High-resolution spectroscopy for exoplanet characterisation

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What did we learn from yesterday’s session?

**Studying exoplanet atmospheres is useful to understand their nature, formation, evolution, and habitability**

High-resolution spectroscopy:

- Amplifies signals through cross correlation
- Robustly identifies species
- Filters out stationary spectral components (telluric lines)
- Measure masses and inclination of non-transiting planets

*A couple of dozen hot Jupiters have atoms and/or molecules detected at high spectral resolution*

Open questions for this lecture:

- Can the method be applied on large scale?
- What’s the effect of the stellar spectrum?
- How do we assess the statistical significance of the cross correlation signals?
From demonstration to comparative exo-planetology

How can we increase the S/N of the cross correlation function?

\[
\frac{S}{N} \propto \frac{N_{\gamma,P}}{\sqrt{N_{\gamma,*}}} \sqrt{n_{\text{lines}}}
\]

- \(n_{\text{lines}}\): spectral range of the instrument
- \(N_{\gamma}\): telescope size
- \(P_{\gamma}\): instrument efficiency
- \(\gamma, \star\): brighter stars

Modern spectrographs can compensate smaller apertures with increased spectral range and efficiency.

Example: \(O_2\) line around 760.45 nm at \(R=10^5\) (black), \(3\times10^5\) (blue), \(5\times10^5\) (green), and \(10^6\) (red)

from Lopez-Morales+19
From demonstration to comparative exo-planetology

Only a small fraction of the current detectable sample has been observed

30-40 exoplanets (transiting and non-transiting) within reach of current facilities

**Sensitivity range:** from warm Neptunes to ultra-hot Jupiters

**Current sample:** most of the measurements still focussed on Jupiter/Saturn-size planets
The TESS mission: small(er) planets around bright stars

Small (4×10cm) telescope on a 2:1 lunar resonance orbit, 2yrs+ mission

Optimised to find small planets (< 4 R⊕) around bright stars

Launched in April 2018, primary mission completed in Aug 2020
Extended mission ongoing (half-way through)

3,300+ candidates (excl. false positives), 156 confirmed
From demonstration to comparative exo-planetology

On paper there should be a few dozen TESS planets already observable.

Confirmation of TESS planets focusses on rocky exoplanets or planets in the evaporation valley.

No significant change to the current observable sample yet.
The most common exoplanets are not giants.

Statistics from *Kepler* detections of transiting planets around FGK stars.

The most common planets have **no analogues** in the solar system (their size is intermediate between Earth and Neptune).
Determining the nature of exoplanets

Combining observational techniques to get the planet density

The most common exoplanets (2-4 Earth radii) can have a wide range of compositions
Determining the nature of exoplanets

Intrinsic degeneracy between interior and envelope mass and composition

Mini-Neptunes
Scaled-down versions of giant gas planets

Super-Earths
Scaled-up versions of rocky planets

Small, dense core
(iron & silicates)

Extended atmosphere
(Hydrogen)

Big, light core
(mostly water ice)

Thin atmosphere
No \( \text{H}_2 \)
\( \text{H}_2\text{O} \) [\(+ \text{CO}_2 \text{ etc.}\)]

Studies of **exoplanet atmospheres** can solve the degeneracies
The cloudy atmosphere of GJ 1214 b

6.5× Earth mass, 2.7× Earth radius orbiting a small M-dwarf star
Planet temperature is 400-550 K

Nearly 100 hours of HST and 13 transits show a spectrum consistent with a flat line

Density is 1.87 g cm$^{-3}$: too low to be lacking an atmosphere
Too big for a pure-water atmosphere: must have significant H$_2$

Most likely explanation is a high-altitude thick cloud layer equalising the planet radius regardless of wavelength
Another cloudy atmosphere: the case of GJ 436 b

Most likely explanation is (again) a high-altitude thick cloud layer equalising the planet radius regardless of wavelength.

HST transit spectroscopy also sees a relatively flat spectrum. The data alone is not excluding a pure-water atmosphere due to lower precision.

