High-resolution spectroscopy for exoplanet characterisation

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Basic concepts

Spectral resolution and spectrographs Exoplanets and their orbits Low-resolution spectroscopy of transiting exoplanets

Basic concepts in spectroscopy: resolution

The ability to distinguish light of similar frequency

How close can two spectral lines be to be considered "spectrally resolved"?

Throughout these lectures we'll adopt the Houston criterion



We'll assume that spectrographs turn a delta function into a Gaussian with FWHM= λ/R

Spectrographs are characterised by a ~constant resolving power R= $\lambda/\Delta\lambda$ This translates into a variable spectral resolution $\Delta\lambda$ according to wavelength λ

Linking resolution to velocity

Objects in motion absorb/emit at shifted wavelengths λ ' due to Doppler effect We will use the non-relativistic Doppler formula

$$\lambda' = \lambda \left(1 + \frac{v}{c} \right) \qquad \Delta \lambda \equiv (\lambda' - \lambda) = \lambda \frac{v}{c}$$
$$R = \frac{\lambda}{\Delta \lambda} = \frac{c}{v}$$

The minimum velocity shift v that can be fully resolved is related to R via

$$v = \frac{c}{R}$$

 $R = 500 \text{ (low-res)} \Rightarrow \Delta v = 600 \text{ km s}^{-1}$ Generally insufficient for most astrophysical sources

R = 5,000 (intermediate-res) $\Rightarrow \Delta v = 60$ km s⁻¹ OK for the broadest spectral lines

R = 50,000 (high-res) $\Rightarrow \Delta v = 6$ km s⁻¹ OK for most of spectral lines, and exoplanet orbital motion too!

Using spectroscopy to find exoplanets

Periodic shift of spectral lines due to reflex motion around the centre of mass



Period of the orbit Eccentricity of the orbit

Only lower limit on planet mass (orbital inclination unknown)

10 cm/s required to do Earth-Sun systems current limits are 30 cm/s (instrumental) and ~1 m/s (stellar)



Proxima Cen b: ~1.4 m/s



Nomenclature for orbital phases φ of exoplanets



Orbital radial velocity of an exoplanet



Additional velocity terms are needed to compute the RV as measured by the observer (day 2)

Light curves of transiting exoplanets

Dimming of starlight due to transit or eclipse of planetary body



Period of the orbit Radius of the planet relative to the star Orbital inclination

Measuring the stellar light accurately is a challenging task from the ground due to instability of the instrument (flexure, pointing, etc.) and of the Earth's atmosphere (transparency, water vapour, etc.)

We live in the golden era of exoplanet discoveries

 $1995-2021 \Rightarrow 4,400$ confirmed exoplanets



Is our solar system rare?

The discovery space corresponding to solar system planets is empty



Both plots are biased by *detection limits!* Smaller and further away planets are harder to detect

The most common exoplanets are not giants

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



What is the nature of the most common exoplanets?

The mini-Neptune / super-Earth dilemma



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The gaseous/rocky transition and the evaporation valley

What shapes the transition between gas and rocky planets?



Studying the **atmospheric composition** (and mean molecular weight) can inform about physical processes shaping the valley

Key questions about exo-atmospheres



Need to measure

Atmospheric composition Temperature structure How do atmospheres form and evolve?

Does composition reflect formation conditions?

What is the range of planetary climates?

What are the driving chemical processes?

What is the prevalence of bio-signatures?

Must balance low measurement precision with sample size (comparative / statistical studies)

Transmission spectroscopy of exoplanets

0.152 CO2 -4 $R_{\rm P} = R_{\rm P}(\lambda)$ Na 0.150 If the opacity increases Transit Depth (R_p/R_s) 0.148 the planet appears bigger Transmission spectroscopy 0.148 D. 0.144 High Low opacity opacity 0.142 0.4 0.5 1.5 2 0.3 3 5 1 Wavelength (µm) WASP-39b, Wakeford+ 2017 Transit Missing stellar light due to opaque planet disk



Optical wavelengths

Dominated by lines of alkali metals (Na / K doublets), Rayleigh scattering from H₂, some (weak) H₂O For very hot giants there can be TiO / VO in gas phase

Infrared wavelengths

Dominated by molecular absorption, mostly H₂O and possibly CH₄, CO, CO₂, HCN, NH₃, C₂H₂.

