Atomic Spectra in Astrophysics

Potsdam University: Dr. Lidia Oskinova
lida@astro.physik.uni-potsdam.de
Fundamentals of stellar classification
- Stars are made of hot, dense gas
- Continuous spectrum from the "photosphere"
- Approximates a BB spectrum.

Hot stars $T > 10000\text{K}$ **Blue**

Solar-type: $T \sim 6000\text{K}$ **Yellow**

Cool: $T \sim 3000 \text{K}$ **Red**
Above the hot and dense photosphere is a thin layer of cooler gas - atmosphere.

Absorption lines are formed in the atmosphere.

Spectrum formation: chemical composition, element ionization and excitation, radiation field, fundamental stellar parameters.

Requirement: quantum mechanics; radiative transfer.
Astrophotography

- Henry Draper (1837-1882) made the first photograph of a star’s (Vega) spectrum showing distinct spectral lines in 1872.

- Other works by HD (degree in medicine):
  - Are there other inhabited worlds?, 1866;
  - Delusions of Medicine, Charms, talismans, amulets, astrology, and mesmerism, 1873;
  - The Discovery of Oxygen in the Sun by Photography, 1877.
Objective Prism Photography

- Henry Draper took hundreds photographs of stellar spectra before his death in 1882 (45yo).

- The objective prism method.

- 1885 Edward Pickering began to supervise photographic spectroscopy at Harvard.

- Obtained spectra of >100,000 stars hired women to analyze spectra.

- 1886 Draper’s widow became interested in Pickering’s research and funded it under the name Henry Draper Memorial.

- 1890 Draper Catalogue of Stellar Spectra, 10 351 stars.
Hyades cluster
Objective prism spectra of Hyades cluster
Edward Pickering (director, Harvard Observatory, 1877 to 1919)
Hired women as “computers” to systematically look at stellar spectra
‘Harvard computers’ incl. Williamina Fleming, Annie Jump Cannon,
Henrietta Swan Leavitt and Antonia Maury
Harvard Classification

Edward Pickering’s first attempt at a systematic spectral classification:  Sort by Hydrogen absorption-line strength; Spectral Type A = strongest Hydrogen - followed by types B,C,..,N (weaker)

Problem: Other lines followed no discernible patterns.
Annie Jump Cannon Leader of Pickerings computers, she noticed subtle patterns among metal lines. Re-arranged Pickerings ABC spectral types, throwing out most as redundant.

Left 7 primary and 3 secondary classes

Unifying factor: Temperature
Be Pickering’s computer: identify the lines
Become a Pickering’s computer: identify the lines

Rydberg: \[ \frac{1}{\lambda} = \frac{R_{\infty}}{1 + \frac{m_e}{m_H}} \left( \frac{1}{j^2} - \frac{1}{f^2} \right) \]

H\(\alpha\) \(\lambda 6563\)Å, H\(\beta\) \(\lambda 4861\)Å, H\(\beta\) \(\lambda 4341\)Å, ...

He\(\text{II}\) \(\lambda 4541\)Å, He\(\text{II}\) \(\lambda 4200\)Å, He\(\text{I}\) \(\lambda 4471\)Å, He\(\text{I}\) \(\lambda 4026\)
The Spectral Sequence is a Temperature Sequence

Gross differences among the spectral types are due to differences in **Temperature**.
Composition differences are minor at best. - Demonstrated by Cecilia Payne-Gaposhkin in 1920s

Why?

What lines you see depends on the state of excitation and ionization of the gas.
Example: Hydrogen Line $H\alpha$ $\lambda_{6564.6}\text{Å}$

B Stars (15-30 000 K): Most of H is ionized, so only very weak $H\alpha$

A Stars (10,000 K): Ideal excitation conditions, strongest $H\alpha$

G Stars (6000 K): Too cool, little excited H, so only weak H lines.

What lines you see depends on the state of excitation and ionization of the gas.
O stars
T > 30,000 K; He+, O++, N++, Si++

B stars
T = 11,000 - 30,000 K, He, H, O+, C+, N+, Si+

A stars
T = 7500 - 11,000 K, H(strongest), Ca+, Mg+, Fe+
F stars
$T = 5900 - 7500 \, K$; H(weaker), Ca+, ionized metals

G stars
$T = 5200 - 5900 \, K$; Strong Ca+, Fe+ and other metals dominate

K stars
$T = 3900 - 5200 \, K$; Ca+(strongest), neutral metals, H(weak), CH & CN
M stars

T = 2500 - 3900 K Strong neutral metals, TiO, VO, no H

L stars

T = 1300 - 2500 K; strong molecular absorption bands particularly of metal hydrides and neutral metals like sodium, potassium, cesium, and rubidium. No TiO and VO bands.

