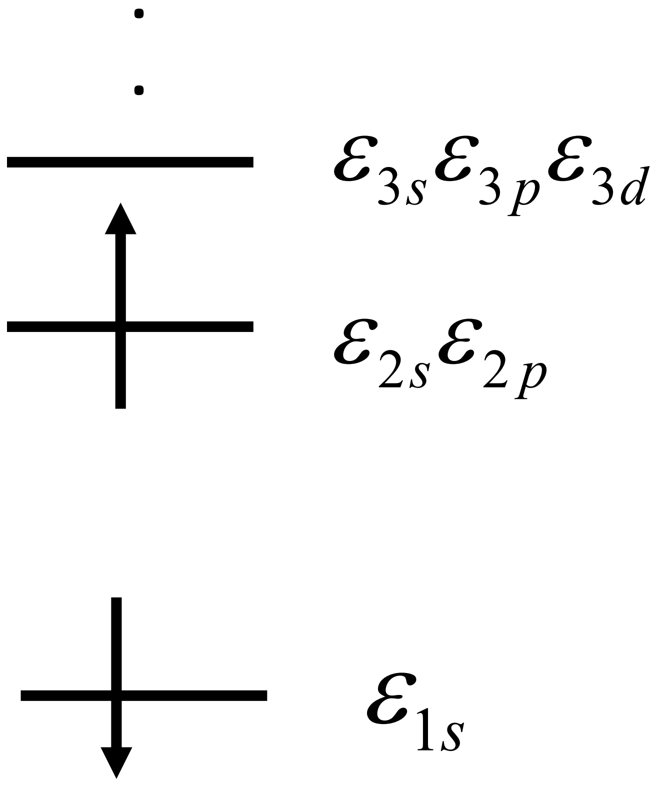
$$= \frac{e^{2}}{2a_{0}}(-4.25)$$

Consider another excited state of He

While these two states are orthogonal to each other, they are mixed by the Hamiltonian, so we must consider them together

$$\psi_A = f^\dagger_{1s\alpha} f^\dagger_{2s\beta} \left|0\right\rangle \qquad \psi_B = f^\dagger_{1s\beta} f^\dagger_{2s\alpha} \left|0\right\rangle$$





Consider another excited state of He -- continued

$$H = \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

$$\psi_A = f_{1s\alpha}^\dagger f_{2s\beta}^\dagger |0\rangle \qquad \psi_B = f_{1s\beta}^\dagger f_{2s\alpha}^\dagger |0\rangle$$

$$\langle \psi_A | H | \psi_A \rangle = \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} = \langle \psi_B | H | \psi_B \rangle$$

$$\langle \psi_A | H | \psi_B \rangle = -v_{1s2s2s1s} = \langle \psi_B | H | \psi_A \rangle$$

Consider another excited state of He – continued

Since the two states are mixed by the Hamiltonian, we need to consider their linear combination:

$$\psi = C_A\psi_A + C_B\psi_B \quad \text{for} \quad \psi_A = f^\dagger_{1s\alpha} f^\dagger_{2s\beta}\left|0\right\rangle \text{ and } \psi_B = f^\dagger_{1s\beta} f^\dagger_{2s\alpha}\left|0\right\rangle$$

$$H = \begin{array}{c|cc} & A & B \\ \hline A & \varepsilon_{1s}+\varepsilon_{2s}+v_{1s2s1s2s} & -v_{1s2s2s1s} \\ B & -v_{1s2s2s1s} & \varepsilon_{1s}+\varepsilon_{2s}+v_{1s2s1s2s} \end{array}$$

Two solutions:

$$\psi = \frac{1}{\sqrt{2}}\left(\psi_A \pm \psi_B\right) \qquad \varepsilon_\pm = \varepsilon_{1s}+\varepsilon_{2s}+v_{1s2s1s2s} \mp v_{1s2s2s1s}$$

Consider another excited state of He – continued

One solution:

$$\psi_+ = \frac{1}{\sqrt{2}}\left(\psi_A + \psi_B\right) \qquad \varepsilon_+ = \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} - v_{1s2s2s1s}$$

