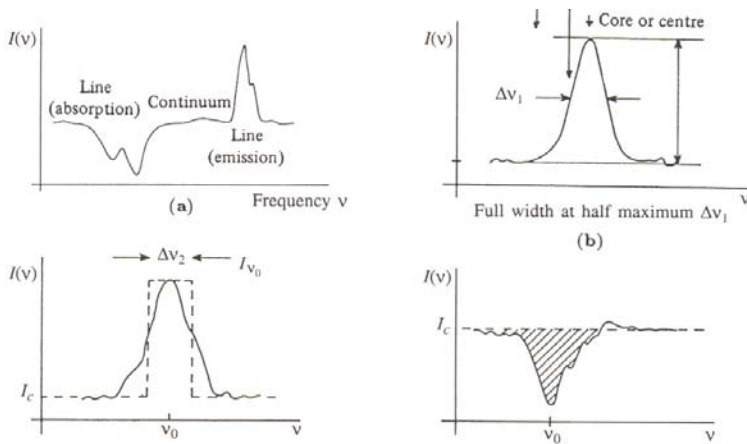


Astronomische Waarneemtechnieken (Astronomical Observing Techniques)

10th Lecture: 12 November 2012



1. Formation of Spectral Lines
2. General Principle
3. Gratings and Filters
4. Advanced Spectrometers
5. Spectral Line Analysis

Based on "Observational Astrophysics" (Springer) by P. Lena,
Wikipedia, ESO, and "astronomical spectroscopy" by Massey & Hanson

ASTRONOMICAL SPECTRA

Excitation Processes

- **Electronic transitions** due to the change of the principal quantum numbers of the electronic states (\rightarrow *visible*).
- **Electronic fine structure transitions** due to the coupling of electron spin and nuclear spin.
- **Electronic hyperfine structure transitions** due to the interaction of the nuclear magnetic moment with the magnetic field of the electron.
- **Molecular transitions** such as rotational (change in angular momentum) and vibrational (change in vibrational energy) transitions*, requiring dipole moment and moment of inertia I (\rightarrow *near-far-IR*).
- **Nuclear lines** due to nuclear excitations or electron-positron annihilation (\rightarrow *MeV range*)
- **Transitions in solids** (ices) due to vibrations \rightarrow phonons (\rightarrow *near-far-IR*).

* rotational transitions are generally weaker and often coupled to vibrational transitions \rightarrow vibrational transitions split further: complex structure of **vibrational-rotational** transitions.

Excitation Processes - Energy Ranges

Transition	Energy [eV]	Spectral Region	Example
Hyperfine structure	10^{-5}	Radiofrequencies	21 cm hydrogen line
Spin-orbit coupling	10^{-5}	Radiofrequencies	1 667 MHz transitions of OH molecule
Molecular rotation	10^{-2} – 10^{-4}	Millimetre and infrared	1–0 transition of CO molecule at 2.6 mm
Molecular rotation-vibration	1 – 10^{-1}	Infrared	H ₂ lines near 2 μ m
Atomic fine structure	1 – 10^{-3}	Infrared	Ne II line at 12.8 μ m
Electronic transitions of atoms, molecules and ions	10^{-2} – 10	Ultraviolet, visible, infrared	Lyman, Balmer series, etc. of H; resonance lines of C I, He I; K, L shell electron lines (Fe XV, O VI)
Nuclear transitions	$> 10^4$	X- and γ -rays	¹² C line at 15.11 keV
Annihilations	$\gtrsim 10^4$	γ -rays	Positronium line at 511 keV