22x Earth mass, 4.2x Earth radius orbiting a small M-dwarf star. Planet temperature is 400-550 K.

Knutson+14

Massive H$_2$ evaporation has been measured. The planet has an extended hydrogen envelope.
Peeking above the clouds: the Neptune-size GJ 3470 b

14× Earth mass, 4.6× Earth radius orbiting a small M-dwarf star

Much less telescope time: data cannot exclude a water world, but we have seen H2.

Density is 0.80 g cm\(^{-3}\): too low to be lacking an atmosphere

Massive H\(_2\) evaporation has been measured
The planet has an extended hydrogen envelope

Benneke+19: Mie scattering from ~0.6\(\mu\)m particles - opacity “drop-off” around 2-3\(\mu\)m
Seeing above the clouds at high spectral resolution

H$_2$O transmission spectrum of a hot Neptune across the NIR spectral range

High-altitude cloud deck (0.1-1 mbar) completely mutes “weak” water lines
Peaks of H$_2$O band still form above the clouds

Observations at low spectral resolution produce flat spectra for clouds top $\leq$ 1 mbar
At high spectral resolution there is still residual spectrum above the clouds

(see Gandhi+20, Hood+20)
Solving the cloud-metallicity degeneracy

Cloud decks extending to high altitudes are degenerate with high metallicity (= high mean molecular weight) at low spectral resolution.

High metallicity and high clouds both contribute to mute the spectral features.
Simulating observations with HR spectrographs

Need to account for telluric absorption cancelling some of the advantages of HRS

8 hrs of observations (~4 transit) sufficient to confidently detect the Benneke+19 scenario
Estimating significance and error bars

S/N versus statistical significance
Injection and retrieval of models
Bayesian retrievals via MonteCarlo
From detecting to measuring: detection significance

Quantifying the “goodness of fit” of a model is not (yet) possible at high-res

Low-res spectroscopy

WASP-39b, Wakeford+ 2017

High-res spectroscopy

Brogi+ 2012

Low-res spectroscopy recovers an actual spectrum
Models can be matched to observations via chi-square fitting (also in a Bayesian way)

High-resolution spectroscopy measures a level of correlation

How do we even quantify significance?
How do we “select” models?
**S/N as a proxy for detection significance**

Noise: the standard deviation of all the other cross correlation values

Signal: the peak value of the total cross correlation

\[ S/N = \frac{\text{Peak CC}}{\text{stdev(CC)}} \]

Immediate and intuitive quantity to compute

Some of the “noise” is actually auto-correlation / aliasing signal

Some \((V_{\text{sys}}, K_P)\) values will have increased noise due e.g. to residual telluric or stellar lines

At low SNR peaks can arise by just noise fluctuations

Error bars are usually defined by \((V_{\text{sys}}, K_P)\) values corresponding to \((S/N)_{\text{max}} - 1\)
Detection significance from statistical tests on the CCFs

Testing the means of the in-trail and out of trail cross-correlation values

Null hypothesis $H_0$: in-trail and out-of-trail sample have the same mean

- **Welch t-test** (data samples can have ≠ size and variance) used to reject $H_0$
  - $p$-value $\Rightarrow$ detection significance $\sigma$

Hp #1: the cross correlation values follow a Gaussian distribution (usually true)

Hp #2: the cross correlation values are independent (depends on RV sampling)

Dependence on the “width” of the in-trail sample (at least 1 FWHM)

$n$-σ error bars can correctly be determined as $\sigma_{\text{max}} - n$
Five carbon- and nitrogen-bearing species in a hot giant planet’s atmosphere


4 transits of hot Jupiter HD 209458b (1,500K) $\Rightarrow$ H$_2$O + 5 species simultaneously detected

**What does it mean for the atmosphere of HD 209548 b?**

Need to move *beyond detecting* and towards *measuring* (We will see this in the next lecture!)
Need to: account for any biases of the analysis
understand what’s the information content at high-res
design a method to select the best model within a grid
explore the whole parameter space to understand degeneracies
The data analysis is not completely harmless

