The Imperial College London Spectroscopy Group

Atomic Data Measured Using High Resolution Spectroscopy

Christian Clear (Research Fellow, Imperial College London)

The 14th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (ASOS14), Paris, July 2023
The Imperial College Group

People:
- Prof. Juliet Pickering (PI)
- Dr. Christian Clear (PDF)
- Dr. Florence Concepcion (PDRA)
- Milan Ding (PhD)
- Ruairi Shannon (PhD – Oct 2023)

Focus:
- Measure atomic data
  - High-resolution, high-accuracy fundamental properties of atoms
- Use high resolution spectroscopy to measure:
  - Transition wavelengths
  - Energy Levels
  - Transition probabilities, oscillator strengths, f-values
  - Nuclear effects - hyperfine & isotope structure
- Regularly collaborate with other experimental and theoretical groups.
Collaborations
Why Atomic Physics?

- Atomic data is vital for many fields:
  - Astrophysical spectra
  - Laboratory plasmas
  - Medical
  - Industrial
  - Fundamental physics in general
- 99% of observable universe in plasma form
  - Atomic data is vital to understanding the processes involved
- Very high accuracy needed
  - no other field of science places such higher demands on atomic data

High dispersion spectra of χ Lupi [1]

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  - Measured a long time ago
  - Using lower resolution techniques than are available now

- Our group focuses on astrophysically important elements:
  - Iron group (scandium to copper)
  - Rare earth

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Fourier Transform Spectroscopy (FTS)

- 1 fixed and 1 moving mirror
- Partially reflective beamsplitter
- Intensity recorded as function of path difference

Schematic of a Fourier transform spectrometer

\[ R = \frac{2L}{\lambda} \]

\[ L = \text{maximum mirror travel} \]
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Schematic of a Fourier transform spectrometer

Interferogram

Spectrum

FT

SNR

Wavenumber (cm\(^{-1}\))
Fourier Transform Spectroscopy (FTS)

- Max. path difference: 20 cm
- Resolving power: $2 \times 10^6$ at 200 nm
- Maximum resolution: 0.025 cm$^{-1}$
- Range: 74,000 – 12,000 cm$^{-1}$ (135 – 850 nm)
- Wavenumber accuracy: ±0.001 cm$^{-1}$
Fourier Transform Spectroscopy - Advantages

• High Resolving Power:
  • Doppler-limited resolving power – fully resolve 3d group line at 50,000 cm\(^{-1}\) (widths are few hundredths of a wavenumber).
  • High enough for nuclear effects such as Hyperfine and Isotope Structure.

• Linear wavenumber scale and high wavenumber accuracy:
  • 1 part 10\(^{8}\) achievable.

• Slowly-varying photometric response:
  • Reliable and accurate intensity calibration.
  • Comes from the fact that all elements are measured at once therefore small drifts in source won’t affect relative intensities.

• Large and variable free spectral range:
  • V. important for large-scale studies.
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**Which other tools are available?**

- Grating spectroscopy
  - Wide spectral ranges
  - Lower resolving powers
  - Lower accuracies

- Fabry-Perot interferometer and Laser spectroscopy
  - High resolution and accuracy
  - Line-by-line techniques

- Theoretical calculations
  - Extensive but with large uncertainties
  - Provide essential data for experimentalists as well
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Sources – Hollow Cathode Discharge
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Noble carrier gas ionised → Gas ions sputter cathode material → Metal atoms excited and ionised in plasma

Predominantly neutral and singly-ionised species

• High stability
• Water-cooled:
  • High currents
  • Reduction of Doppler widths
Sources – Penning Discharge

- Same excitation method as HCD with addition of static magnetic field
- Magnetic field confines plasma, leading to higher ionisations

Predominantly *singly*- and *doubly-ionised* species
Wavelengths

• Record spectra. **Coadding** $n$ spectra improves SNR by $\sqrt{n}$

• Fitting – Voigt or Centre of Gravity

• Extracted Parameters:
  • Peak position ($\sigma$ in cm$^{-1}$)
  • Width of line (FWHM)
  • Area under curve – **intensity**
Wavelengths