Three General Types of Spectra

Continuous spectrum



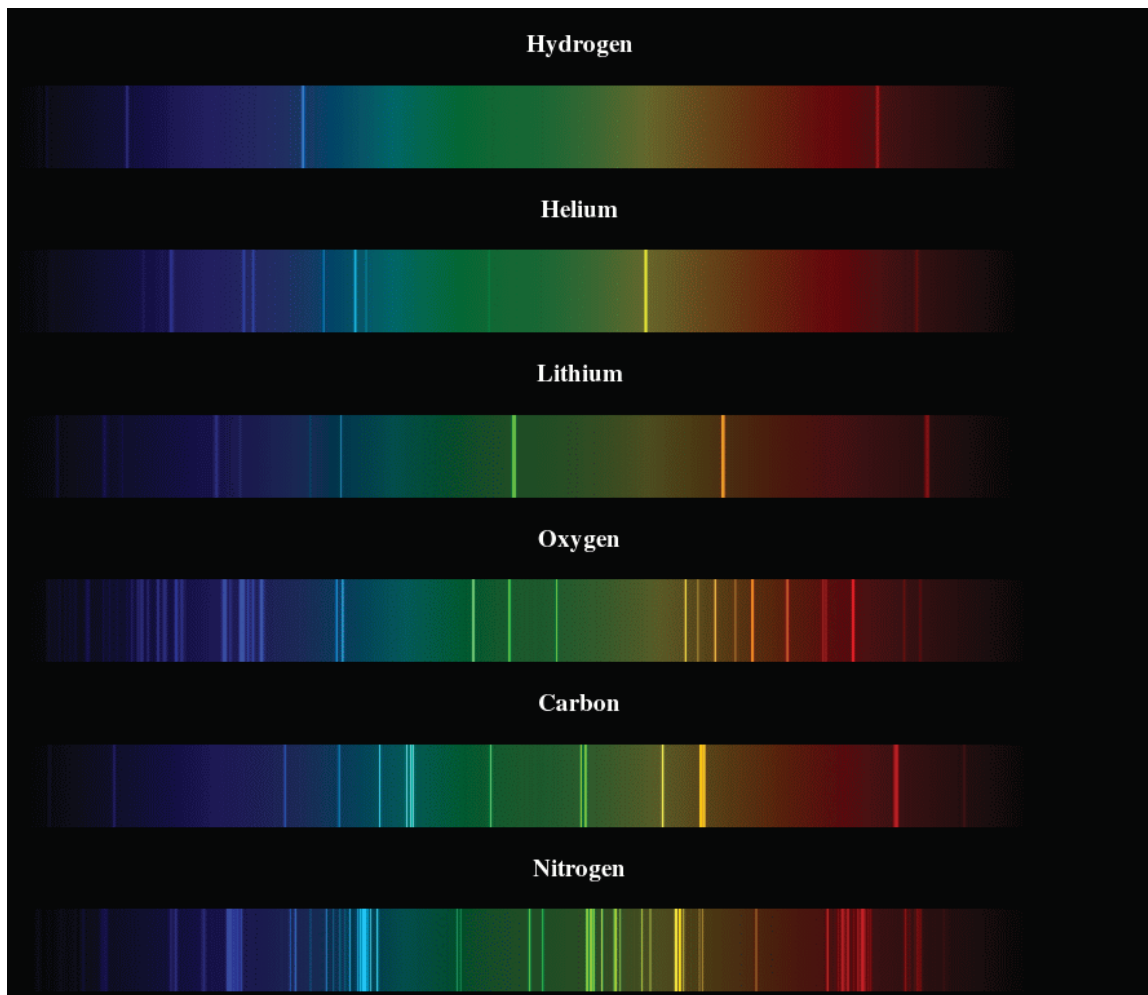
Emission line spectrum

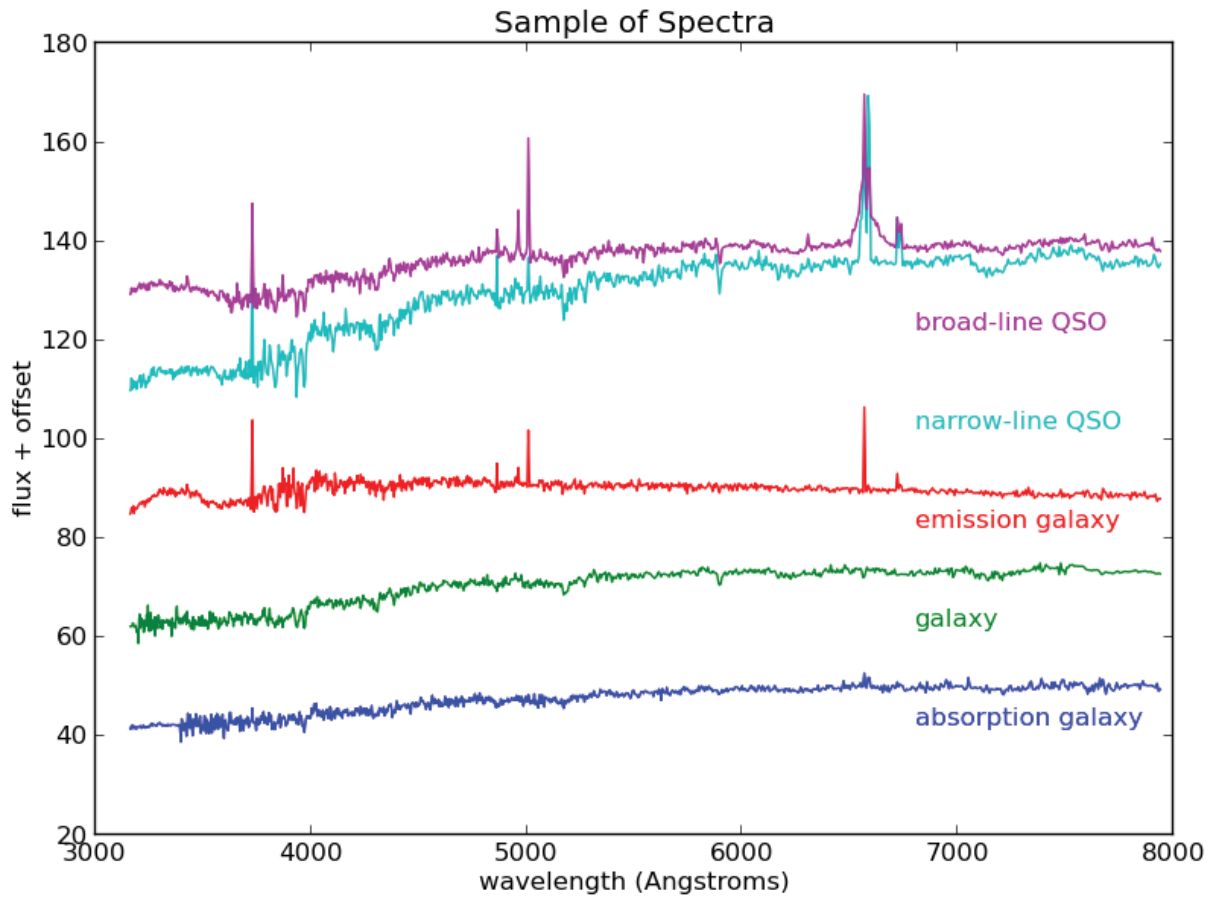