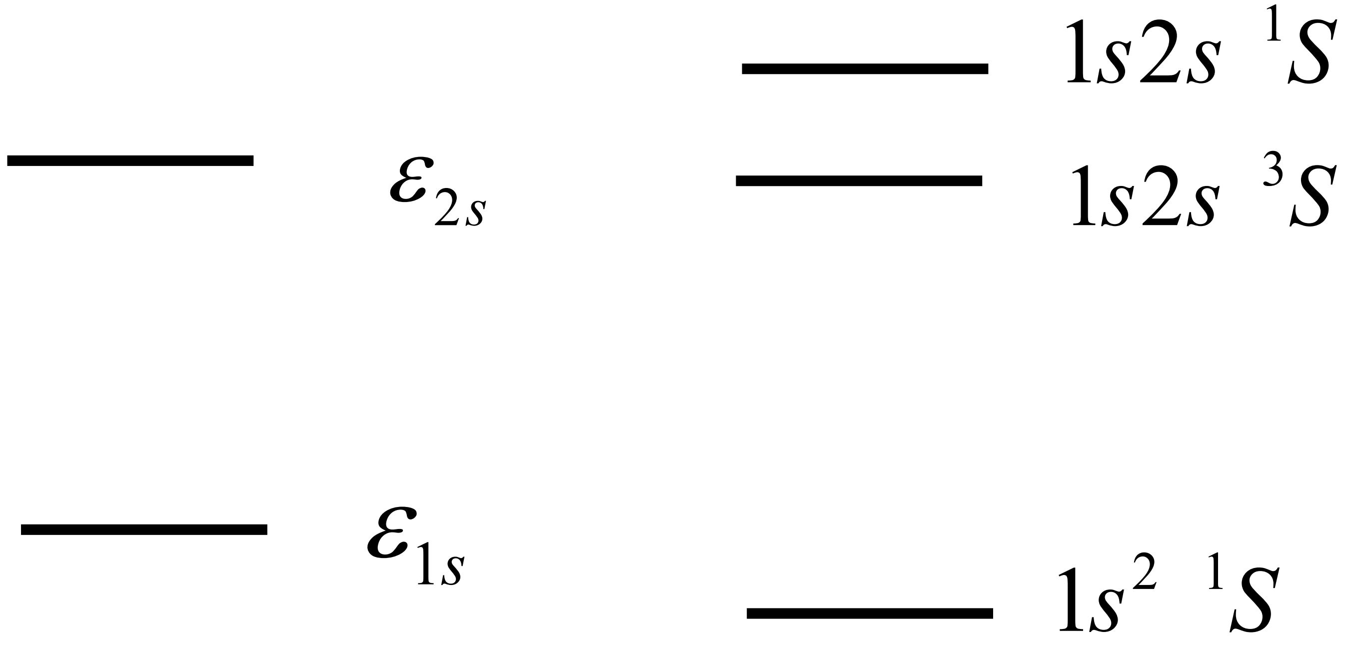
$\Rightarrow$ This solution is another example of the spin triplet (S=1) solution that we analyzed previously

Another solution:

$$\psi_- = \frac{1}{\sqrt{2}}\left(\psi_A - \psi_B\right) \qquad \varepsilon_- = \varepsilon_{1s} + \varepsilon_{2s} + v_{1s2s1s2s} + v_{1s2s2s1s}$$

$\Rightarrow$ This solution is a spin singlet (S=0) solution with higher energy

Summary of analysis of ground state and lowest excited states of He atom



Single particle states	Two particle states (first order perturbation)	Energies Calc. (eV)	Energies NIST (eV)
	$1s2s\ ^1S$	19.4	20.6
ε_{2s}	$1s2s\ ^3S$	17.0	19.8
ε_{1s}	$1s^2\ ^1S$	0.00	0.00