A first-order estimate of transmission signals

 $R_{\rm P}$

Transit depth $D = (R_{\rm P}/R_{\star})^2$

Jupiter-Sun ~ 1% Earth-Sun ~ 0.008%

 R_{\star}

Change in transit depth ΔD due to atmospheric opacity $\Delta D \approx A_{ring} / A_{star}$

 $A_{ring} = area \ outer \ radius - area \ inner \ radius$ $Outer \ radius = R_P + \delta$ $Inner \ radius = R_P$

$$A_{\rm ring} = \pi (R_{\rm P} + \delta)^2 - \pi R_{\rm P}^2$$
$$= \pi (R_{\rm P}^2 + 2\delta R_{\rm P} + \delta^2 - R_{\rm P}^2)$$
$$= \pi \delta (2R_{\rm P} + \delta) \approx \pi \delta R_{\rm P}$$

$$\Delta D = \frac{A_{\rm ring}}{A_{\star}} = \frac{\delta R_{\rm P}}{R_{\star}^2}$$

What is δ ?

A first-order estimate of transmission signals



A first-order estimate of transmission signals









Example: the "cloudiness" levels of hot Jupiters



Key comparative study by Sing et al., *Nature* (2016)

10 exoplanets high-quality optical-NIR data (HST STIS & WFC3)

Weak IR water features are either due to low water abundance, or to muting effects of clouds

Answer is still not definitive

Ongoing research

Large HST proposals (100s hours) to increase the sample and complete the 0.8-1.3 µm region

Reflected starlight from exoplanets

At visible wavelength, secondary eclipse depth = missing reflected starlight Very challenging measurements, especially spectrally-resolved



Hot Jupiters are not reflective at visible wavelengths (Na and K lines absorb radiation)



Stellar flux at planet: $F_{\star,\text{pl}} = L_{\star}/(4\pi a^2)$ $L_{\star} = 4\pi\sigma R_{\star}^2 T_{\text{eff}}^4$

Luminosity: energy / s \Rightarrow [W s⁻¹] Flux: energy / s / unit area \Rightarrow [W s⁻¹ m⁻²]



Stellar flux at planet: Energy reflected / s:

$$F_{\star,\text{pl}} = L_{\star} / (4\pi a^2) \qquad L_{\star} = 4\pi \sigma R_{\star}^2 T_{\text{eff}}^4$$
$$E_{\text{refl}} = A\pi R_{\text{P}}^2 F_{\star,\text{pl}}$$

The planet is a disk of area $\pi(R_P)^2$



Stellar flux at planet: $F_{\star,\text{pl}} = L_{\star}/(4\pi a^2)$ $L_{\star} = 4\pi\sigma R_{\star}^2 T_{\text{eff}}^4$ Energy reflected / s: $E_{\text{refl}} = A\pi R_{\text{P}}^2 F_{\star,\text{pl}}$

Flux ratio at the observer (distance D)



Stellar flux at planet: $F_{\star,pl} = L_{\star}/(4\pi a^2)$ $L_{\star} = 4\pi\sigma R_{\star}^2 T_{eff}^4$ Energy reflected / s: $E_{refl} = A\pi R_P^2 F_{\star,pl}$

Flux ratio at the observer (distance D)



Emission spectroscopy of exoplanets

At infrared wavelength, secondary eclipse depth = missing planet thermal emission



A first-order estimate of emission signals

Approximating the star and the planet as black bodies

Stellar flux at planet:

 R_{\star}

$$F_{\star} = L_{\star} / (4\pi a^2) \qquad \qquad L_{\star} = 4\pi\sigma R_{\star}^2 T_{\rm eff}^4$$