The removal of telluric and stellar lines affects exoplanet lines

Shown by Brogi & Line (2019) on simulated data - easy to see in the noiseless case

Different telluric removal techniques show different biases
(e.g. airmass de-trending, PCA, Sysrem)

Altered shape & depth of spectral lines ⇒ biased abundances and T

Model reprocessing is **unavoidable** to obtain **unbiased measurements** from HRCCS
Model reprocessing: an unavoidable step

The model planet spectrum is injected in the data or a synthetic sequence is created

Can we translate cross correlation into a statistically meaningful quantity (a likelihood)?
What is the information content in high-res data?

High-res data is normalised to remove stellar & telluric spectrum
(loss of absolute level of continuum in both emission and transmission)

No actual “spectrum” is visible
(no ground truth - consequences for goodness of fit)

Data is still expressed in units of stellar spectrum
(absolute line-to-line and line-to-continuum depths can still be recovered)

Line ratios and line shape change with absolute abundances and temperatures

HRCCS can measure absolute and relative abundances with the right framework
Building a likelihood function for high-res data

Brogi & Line (2019), but also Zucker (2003) and Gibson et al. (2020)

We would like to:

- use the match in line position
- distinguish between +ve and -ve correlation
- use information about line shape and amplitude

\[
\log(L) = -\frac{N}{2} \log \left[ s_f^2 - 2R(s) + s_g^2 \right].
\]

\(\log L\) contains the \textbf{model} and \textbf{data variances} \(s^2\)

(it accounts for the amplitude of lines)

\[
C(s) = \frac{R(s)}{\sqrt{s_f^2 s_g^2}}.
\]

\(\log L\) contains the \textbf{cross covariance} \(R\)

(not normalised - accounts for amplitude of lines)

(penalises anti-correlation - accounts for emission/absorption)
Model selection through likelihood-ratio tests

Exploring a grid of equilibrium models by varying metallicity and C/O
Giacobbe, Brogi, Gandhi et al., Nature (2021)

Addition of clouds (with LR parameters) highly favoured (17 sigma)

Disequilibrium chemistry disfavoured

HD 209458b formed beyond the snow line and subsequently migrated w/o accreting ice planetesimals
Running a Bayesian retrieval on HR data

Letting the data “inform” model selection to explore full parameter space

Input parameters
Abundances, T-p profile, Velocities

Radiative transfer

Model spectrum

Observed Data
Analysis
Processed Data (noisy)

Modelled Data
Analysis
Processed Model (noiseless)

Cross Correlation
log-Likelihood

Your favourite MCMC sampling algorithm
The emission spectrum of WASP-77 A b

Line, Brogi, Gandhi et al., *Nature*, accepted (coming soon!)

IGRINS@Gemini-S (8.1m)

R\(\sim\)45,000
1.45 - 2.45 \(\mu\)m simultaneously
Silicon immersion grating
(keeping the instrument compact)
Achieving “solar system” precisions in the chemistry

Full retrieval with the Brogi & Line (2019) likelihood

15-parameter MCMC
7 gases + 5 T-p parameters +
2 velocities + scaling

Bound and very tight
CO and H2O abundances

Upper limits on
CH₄, NH₃, H₂S, HCN

Monotonically decreasing T-p profile
Achieving JWST precisions in the chemistry

0.1-0.2 dex precision in **absolute abundance** for H2O and CO

Validated independently with 2 retrieval frameworks
CHIMERA (Line)
GENESIS/HyDRA-H (Gandhi)

Accuracy tested by changing:
Data processing
T-p parametrisation
Choice of line lists

Computationally intensive
1 model evaluation = 5-10s on a single CPU core (GPU+parallel computing)