What do you think about these results

1. Very discouraging
2. Very encouraging
3. Needs more work

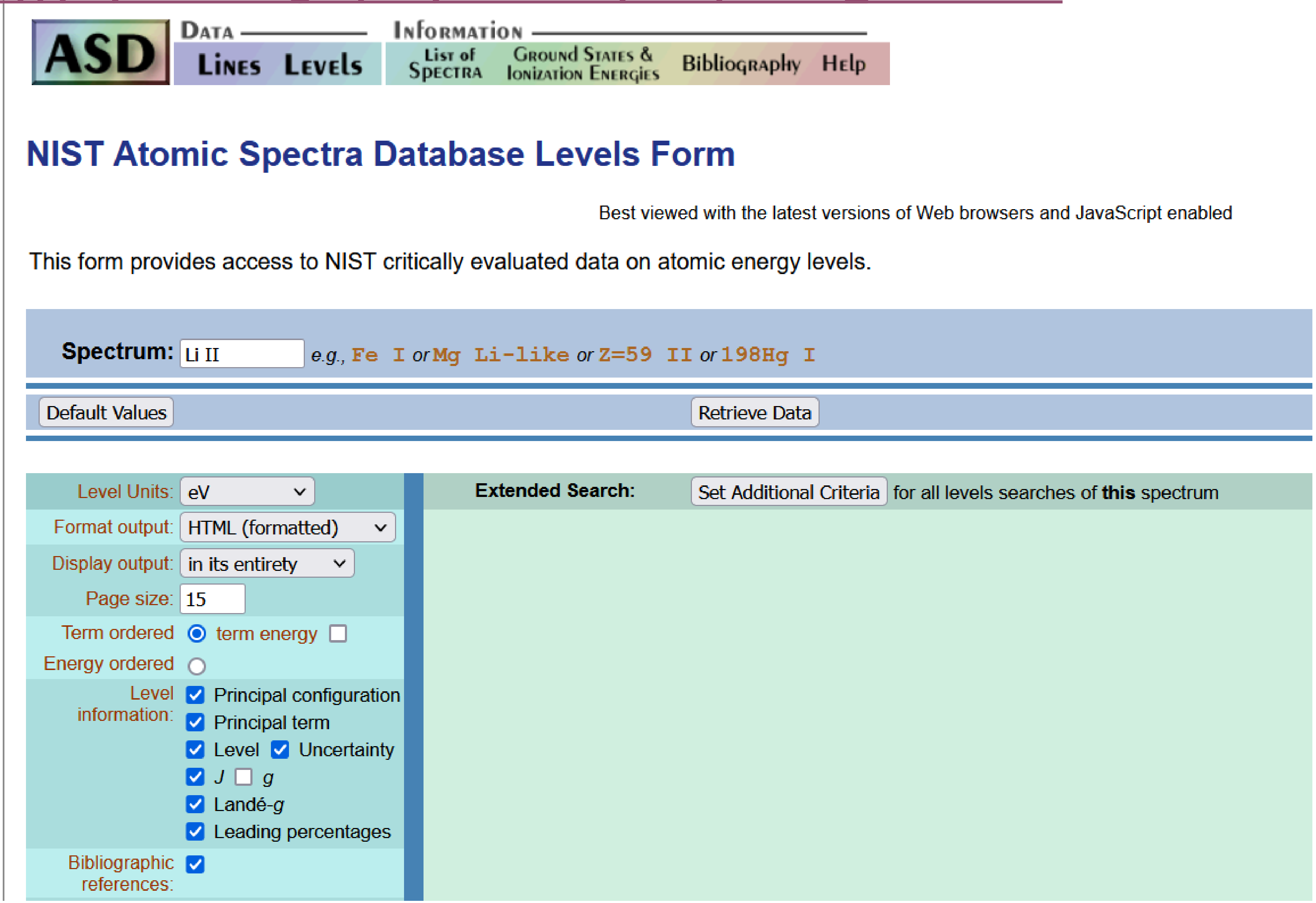
Other formulations

- Form basis functions that are eigenfunctions of total spin
  - Eigenfunctions of total spin may be symmetric or antisymmetric wrt particle exchange.

$$\psi = \psi_{\text{Space}}\psi_{\text{Spin}}$$

	Space	Spin
	Sym	Anti
or	Anti	Sym

https://physics.nist.gov/PhysRefData/ASD/levels_form.html



NIST Atomic Spectra Database Levels Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

This form provides access to NIST critically evaluated data on atomic energy levels.

Spectrum: Li II *e.g.*, `Fe I` *or* `Mg Li-like` *or* `Z=59 II` *or* `198Hg I`

Extended Search: Set Additional Criteria for all levels searches of **this** spectrum

Level Units: eV

Format output: HTML (formatted)