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- Fitting – Voigt or Centre of Gravity
- Extracted Parameters:
  - Peak position (\(\sigma\) in cm\(^{-1}\))
  - Width of line (FWHM)
  - Area under curve – **intensity**
- Wavenumber uncertainties:
  - Both a statistical uncertainty, from fitting, and a calibration uncertainty.
  - FTS wavelength uncertainty: **few** parts in $10^8$

\[
\delta \sigma_{\text{stat}} = \frac{\sqrt{\text{FWHM} \times R_{\text{spec}}}}{\text{SNR}}
\]

\[
= \frac{\text{FWHM}}{\sqrt{N} \times \text{SNR}} \approx \frac{\text{FWHM}}{2 \times \text{SNR}}
\]

\(N = \) number of points across the line
Wavelengths - Calibration

- Small change in path of laser and source light through FTS gives linear wavenumber shift

\[ \sigma_{\text{corr}} = (1 + K_{\text{eff}})\sigma_{\text{obs}} \]

- Match lines to standards (usually Ar II) or to lines in previously calibrated spectra to give \( K_{\text{eff}} \)
Wavelengths - Calibration

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\[ \sigma_{corr} = (1 + K_{eff}) \sigma_{obs} \]

- Match lines to standards (usually Ar II) or to lines in previously calibrated spectra to give \( K_{eff} \)

- Total calibration uncertainty is then sum of all matched line differences:

\[ \delta \sigma_{calib} = \delta \sigma_{prev} + \sum_i \delta k_i \]

- Finally get total uncertainty of a measured line:

\[ \delta \sigma_{total} = \sqrt{\delta \sigma_{stat}^2 + \delta \sigma_{calib}^2} \]

Example wavenumber calibration schema for Ni II
Energy Levels – Term Analysis

- Derivation of energy levels from observed spectral lines
- Energy levels give the fundamental atomic structure of nature

<table>
<thead>
<tr>
<th>line</th>
<th>wavenumber</th>
<th>peak width</th>
<th>delta</th>
<th>eq width</th>
<th>itn</th>
<th>H tags</th>
<th>identification</th>
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<tr>
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<tr>
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<tr>
<td>43</td>
<td>25552.247964</td>
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<td>no id</td>
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<td>80.97</td>
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<td>0 L</td>
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<td>34021±01</td>
<td>100.17</td>
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Energy Levels – Term Analysis

- Derivation of energy levels from observed spectral lines
- Energy levels give the fundamental atomic structure of nature
- Ritz wavelengths often more accurate than observed lines.
- Ritz wavelengths also provide data of experimental accuracy for lines not observed in the lab:
  - very weak lines or,
  - parity-forbidden transitions
- Levels also form one of the key inputs to semi-empirical calculations:
  - Allowing the “fine-tuning” of calculated eigenvalues to the experimental energy levels resulting in more accurate eigenvectors and therefore transition probabilities.

Energy Levels – Term Analysis

- Observed linelist
- Compare linelists
- Identified lines
- Fits: improve level accuracy
- Improved levels
- Search for new levels and lines
- Unidentified lines

Processes:
- Data input/output

Diagram showing energy levels and transitions for Ni II 3d^8 (^3L) nl.
Energy Levels – Term Analysis

Spectral term analysis is like a complicated jigsaw, where:

The pieces never fit exactly - lines have finite uncertainties
Some pieces fit spuriously - accidental wavelength coincidences
Some crucial pieces are missing - missing lines (weak or blended)
There are pieces belonging to a completely different puzzle - impurities
And the picture on the box is not very clear - theory as a guide
Transition Probabilities – Branching Fractions

\[ B_{12} = \frac{g_2}{g_1} \frac{c^3}{8\pi h \nu_{12}^3} A_{21} \]
Transition Probabilities – Branching Fractions

\[ B_{12} = \frac{g_2}{g_1} \frac{c^3}{8\pi \hbar \nu_{12}^3} A_{21} \]