What can we do with such precision?
Constraints in the chemistry

WASP-77 A b has sub-solar metallicity but solar C/O

CO+H₂O \Rightarrow \text{Metallicity, C/O}

\[
\frac{[\text{C+O}]}{\text{H}} = -0.48^{+0.15}_{-0.13}
\]

"High C/O" (>0.8)

C/O & metallicity of hot Jupiters can be connected to formation and early evolution scenarios

2021 has seen three measurements of C/O & metallicity
(Giacobbe+21; Line+21; Pelletier+21)
The host star as a source of noise

Influence on both emission and transmission spectra
Modelling and removal of the stellar spectrum
One example: rotation of giant exoplanets
Stars are not black bodies

Their spectra have an “envelope” (continuum) plus spectral lines

Spectral lines are formed by different atoms / molecules vs. temperature

Spectral lines are formed at various depths, each characterised by $T$ and $v$

Spectral lines are formed at various points on a rotating stellar surface

We expect stellar spectra to be a “nuisance” for exoplanet detections
Stars and hot Jupiters can have “similar” spectra

Especially true for the CO spectrum at 2.3 µm

Stars of spectral type G or later exhibit strong CO lines, as hot Jupiters do!

Cooler stars (M-dwarfs) also have TiO and H$_2$O similarly to hot exoplanets

We expect stellar spectra to be a “nuisance” for exoplanet detections
Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra

\[
RV_P = V_{\text{orb}} \sin(i) \sin[2\pi\varphi(t)] = K_P \sin[2\pi\varphi(t)] \\
RV_\star = K_\star \sin[2\pi(\varphi(t) - 0.5)]
\]

Explicit time dependence of phase:

\[
\varphi(t) = \frac{t - T_0}{P_{\text{orb}}}
\]

This is in the rest frame of the exoplanet system!
Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra

Radial velocity of the system as a whole compared to the centre of mass of the solar system

$$RV_{\text{obs}} = RV_\star(t) + V_{\text{sys}}$$
Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra

\[ RV_{\text{obs}} = RV_\star(t) + V_{\text{sys}} + V_{\text{bary}}(t) \]

Altogether we expect typical changes of 500 m/s over a full set of spectra (5 hrs)
Stellar cross correlation noise in dayside spectroscopy

Case 1: Search for CO in the thermal spectrum of HD 189733 b (de Kok+13)

The star HD 189733 also has CO lines $\Rightarrow$ contaminating signal

Where does stellar noise appear in the $(V_{\text{rest}}, K_P)$ diagram?

The star moves with the system, so it should be at $V_{\text{rest}}=0$
It should also appear at $K_P \sim 0$ because its RV amplitude is $< 1$ km/s

Very strong residuals and small change of the Earth’s barycentric velocity cause stellar residuals to propagate to $K_P \neq 0$ and peak at small $K_P$

Planet detection is not prevented but highly confused
Applications to emission spectroscopy

Results from Chiavassa & Brogi (2019)

HD 189733b

Stellar spectra in emission spectroscopy can be corrected with both 1D and 3D stellar models.
A transiting planet distorts the stellar spectrum

Stellar intensities vary according to distance from centre (limb darkening)
Stars are rotating with a spin-orbit angle that can be non-zero

**Centre-to-limb variations**
A transiting planet blocks regions of the stellar surface with different intensities

**Rossiter-McLaughlin effect**
A transiting planet blocks regions of the stellar surface with different rotation

If uncorrected, stellar residuals during transit can dominate the cross correlation signal
The Rossiter-McLaughlin effect

A transiting planet blocks a (changing) portion of a rotating star
The line profile gets distorted, and the CCF is also asymmetric

Problem: stellar RVs are determined by fitting the CCF with a symmetric profile

Beginning of the transit
Blue-shifted part of the rotating disk is blocked ⇒ red-shifted CCF

End of the transit
Red-shifted part of the rotating disk is blocked ⇒ blue-shifted CCF

Adapted from Gaudi & Winn 2007
RM effect shifts centroid of cross correlation functions

Distorted line profiles are fitted with Gaussian profiles

The shape of the RM effect can be used to estimate the angle between the orbit of the planet and the spin of the star: the spin-orbit angle

Smaller planets or highly misaligned planets can have very small RM effect
RM effect visualised through Doppler tomography

Requires dividing each CCF by the out-of-transit (symmetric) CCF

This allows us to see the planet shadow sweeping in radial velocity between ±vsini

Kelt-7b, Zhou+16
But wait... isn’t that what the planet does too?