Let's make it wavelength dependent $B(T_{\text{eff}}, \lambda)$ is the Planck function for black-body radiation

$$B(T,\lambda) = \frac{2hc^2}{\lambda^5} \frac{1}{\exp[hc/(\lambda kT)] - 1}$$

It has units of [W s⁻¹ m⁻² m⁻¹ sr⁻¹] (energy / time / area / wavelength / solid angle)

R_P

Radiation is isotropic so for the flux

 $F(T, \lambda) = \pi B(T, \lambda)$ $L_{\star}(\lambda) = 4\pi^2 R_{\star}^2 B(T_{\text{eff}}, \lambda)$

A first-order estimate of emission signals

Approximating the star and the planet as black bodies

Stellar flux at planet:

Energy absorbed / time:

$$F_{\star}(\lambda) = L_{\star}(\lambda)/(4\pi a^2) \qquad L_{\star}(\lambda) = 4\pi R_{\star}^2 B(T_{\text{eff}}, \lambda)$$
$$E_{\text{abs}}(\lambda) = (1 - A)\pi R_{\text{P}}^2 F_{\star}(\lambda)$$

Energy absorbed = Energy re-emitted (over all wavelengths)



A first-order estimate of emission signals

Approximating the star and the planet as black bodies Estimating the planet / star flux as measured by an observer at distance D



Phase curves: light modulation along the orbit



All together these measurements inform the chemical make-up and the energy balance in exoplanet atmospheres

Thermal vertical structure from dayside spectroscopy

Best-case scenario: the phase curve of WASP-43b (Stevenson+14)



Large day-night temperature contrast, 18% albedo Temperature monotonically decreasing with altitude

Thermal vertical structure from dayside spectroscopy

Best-case scenario: the phase curve of WASP-43b (Stevenson+14)



Large day-night temperature contrast, 18% albedo Temperature monotonically decreasing with altitude

Only possible for a handful of objects so far

High-resolution spectroscopy of exoplanets

Key characteristics The signal-to-noise formula Cross correlation and data analysis

Exoplanets at high spectral resolution



Each species has a **unique** pattern of spectral lines Species can be "matched" line by line to templates, e.g. via **cross correlation**



Water is key to study exoplanet atmospheres

H₂O abundant for a wide range of temperatures relevant to hot Jupiters



Relative abundances (especially [H₂O]/[CH₄]) are a strong function of C/O ratio



Connecting C/O to the origin of giant exoplanets

Hot Jupiters might form far away from the star and then migrate inward Atmospheres will have different composition according to the formation location



(see Öberg+11; Piso+15; Eistrup+18)

Atmospheres to investigate formation and evolution

For the hottest exoplanets mostly in equilibrium (inverting observations into composition)



Planets can form at various distances from the star \Rightarrow different C and O content in solids/gas due to snowlines

Planets migrate through a disk and/or re-accrete planetesimals \Rightarrow C/O can change from the formation value

Cores can be partially eroded to "enrich" the metal content of the envelope ⇒ metallicity can change

Uncertainties on timescales / dominance of processes makes predictions hard ⇒ need for statistical studies of exoplanet atmospheres in metallicity-C/O

Possible formation/evolution predictions to test

Need to measure "metallicity" and C/O ratio

The mass-metallicity correlation

The C/O ratio



There should be a mass-metallicity relation as in the solar system but core erosion can alter it (e.g. Madhusudhan+17)



Planets formed beyond the water snowline should have high C/O (e.g. Öberg+11, Piso+16)

unless they re-accrete planetesimals, which lead to C/O<0.5 (e.g. Mordasini+16)

Detecting the orbital motion of close-in planets



High spectral resolution of non-transiting planets



Wavelength (µm)

Understanding the data: the noise balance

Star and planet are not spatially separated We measure photons coming from both, but stars are o.o.m. brighter!

