Problem set 2: Dirac Hydrogen, Helium and Alkali Elements

Due: COB, Tuesday, 24 January, 2022

Background & Motivation. *This homework assumes that you are familiar with Schrodinger solution for Helium including Direct and Exchange integrals, are conversant with Dirac's solution for hydrogen and familiarity with spectral terms (which arise from L-S coupling). The problems range from simple but useful to the zany through the standard textbook type problems. Problem [1] is straightforward. It requires you to download data from NIST and build a Grotrian (energy-level) diagram. The principal goal of this simple exercise is to devise necessary steps (down-loading and filtering out exactly the data that are needed; rapid plotting) that are fast and efficient. The instructor will illustrate his approach to this problem in an upcoming lecture. The textbook problems are [2] and [5]. Problem [3] is to make appreciate the amazing success of QED. Problem [4,5] are simple. However, [4] informs teaches something fundamental to the physics of the ISM while [5] helps you confront data with assumptions (in this case L-S coupling). Finally, the last (un-numbered) un-numbered problem is truly zany problem. To my knowledge, this is an original problem!*

All problems are 10 points each. The last problem is a bonus. You need not solve it but you will be graded should you elect to answer and the resulting score will be added to the score. So it is possible to get $> 100\%$ in this course.

[**1**] **Excited States of Helium.** Using NIST[1] plot the Grotrian diagram for the ground state and the first two excited states of Helium (Figure 1). Superpose a marker for $n = 1, 2, 3$ levels of H I. Comment on (1) the relative placement of triplet and singlet energy levels and (2) the relative placement of excited levels of helium with that of hydrogen. [If you are so inclined: write a program that, given name of species (e.g., "He I") accesses the NIST gateway and builds an elegant Grotrian diagram (of the sort shown in Draine's book). Caution: This may be time consuming but very useful for future use].

[**2**] **The Direct Integral.** In the class we discussed a variational approach to compute the total binding energy of Helium. For the principal Hamiltonian we assumed that the two electrons interact only with the nucleus but we let the nuclear charge be Z^* ("screening of charge by one electron for the other"). The perturbing Hamiltonian is e^2/r_{12}. We adopt $\Psi = \psi_{1s}(r_1)\psi_{1s}(r_2)$ where $\psi_{1s}(r_i)$ is the hydrogen $1s$ wave-function for electron with index i. Show that the electrostatic energy that arises from the perturbing Hamiltonian is

$$J_{1s^2} = 2\int_0^\infty V_{12}\rho(r_2)4\pi r_2^2 dr_2 \quad (1)$$

[1] `https://physics.nist.gov/PhysRefData/ASD/levels_form.html`

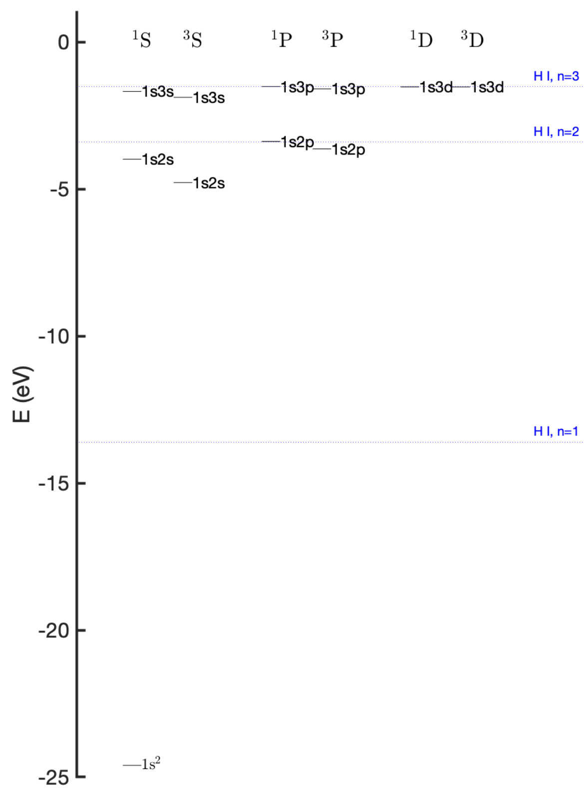

Figure 1: Partial Grotrian diagram for He I.

where $V_{12} = Q(r_2)/r_2$. and $Q(r_2)$ the charge within radius of r_2,

$$Q(r_2) \;=\; \int_0^{r_2} \rho(1) 4\pi r_1^2 dr_1 \; . \qquad (2)$$

Here $\rho(r_i) = e\psi_{1s}(r_i)\psi^*_{1s}(r_i)$ Show that $J_{1s^2} = {}^5\!/\!_8 Z^*$ Hartree.