Absorption line spectrum



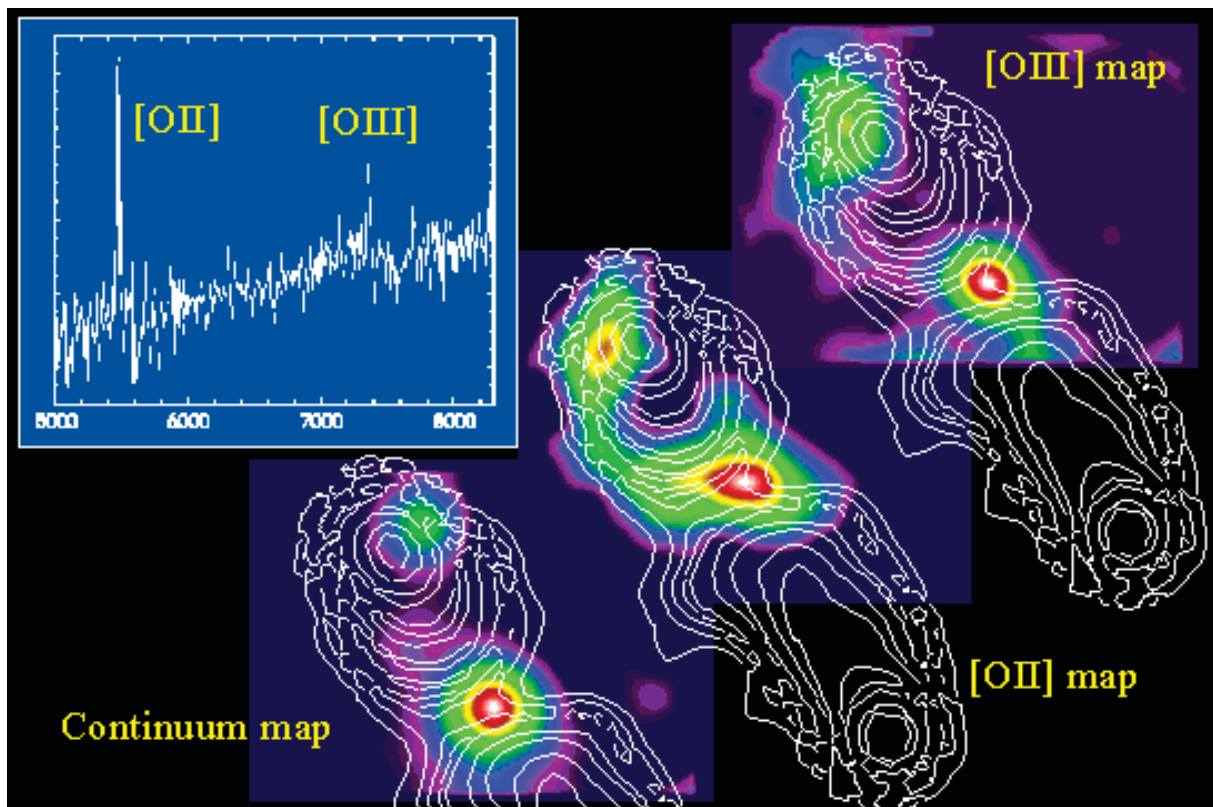
Courtesy:
<http://home.achilles.net/~ypvsj/data/elements/index.html>