Display output: in its entirety

Page size: 15

Term ordered ● term energy ☐

Energy ordered ○

Level information: ☑ Principal configuration

☑ Principal term

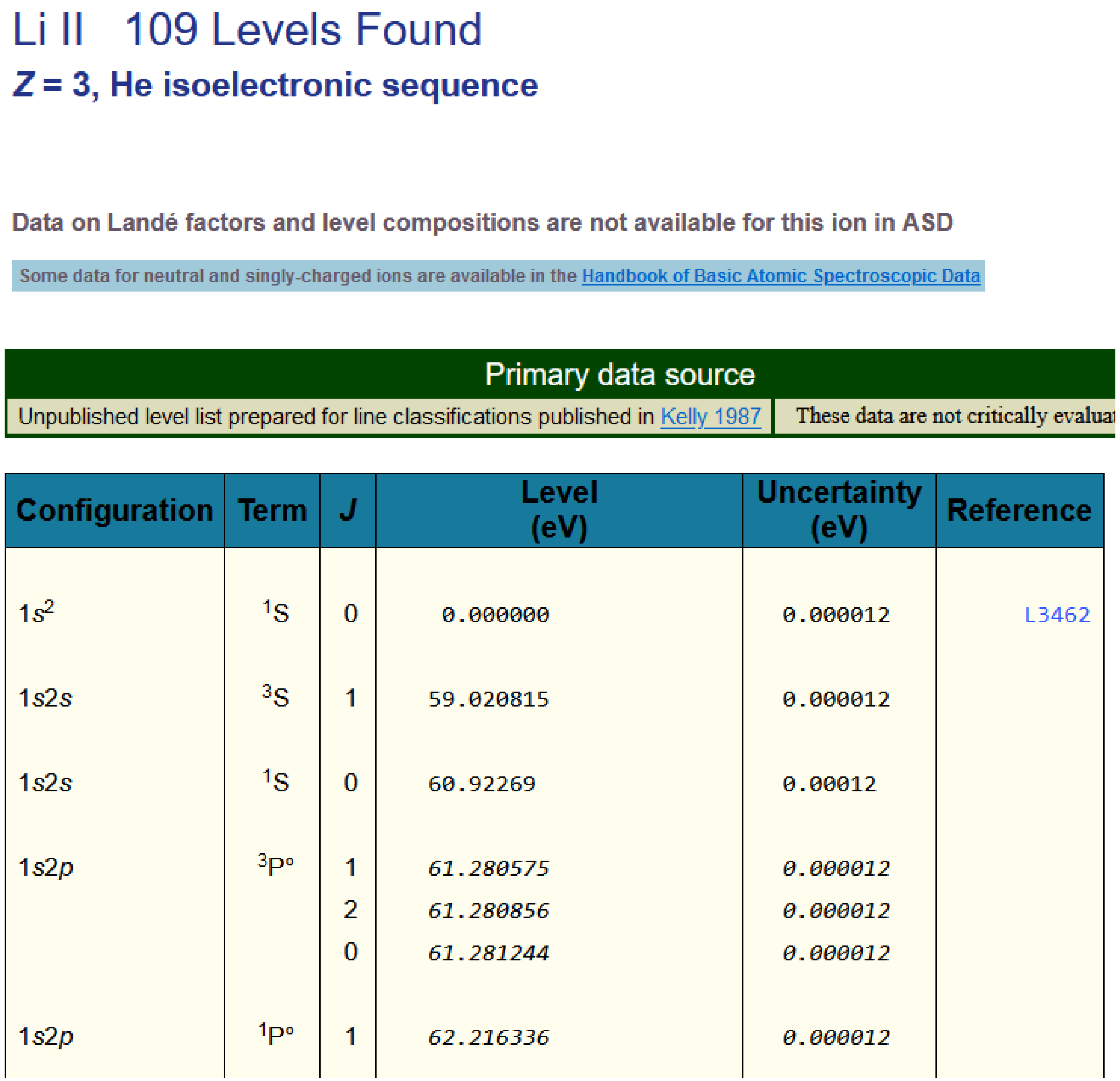
☑ Level ☑ Uncertainty

☑ *J* ☐ *g*

☑ Landé-*g*

☑ Leading percentages

Bibliographic references: ☑



Li II 109 Levels Found

Z = 3, He isoelectronic sequence

Data on Landé factors and level compositions are not available for this ion in ASD