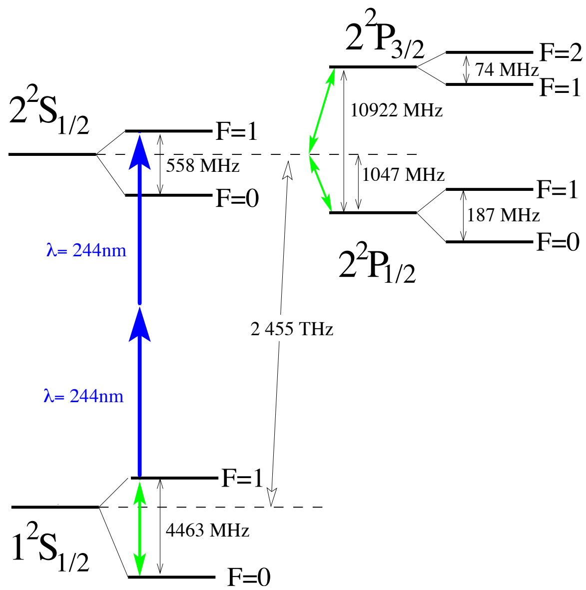

Figure 2: Energy level diagram for muonium (from K. P. Jungman, "Past, present and future of muonium". `https://ui.adsabs.harvard.edu/abs/2004shvw.conf..134J/abstract`. The blue lines show two-photon excitation from $1\,^2\mathrm{S}_{1/2} \rightarrow 2\,^2\mathrm{S}_{1/2}$. The effective wavelength to excite $1^2\mathrm{S}_{1/2}, \mathrm{F}=1$ to $2^2\mathrm{S}_{1/2}, \mathrm{F}=1$ is 2455 THz (about 122 nm).

[3] Muonium. Leptons and neutrinos have no internal structure, as shown by lack of scattering in scattering experiments. Furthermore leptons interact with other particles only via electromagnetism, weak force (and gravity). In contrast, protons and neutrons, being hadrons, exhibit structure (quarks) and interact with other particles via all forces. For this reason, *muonium*[2], μ^+e^- , variously given the label Mu or M, is prized as a laboratory for quantum electrodynamics. This is superior to hydrogen which is sensitive to the structure of the proton. The Grotrian diagram for muonium is given in Figure 2. Apply the best values for the masses, charges and magnetic moments from the Particle Data Group[3] to the Dirac Equation and see if you can reproduce Figure 2; for now ignore the hyperfine structure (indicated by quantum number F). Compare and contrast with a similar diagram for hydrogen (found in any textbook).

[2] The entity, $\mu^+\mu^-$, which is yet to be observed, is called as "true muonium".
[3] `https://pdg.lbl.gov/`

4. Ionization Potential. The first (and occasionally) second ionization potential of elements is an important input to physical models of the ISM. As you will learn later in the course, the opacity of hydrogen ground state lines (Lyman series and Lyman continuum) is very large in the ISM and as such interstellar radiation cuts off at the Lyman edge, 912 Å (corresponding to 13.6 eV). With this as background try to figure out why I assigned this straightforward problem.

The *Madelung* and the *Aufbau* rules help explain the periodic table. Review the run of ionization potential with Z, the nuclear charge (Figure 3). Explain the figure given your rudimentary knowledge of self-consistent models for atomic structure and discussion of the alkalis in the class room. Next, review Table 1.4 of Draine and become familiar with elements whose abundance, relative to that of hydrogen by number, is greater than 1 ppm (parts per million).[4] Of these, which elements have first ionization potential greater than that of hydrogen?

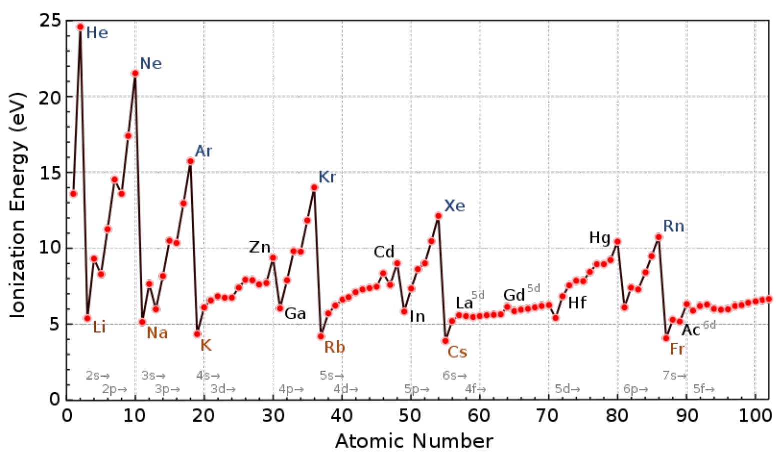

Figure 3: First ionization potential of elements.

[In tandem with Figure 3 may wish to review Figure 4, given in the Appendix. The latter figure follows from the former but is, in my view, visually more compelling.]

5. L-S Coupling. The L-S coupling model, first proposed by astronomer Henry Norris Russell (of the H-R fame)[5] and Frederick Saunders was motivated by data and not by theoretical ideas. Recall that in L-S coupling spin-spin interaction (i.e. Pauli Exclusion principle) and residual electro-static correction account for the splitting of gross energy levels (characterized by n quantum number) into *terms* ${}^{2S+1}\mathcal{L}_J$ where $\mathcal{L} = S, P, D, \ldots$. The

[4]Success in astronomy requires having a command of data. I have memorized to appropriately low precision the relative abundance of the top eight elements, He, O, C, Ne, N, Mg, Si, Fe,. Sounds trivial but this has been very helpful in my research.