Yes, planet transmission spectra and planet shadows both sweep in RV during transit

Example: the transmission spectrum of HD 189733b

Stellar RM
Sweeping \( \pm v\sin i = \pm 3.3 \text{ km/s} \)

Planet signal
Changing by \( \pm 16 \text{ km/s} \)

The stellar RM is \( \sim \) transit depth, the planet signature is 10-100\( \times \) smaller!

Even if the slope of the RM effect is significantly different, it can still contaminate the planet signal due to its big amplitude!
Modelling the distorted stellar spectrum

Spectrum as $f(\phi, \mu)$
Planet occupancy (0,1)
Doppler shift (rotation)

see e.g. Chiavassa & Brogi 2019

Example: Doppler tomography of modelled CO stellar lines in HD 189733

Uncorrected
1D line modelling
3D stellar modelling

HD 189733b transmission
Bridging the gap towards habitable planets
(in the next 10-15 years)
Planets around M-dwarf stars

The Sun

You are here!

Proxima Cen
(M5.5)

Trappist-1
(M8)
The key sample: M-dwarf planets

M-dwarfs are smaller and cooler than the Sun, but still bright in the infrared. Warm sub-Neptunes around (nearby) M-dwarfs are within reach of current techniques.

Transit
1.3% depth

Thermal emission relative to star
(2.3 µm)
140 ppm

Thermal emission relative to star
(3.5 µm)
470 ppm

Solar-type star

1.200 K, 1.15 R_{Jup}

M5.5 star

2.0 R_{Earth}
800 K, 4 R_{Earth}
700 K, 4 R_{Earth}
Planets around M-dwarf stars are abundant

Dressing & Charbonneau (2015): 2.5 planets / star, 30% in the classic habitable zone
M-dwarf stars are abundant ⇒ Temperate M-dwarf planets are nearby

Current (incomplete) census: 70 planets within 10 pc, 35 within 5 pc
Notable examples: Proxima Cen b,c (1.3 pc) & Trappist-1 a-g (12 pc)
Habitable zones around M-dwarfs

Habitable zone (Earth-based) moves inward with decreasing stellar mass
Potentially habitable planets orbit very close to M-dwarfs

Key observational consequences
Temperate planets have an increased probability to transit M-dwarfs
Transits repeat every few days only and can be stacked quickly to increase S/N

Kopparapu+ 2013

Graph showing the habitable zones for M-dwarfs with Earth and Proxima Cen b indicated.
Transiting terrestrial planets around M dwarfs

Oxygen in high-resolution transmission spectra
Average line depth is 1/3 of the CO dayside signal from τ Boo b

Challenge: even the closest M-dwarf is much fainter than τ Boo (at least 6 magnitudes)
Extremely Large Telescopes + Hi-res spectroscopy are needed to reach the S/N

39m E-ELT, 30 transits (3 years) ⇒ 3σ detection

High instrumental efficiency and RV separation from telluric oxygen is key
(Snellen+13, Rodler & Lopez-Morales14; Serindag & Snellen 19; Lopez-Morales+19)
The star is faint in the optical (B=12.95, $V=11.13$, $R=9.45$) $\Rightarrow$ low S/N

Gain in S/N from cross-correlating with thousands of lines: $65-80\times$

Current spectrographs are starting to be optimised to observe M dwarfs

Gain in S/N from cross-correlating with thousands of lines: $65-80\times$
Reflected light from Proxima Centauri b

The planet/star contrast is between $7 \times 10^{-7}$ and $2 \times 10^{-6}$ times the albedo

High-resolution spectroscopy (350-1000nm, 10% throughput): challenging even with 100 hours of Extremely Giant Telescopes
Combining spectral and spatial resolution

Direct imaging state-of-the-art
Playing with the S/N formula
Simulations and future prospects
Direct imaging of exoplanets

Technology can detect planets 1 million times fainter than the star. Some of these planets can be seen orbiting their star!