Photons obey Poisson statistics: $\sigma = N^{1/2}$

The signal: number of photons emitted / absorbed / reflected by the planet

$$\frac{S}{N} = \frac{N_{\gamma,P}}{\sqrt{N_{\gamma,\text{tot}} + N_{\gamma,\text{sky}} + N_{\text{dark}} + \sigma_{RO}^2}}$$

The noise budgetTotal number of photons $N_{\gamma,tot} = N_{\gamma,P} + N_{\gamma,star}$ Photons from the sky (Earth) $N_{\gamma,sky}$ Photons from the thermal current of the detector N_{dark} Read-out noise from the detector electronics (σ_{RO})

Understanding the data: the noise balance

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of noise - summed in quadrature

Sources that come from **photon counting** have noise $\approx \sqrt{N_Y}$ Detector **readout** is just an extra noise budget \Rightarrow noise = σ_{RO}

Understanding the data: the noise balance

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Even for the brightest stars $N_{Y} \leq 10^{6}$ / pixel

 \Rightarrow We expect each spectral line to be detected at most at S/N = 1 Some technique to "amplify" the signal is needed \Rightarrow cross correlation

The cross correlation function

Measuring correlation between (noisy) data and a moving template



The cross correlation function

Measuring correlation between (noisy) data and a moving template



Typical hot-Jupiter has S/N~0.8/line and n=50 \Rightarrow We expect a S/N~5-6 from cross correlation with strong lines (e.g. CO)

Understanding the data: a time sequence of spectra



Planet spectral lines ~10⁻⁴ of stellar continuum

Radial component of planet orbital motion changes by ~10 km / s per hour of observation

Dominant by orders of magnitude over the planet signal (up to 50-60% depth)

20-30% variation in overall measured flux (telescope pointing, atmospheric transparency, etc.)

Reverse-engineering the exoplanet spectrum



Wavelength



All the steps after normalisation can be done "automatically" by algorithms that decompose the data into a linear combination of eigenvectors (e.g. PCA) Every spectral line stationary in wavelength (vertical in our figures) is removed **The process "auto-calibrates" the data: no reference star required!**

Extracting the (faint) planet signal: cross correlation

5 hours of real data + 20x planet signal (CO)



Wavelength

Cross-correlation with model spectra

Cross-correlation matrix CC(RV, t)



Planet radial velocity

The peak CC tracks the planet radial velocity in time

Phase-resolved cross-correlation: transmission



Phase-resolved cross-correlation: emission



Extracting the (faint) planet signal: cross correlation

5 hours of real data + 20x planet signal (CO)



Wavelength

Cross-correlation with model spectra

Cross-correlation matrix CC(RV, t)



Planet radial velocity

The peak CC tracks the planet radial velocity in time

Shifting and co-adding to planet rest-frame requires knowledge of planet orbital velocity (two parameters: *slope* and *shift*)

Star and planet as spectroscopic binaries Pilot study: T Boo b (Brogi+ 2012)

+6σ

+4σ

+2σ

0

-2σ

15 hours of VLT/CRIRES, 2.3μm Carbon monoxide detected at 6σ



Measured:

RV semi-amplitude ratio: K_P/K_S \Rightarrow Mass ratio: M_P/M_S

Inferred:

Orbital inclination i Planet mass $M_P = f(M_S)$

Uncertainties in planet mass dominated by uncertainties in stellar mass.

Star and planet as spectroscopic binaries

Deriving the true planet mass



	Inclination (degrees)	Mass (M _{Jup})	Reference
τ Boötis b	45.5±1.5	5.95±0.28	Brogi+12
51 Pegasi b	>79.8	0.46±0.02	Brogi+13
HD 179949 b	67.7±4.3	0.98±0.04	Brogi+14
HD 88133 b	15 ⁺⁶ –5	1.02+0.61_0.28	Piskorz+16
υ And b	24±4	1.70+0.33_0.24	Piskorz+17
HD 102195 b	>72.5	0.46±0.03	Guilluy+19

The chemical inventory at high spectral resolution



Five carbon- and nitrogen-bearing species in a hot giant planet's atmosphere

P. Giacobbe, M. Brogi, S. Gandhi et al., *Nature* **592**, 205-208 (2021)



4 transits of hot Jupiter HD 209458b (1,500K) \Rightarrow H₂O + 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!)