ASTR 541 - Interstellar Medium

Final Project Proposal

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1 General Idea

I enjoyed the lectures on electronic configuration and spectroscopic terms and I was intrigued by the concept of implementing an algorithm to solve the problems that we did in class by hand. Therefore, for my project I intend to write some code to work out electronic configurations, spectroscopic terms and also create energy level diagrams.

2 Intended Products

2.1 Code

I'd like to design a small bit of code to do the following. Note in several places I have to say *"(only guaranteed to work for atoms)"* because it seems that Hund's rules and the Aufbau Principle do not apply to ions in the same way - there don't seem to be rules for ions as far as I can tell.

Electronic Configurations

- **Input:** either a number of electrons and ionisations or a string like "HII" or "O3+"
- **Output:** the electronic configuration in a list of $[n, l, n_e)$ tuples - *(only guaranteed to work for atoms)*
- Add options to return in ASCII or LaTeX format

Spectroscopic Terms

- **Input:** Subshell parameters, n, l and number of electrons for the shell, n_e
- **Output:** the spectroscopic terms in the a list of $(2S + 1, L, J)$ tuples - *(only guaranteed to work for atoms)*
- Add options to return in ASCII or LaTeX format
- Sort terms by energy based on Hund's rules
- Work out the ground state spectroscopic terms given an electronic configuration

Energy Level diagrams

- **Input:** a list of spectroscopic terms (or a string to be parsed and it'll calculate them) for a series of levels, a list of transitions between levels as tuples $(n_u p, n_l o w, \lambda)$ - these transitions could be pulled directly from `linetools`
- **Output:** an energy level diagram with levels labelled with their terms, colour coded and annotated with transition wavelengths

- I'm also interesting in adding conditions for whether a transition is forbidden and changing the style of the arrow if it is
- So big picture I could get to a point where I write something like `plot_energy_levels("SII", transitions)` and it'll work out the electronic configuration, then the spectroscopic terms, plot up the levels and then add the transitions that you specify.

2.2 Discussion

I also think I could write/talk about a couple of different things that I found whilst reading:

- My implementation of the algorithms for working out the configurations/terms *(writing only, no one wants to hear this in the presentation haha)*
- There is a reason for the periodic table's weird shape, we can talk about it!
- Symmetry of spectroscopic terms within subshells
- The problems with the Aufbau Principle and how electron shielding plays a role in messing it up

3 Format

My intended format will be a link to the GitHub repository containing the code (which will be fully comments and docstringed), as well as a Jupyter Notebook that demonstrates its use and discusses the points above.