[5]and also my academic grand-father; see `https://academictree.org/astronomy/tree.php?pid=60768`

further splitting of a given term into various J levels is due to spin-orbit interaction. A basic expectation is that J levels have energy $\propto J(J+1)-L(L+1)-S(S+1)$. In a given term, L and S are fixed. Thus, the separation of $J-1$ to J level is $\propto J$.

Test this expectation by reviewing, with help of NIST energy level portal, the J levels of the ground term of atoms whose valence electrons are p^2 (e.g., C, Si, Ge, Sn) or p^4 (e.g., O, S, Se, Te, Po).

6. Spectroscopic Terms. Consider carbon, $1s^2s^22p^2$. Let us excite this atom to $1s^22s^22p3p$. List the six terms ıterms resulting from this electronic configuration.[6] In contrast, the ground electronic state, $1s^22s^22p^2$ shows only three terms, ^{3}P, ^{1}D and ^{1}S. Work though the micro-states for p^2 and show that indeed the ground state admits of only three terms. Apply Hund's rule to the ground state terms of C I and O I and compare your answer against the Grotrian diagrams given in Appendix E of Draine.[7]

Bonus: A Zany UPS. Review the Grotrian diagram for Helium (Draine, Figure 14.3). You will note that a helium atom excited to the $1s2s\,{}^3\mathrm{S}_1$ level will decay to the ground state ($1s^2\,{}^1\mathrm{S}_0$) in about 2.2 hours. This is one of the longest "meta-stable" states in nature (excluding long-wavelength hyper-fine structure lines; more on those later in the course). Separately, your friend has invented an efficient laser which can excite helium atoms in ground state to this level. The combination of this laser and the long duration of the metastable state suggests an energy storage device – an UPS! An excited He atom is directed towards an anode where it will deposit a 19.8 eV electron. This UPS can tide over an interruption lasting less than an hour. For this scheme to work you need to filter out the excited helium atoms from those in the ground state. Can you think of a mechanism to do so?

Appendix

[6] These are all highly excited states. The Grotrian diagram in Appendix E of Draine shows only the lowest level of this excited sequence.

[7] You can work out the p^2 case by hand since the number of distinct micro-states are 15. For d^2 there are 45 distinct micro-states and the resulting terms are ^{1}S, ^{3}P, ^{1}D, ^{3}F, ^{1}G. If you are so inclined and have the time write a program to compute the surviving terms for pairs of identical electrons for $l=0,1,2,3$. A shortcut to be used only after doing the hard work: only terms with even $L+S$ survive Pauli Exclusion rule!

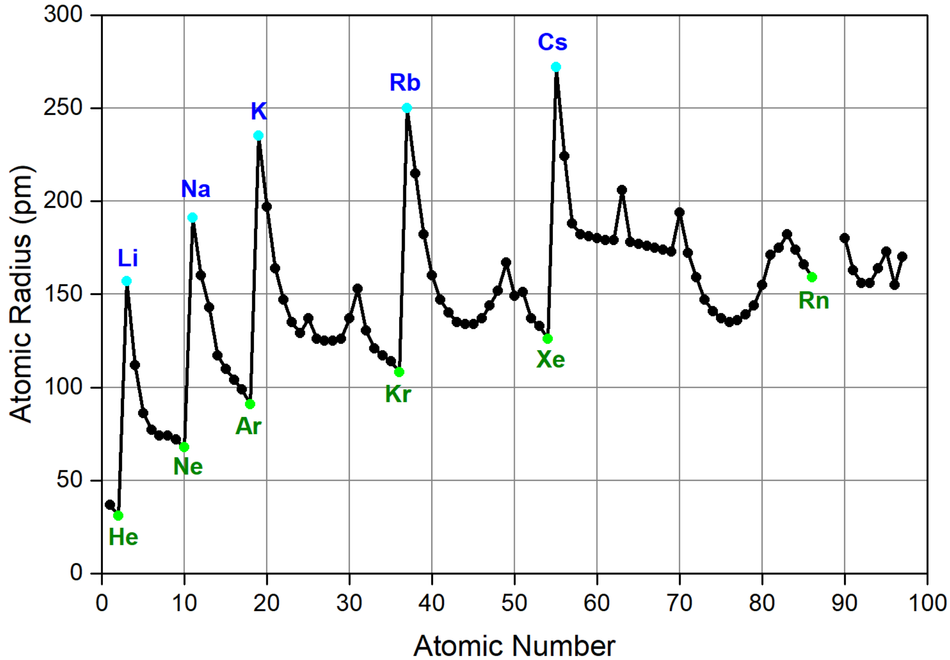

Figure 4: The run of radii of atoms with Z. Notice shrinking of the radius from alkali elements to noble gases, within each group (Ref: University of Wisconsin, Chemistry 109).