Plot courtesy: SDSS

Spectral Line Maps



Radiogalaxy 3C435A radiogalaxy 3C435A

Plot courtesy: Universite de Lyon, Recent TIGER Scientific Results

GENERAL PRINCIPLE OF A SPECTROMETER

The Basic Principle

Main ingredients of a spectrometer:

1. A **slit** (ont which the light of the telescope is focused)
2. A **collimator** (diverging → parallel/collimated light)
3. A **disperser** (to spectrally disperse the light)
4. A **camera** (to focus the spectrum onto the detector)

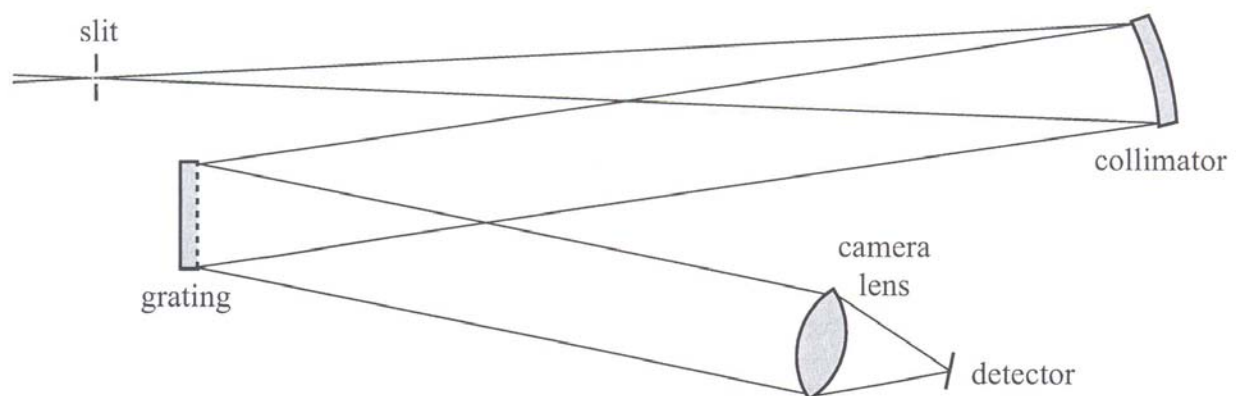
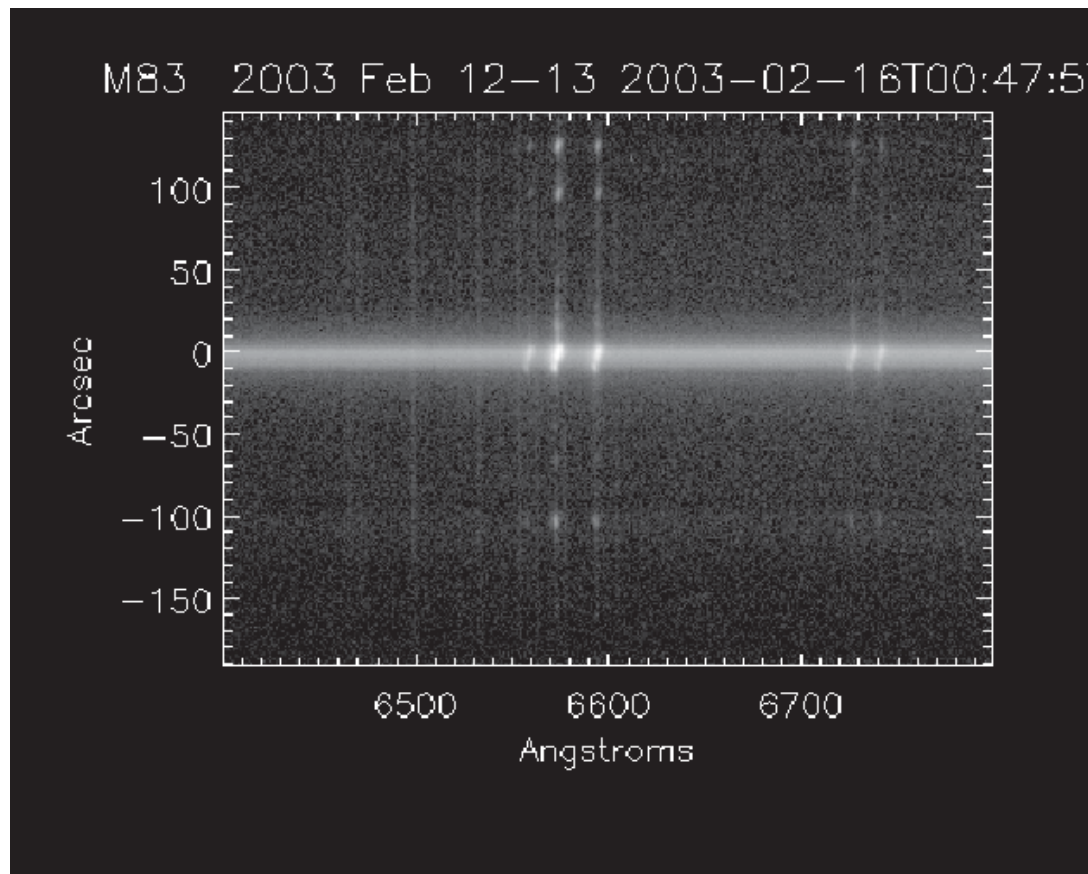