HR 8799 b-c-d-e
Seen “face on”

β Pictoris b
Seen “edge on”
Direct spectroscopy of young giant exoplanets

Possible with state-of-the-art instrumentation (SPHERE, GPi) at low spectral resolution

Direct imaging of HR 8799 system: 4 planets

Only possible for young planets (still contracting) on wide orbits (far from the star)
Observations possible down to planet / star contrasts of $10^{-6}$ (1 ppm)

Our Solar System would be well below our sensitivity
Direct spectroscopy of young giant exoplanets

Keck-OSIRIS K-band spectrum of HR 8799 b,c at medium resolution (R=4,000) (Konopacky+ 2015)

CO head-band + hints of CH$_4$ in planet b
Combining spectral and spatial resolution

Snellen+ 2014, 2015; Lovis+ 2016; Mawet+ 2017; Wang+ 2017

\[
\frac{S}{N} = \frac{S_{\text{planet}}}{\sqrt{S_{\text{star}}/K + \sigma_{\text{bg}}^2 + \sigma_{\text{RN}}^2 + \sigma_{\text{Dark}}}} \sqrt{N_{\text{lines}}}
\]

Direct imaging suppression  Cross-correlation gain

**Implementation:** Integral Field Unit w/ high-res spectroscopic capabilities

Stage 1: classic AO + DI algorithms to suppress starlight

**Stage 2:** cross-correlation of residual spectra at each pixel

Stage 1: classic AO + DI algorithms to suppress starlight

Stage 2: cross-correlation of residual spectra at each pixel
Testing spectral + spatial resolution: long-slit spectroscopy

CRIRES@VLT, 1hr @ 2.3µm, seeing 1.0-1.3”, 22 spectra (Snellen+ 2014)

**β Pic b**
12-21 Myr
2.6×10⁻⁴ contrast
S/N = 6.5
FWHM = 27 km/s
$P_{\text{rot}} \sim 8$ hours

See also Schwarz+ 2015: H₂O+CO in GQ Lupi b, S/N = 12
Thermal emission from Proxima Cen b

R = 1.1 R⊕, T = 250-265K, a = 0.0485 AU \Rightarrow 0.0373'' separation (I. Snellen)

Contrast curve

Contrast (1σ)

Angular separation ('')

1σ @ 0.037'' \approx 2\times 10^{-8}

METIS observations centered at 4.85 μm, 30 hrs

α Cen B planet

(Snellen+ 2015)
Spectral + spatial resolution with the ELT

Simulating ~30 hours of observations on our nearest neighbours (I. Snellen)

**Thermal emission** of “Earth-like” planet (1.5 R$_\oplus$, 300 K, 30 km/s) orbiting α Cen B

**Reflected light** from Proxima Cen b (1.1 R$_\oplus$, 0.048 AU, 40 km/s)

Credits: I. Snellen
Proxima Centauri b: reflected light

The planet/star contrast is between $7 \times 10^{-7}$ and $2 \times 10^{-6}$ times the albedo.

High-resolution spectroscopy only (350-1000nm, 10% throughput): challenging even with 100 hours of Extremely Giant Telescopes.

Spectral and spatial resolution combined would easily succeed! (Revised Snellen+ 2015 estimates, strehl ratio 0.3, 10% throughput)
Testing spectral + spatial resolution: mid-res IFUs

Medium-resolution (R = 5,000)
2.5h on β Pic b
1σ limit: <8 ppm!
Molecular “maps” also possible

See also: HR 8799b with Keck/OSIRIS at R = 5,000 (Konopacky+ 2013)