Spontaneous Emission

Absorption

Stimulated Emission

Decay to multiple levels

Einstein coefficients

Decay to multiple levels

\[ A_{21} = \frac{BF_{21}}{\tau_2} \]

\[ BF_{21} = \frac{I_{21}}{\sum_i I_{2i}} = \frac{EW_{21}}{\sum_i EW_{2i}} \]

BF = Branching fraction

EW = Line equivalent width

\( \tau \) = Level lifetime (s)
Transition Probabilities – Intensity Calibration

- Branching fraction:
  \[ BF_{21} = \frac{I_{21}}{\sum_i I_{2i}} = \frac{EW_{21}}{\sum_i EW_{2i}} \]

- Relative intensities = intensity calibration

- \( D_2 \) from 1650 – 3600Å, W at longer

- Many sources of uncertainty:
  - Lifetimes
  - Lamp calibration
  - Alignment
  - Separation of spectral lines
  - Missing lines
  - Self-absorption

- Typical log\((gf)\) uncertainties 5% - 10%
Nuclear Effects

• Hyperfine Structure:
  • Orders of magnitude smaller than fine structure
  • Caused by interactions of the nuclear dipole moment ($I$) with atomic magnetic and electric fields
  • Affects isotopes with odd mass numbers

Mn I transition from $3d^6(^5D)4s - 3d^5(^6S)4s4p(^3P)$ [1]

Nuclear Effects

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  - Orders of magnitude smaller than fine structure
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- **Isotope Structure:**
  - Additional neutrons give:
    - Mass effect
    - Volume effect
  - Component intensities are proportional to relative abundance

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**Isotope structure in Ni II λ 6884 Å** [1]

<table>
<thead>
<tr>
<th>$^\text{xNi}$</th>
<th>%</th>
</tr>
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<tbody>
<tr>
<td>58</td>
<td>68.1</td>
</tr>
<tr>
<td>60</td>
<td>26.2</td>
</tr>
<tr>
<td>61</td>
<td>1.14</td>
</tr>
<tr>
<td>62</td>
<td>3.63</td>
</tr>
<tr>
<td>64</td>
<td>0.93</td>
</tr>
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Nuclear Effects

- Well resolved in experiment, but blended in stellar spectra
- Wavelengths shifted
- Systematic errors in width – lead to incorrect abundances
- FTS able to determine HFS A values to few %

## Recent Successes

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<td>Magnetic hyperfine interaction constants for 292 energy levels, only 28 were previously known. Characterises broadening of stellar absorption lines, essential for accurate abundance analyses.</td>
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Ding et al., in preparation (2023)
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Summary

- Line identifications and accurate line wavelengths
  - accurate to at least 1 part in $10^7$ (0.15 mÅ at 1500 Å, 0.001 cm$^{-1}$)

- Atomic energy levels
  - Typically, 0.001 – 0.006 cm$^{-1}$ uncertainty

- Hyperfine and isotope structure parameters (line broadening)
  - Fitting to a few %

- Oscillator strengths, transition probabilities, f-values
  - accurate to <10%

- Able to measure from VUV to visible
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• Conclusion: Imperial needs an IR FTS!
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</tr>
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<tbody>
<tr>
<td>Max. path difference</td>
<td>50 cm</td>
</tr>
<tr>
<td>Resolving power</td>
<td>1 x 10^6 at 1000 nm</td>
</tr>
<tr>
<td>Maximum resolution</td>
<td>0.018 cm⁻¹</td>
</tr>
<tr>
<td>Range</td>
<td>~400 – 1720 nm</td>
</tr>
<tr>
<td>Wavenumber accuracy</td>
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Bruker IFS 125HR
## Future work

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We are open to data requests and collaborations!

Please come and discuss your atomic data needs with us.