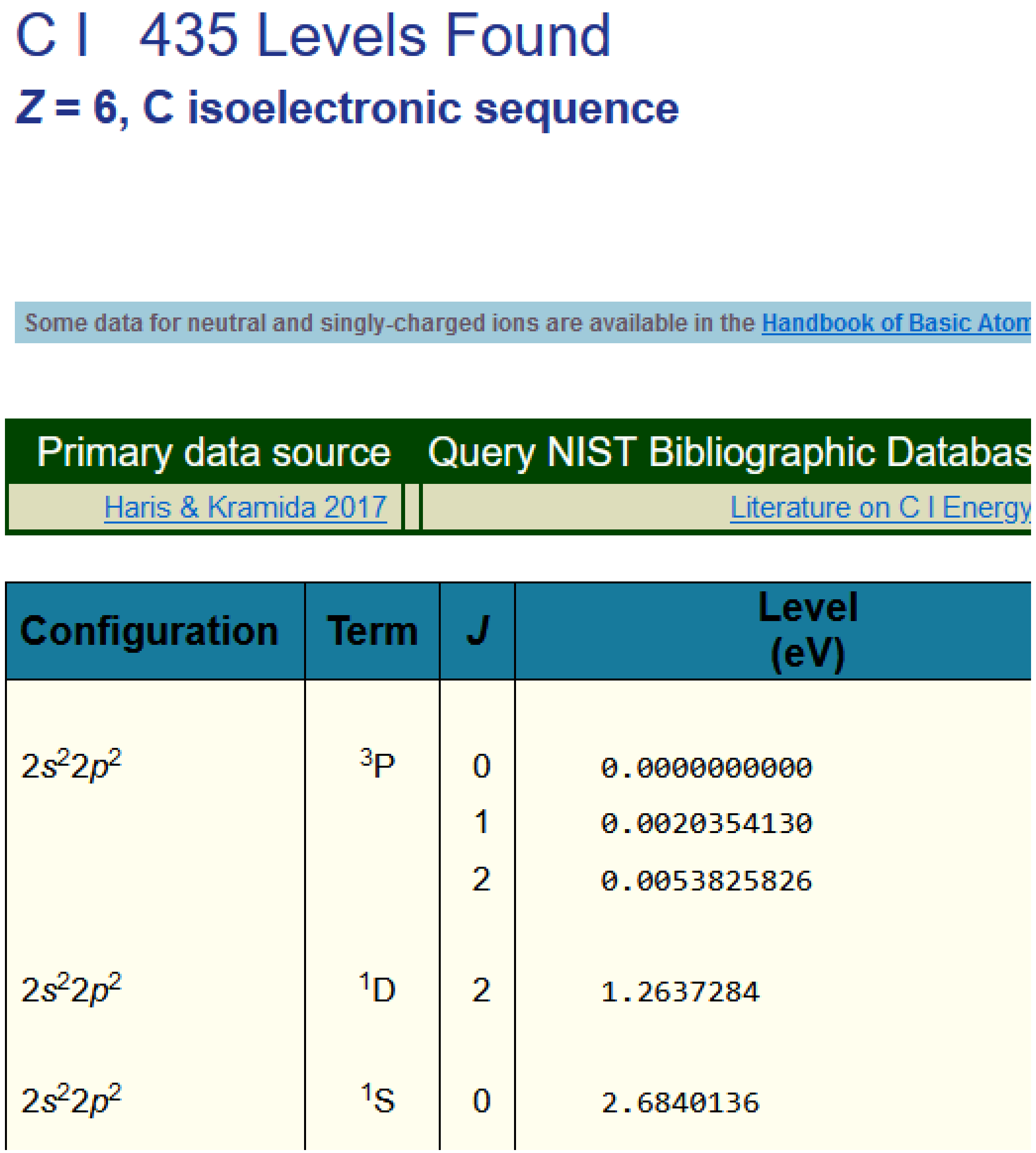
Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

Primary data source	
Unpublished level list prepared for line classifications published in Kelly 1987	These data are not critically evalua

Configuration	Term	J	Level (eV)	Uncertainty (eV)	Reference
$1s^2$	^1S	0	0.000000	0.000012	L3462
$1s2s$	^3S	1	59.020815	0.000012	
$1s2s$	^1S	0	60.92269	0.00012	
$1s2p$	$^3P°$	1	61.280575	0.000012	
		2	61.280856	0.000012	
		0	61.281244	0.000012	
$1s2p$	$^1P°$	1	62.216336	0.000012	

What do you expect to be the atomic term for the lowest energy of Li I?