T dwarfs / Brown Dwarfs

T < 1300 K; very low-mass objects, not technically stars anymore because they are below the Hydrogen fusion limit (so-called "Brown Dwarfs"). T dwarfs have cool Jupiter-like atmospheres with strong absorption from methane (CH4), water (H2O), and neutral potassium.
Stellar Spectra
main sequence stars

The diagram shows the relative intensity of stellar spectra as a function of wavelength (nm) for different temperatures (K). The lines represent:
- Black: $T = 44,500$ K
- Purple: $T = 17,900$ K
- Blue: $T = 9000$ K
- Green: $T = 5900$ K
- Yellow: $T = 4350$ K
- Red: $T = 3580$ K

The x-axis represents wavelength in nanometers (nm), and the y-axis represents relative intensity.
Complex Atoms

Bohr atomic model of a nitrogen atom

- electron orbits
- electron
- proton
- neutron

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Non-relativistic Schrödinger Equation

\[
\sum_{i=1}^{N} \left( \frac{-\hbar^2}{2m_e} \nabla_i^2 - \frac{Ze^2}{4\pi\epsilon_0 r_i} \right) + \sum_{i=1}^{N-1} \sum_{j=1+1}^{N} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} - E \right] \times \psi(\vec{r}_1, ..., \vec{r}_N) = 0
\]

The first sum is a kinetic energy operator for the motion of each electron and the Coulomb attraction between this electron and the nucleus.

The second term: electron-electron repulsion term. Because of this term the equation cannot be solved analytically even for N=2.

Therefore, to understand such systems it is necessary to introduce approximations.
Central Field model

The easiest approximation → reduce the problem to a single particle situation. I.e. a potential does not depend on the angular position of electrons around the nucleus. **Central field potential** - the force acting on each electron only depends on its distance from the nucleus. The Schrödinger eq. can be written for ith electron

\[
\left(\frac{-\hbar^2}{2m_e} \nabla_i^2 + V_i(r_i)\right) \phi_i(r_i) = E_i \phi_i(r_i)
\]

where \(V_i(r_i)\) is the angle-independent central potential of each electron.

The total energy of the system is then \(E = \sum_i E_i\)

- The solutions, \(\phi_i(r_i)\), are called **orbitals**. Important to remember that this is an approximation.
By analogy with H, each atomic orbital can be written as the product of a radial and an angular function.

\[ \phi_i(\vec{r}_i) = R_{n_i l_i}(r_i)Y_{l_i m_i}(\theta_i, \phi_i) \]

The angular part is independent of the other electrons.

To specify central potential \( V_i(r_i) \), one usually considers a position of an electron in the central field of all the other electrons.

\[ V_i(r_i) = \frac{Ze^2}{4\pi\varepsilon_0 r_i} + \sum_{j\neq i} \left\langle \frac{e^2}{4\pi\varepsilon_0 |\vec{r}_i - \vec{r}_j|} \right\rangle \]

where \( <> \) represent average. Hence the radial part, \( R_{n_i l_i}(r_i) \) depends on all other electrons and cannot be obtained analytically.

Usually it is done iteratively - the self-consistent field (SCF) problem
It is standard to use the H-atom orbital labels: \(n, l, m\). The angular behaviour, given by \(l\) and \(m\) is the same. However, radial part is not the same as in case of H.

- The total wavefunction of the system
  \[
  \psi(\vec{r}_1, ..., \vec{r}_N) = \phi_1(\vec{r}_1), ..., \phi_N(\vec{r}_N)
  \]

- Let's consider spin and generalize orbital to spin-orbital
  \(\Phi_i(j) = \phi_i(\vec{r}_j, \sigma_j)\), where \(\Phi_i(j)\) means that spin-orbital \(i\) is a function of the space-spin coordinates of electron \(j\).

- The space-spin wavefunction for the total system then
  \[
  \Psi(1, ..., N) = \Phi(1), ..., \Phi(N)
  \]
**Indistinguishable Particles**

Consider a system with two identical particles. If the wavefunction of these particles is \( \Psi(1, 2) \), and the particles are indistinguishable, what property their wavefunction must have?

Physically observable is \( |\Psi|^2 \). Then, if particles are indistinguishable \( |\Psi(1, 2)|^2 = |\Psi(2, 1)|^2 \).