Examples of atoms in their ground state with complicated multiplet term splittings



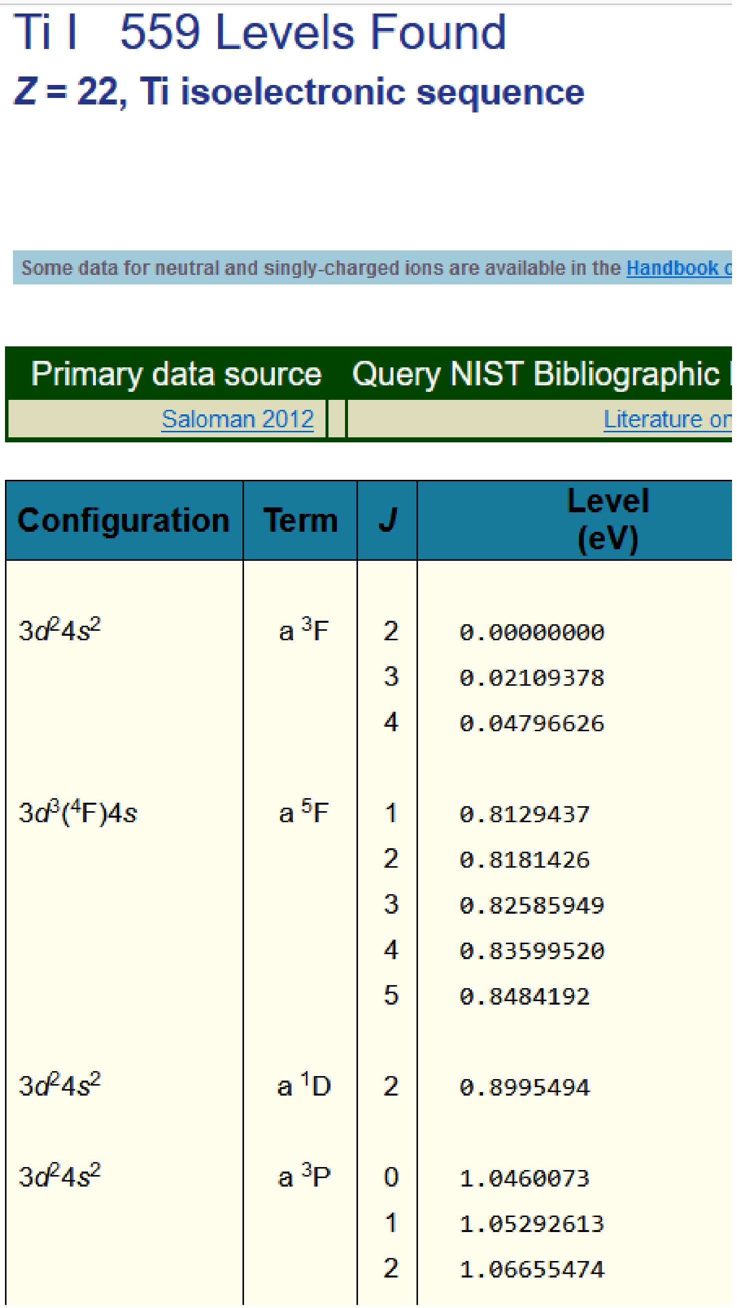
C I 435 Levels Found

Z = 6, C isoelectronic sequence

Some data for neutral and singly-charged ions are available in the Handbook of Basic Atom

Primary data source	Query NIST Bibliographic Databas
Haris & Kramida 2017	Literature on C I Energy

Configuration	Term	J	Level (eV)
$2s^2 2p^2$	^{3}P	0	0.0000000000
		1	0.0020354130
		2	0.0053825826
$2s^2 2p^2$	^{1}D	2	1.2637284
$2s^2 2p^2$	^{1}S	0	2.6840136



Ti I 559 Levels Found

Z = 22, Ti isoelectronic sequence

Some data for neutral and singly-charged ions are available in the Handbook o

Primary data source	Query NIST Bibliographic I
Saloman 2012	Literature or

Configuration	Term	J	Level (eV)
$3d^2 4s^2$	a ^{3}F	2	0.00000000
		3	0.02109378
		4	0.04796626
$3d^3(^4F)4s$	a ^{5}F	1	0.8129437
		2	0.8181426
		3	0.82585949
		4	0.83599520
		5	0.8484192
$3d^2 4s^2$	a ^{1}D	2	0.8995494
$3d^2 4s^2$	a ^{3}P	0	1.0460073
		1	1.05292613
		2	1.06655474