Symmetric solution \( \Psi(1, 2)| = +\Psi(2, 1) \), antisymmetric \( \Psi(1, 2)| = -\Psi(2, 1) \). **Pauli Principle:**

*Wavefunctions are antisymmetric with respect to interchange of identical Fermions*

**Fermions** - any particles with half-integer spin (electrons, protons, neutrons).

A two-electron wavefunction which obeys the Pauli Principle can be written as

\[
\Psi(1, 2) = \frac{1}{\sqrt{2}} [\Phi_a(1)\Phi_b(2) - \Phi_a(2)\Phi_b(1)] = -\Psi(2, 1)
\]

where \( \frac{1}{\sqrt{2}} \) is to preserve normalization.
The Pauli exclusion principle

Consider a two-electron wavefunction. If the two spin-orbitals, $\Phi_a = \Phi_b$, then $\Psi(1, 2) = 0$. This solution is not allowed.

Hence solutions which have the two particles occupying the same spin-orbital are excluded. The Pauli exclusion principle:

*No two electrons can occupy the same spin-orbital*

This exclusion is the key to atomic structure.

It also provides the degeneracy pressure which holds up the gravitational collapse of white dwarfs and neutron stars.
Electron Configurations

- For a H-like atom, the energy is determined only by principle quantum number: $E(1s) < E(2s) = E(2p) < E(3s) = E(3p) = E(3d) < E(4s) ...$

- For complex atoms the degeneracy on $l$ is lifted.

**Order of orbitals (filling) in multi-electron atom**

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s$
Following the Pauli exclusion principle, each orbital labeled $nl$ actually consists of orbitals with $l+1$ different $m$ value, each with two possible values $s$. Thus the $nl$ orbital can hold a maximum $2(2l+1)$ electrons.

- Write possible combinations of magnetic and spin quantum numbers for a $p$ electron.
Following the Pauli exclusion principle, each orbital labeled $nl$ actually consists of orbitals with $l+1$ different $m$ value, each with two possible values $s$. Thus the $nl$ orbital can hold a maximum $2(2l+1)$ electrons.

- An atomic configuration is given by distributing electrons among orbitals. First fill the atomic orbitals in energy order from the lowest energy orbitals upwards.

- Write the ground state configuration for carbon.

- Write the ground state configuration for neon.
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- An atomic configuration is given by distributing electrons among orbitals. First fill the atomic orbitals in energy order from the lowest energy orbitals upwards.

- The ground state configuration for carbon $1s^2 2s^2 2p^2$
- The $2p$ orbital is not full.
- The ground state configuration for neon $1s^2 2s^2 2p^6$
- The $2p$ orbital has closed shell configuration. A closed shell or sub-shell makes no contribution to the total orbital or spin momentum, $L$ or $S$.

- Atomic ions which have the same number of electrons form *isoelectronic series*. E.g. neon-like iron is
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- Atomic ions which have the same number of electrons form *isoelectronic series*. E.g. neon-like iron is \( \text{Fe XVII (Fe}^{16+}) \)
The Periodic Table Dmitry Mendeleyev (1834-1907)

The structure of peridic table-electron configurations of elements

Closed shells: \( n=1 \) orbitals \( K \)-shells

Closed shells: \( n=2 \) orbitals \( L \)-shells

Closed shells: \( n=3 \) orbitals \( M \)-shells etc.

Atoms with the same electron configuration outside a closed shell share similar chemical and optical properties.

Li, Na, K - a single electron outside a closed shell. *Alkali metals.*

Excited states - when one of the outermost electrons jumps to a higher orbital. He: \( 1s^22s, 1s^22p, 1s^3s \).

<table>
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<th>#</th>
<th>Element</th>
<th>Electron configuration</th>
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</table>
Angular Momentum in Complex Atoms

Complex atoms have more than one electron, hence several sources of angular momentum. Ignoring nuclear spin, the total conserved angular momentum, $J$ is the sum of spin plus orbital momenta of all electrons.

There are two coupling schemes of summing the individual electron angular momenta.

**L-S or Russell-Saunders coupling**

The total orbital angular momentum $\vec{L} = \sum_i \vec{l}_i$ and the total electron angular momentum $\vec{S} = \sum_i \vec{s}_i$

These are then added to give $\vec{J} = \vec{L} + \vec{S}$

Pauli Principle → closed shells and sub-shells (e.g. $1s^2$ or $2p^6$), have both $L=0$ and $S=0$. Hence, it is necessary to consider only electrons in open or partly-filled shells.