Fig. 1.— The essential components of an astronomical spectrograph.

Data Products (1): Long Slit Spectra



Main Characteristics of a Spectrometer

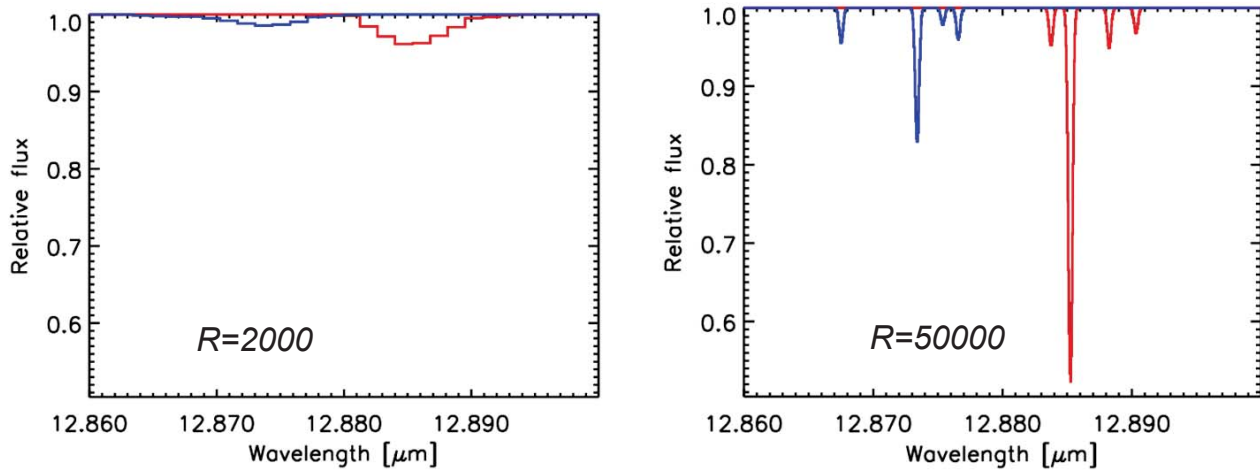
- the **spectral resolution** or **spectral resolving power** is: $R = \frac{\lambda}{\Delta\lambda}$
 $\Delta\lambda$ is called a **spectral resolution element**.
- the **instrumental profile** $P(\nu)$ broadens a theoretically infinitely narrow line $I_0(\nu) = \delta(\nu - \nu_0)$ to the observed line width:
$$I(\nu) = P(\nu) * I_0(\nu)$$

Usually the instrumental profile determines the spectral resolution element, which is typically Nyquist-sampled.
- the **beam étendue** determines the light gathering power of the instrument. Larger étendues require larger dispersive elements (A) or highly inclined beams (Ω).

- the **transmission** determines the throughput $\eta(\nu) = \frac{I_{out}(\nu)}{I_{in}(\nu)}$

Spectral Resolution and S/N

For unresolved lines, both the S/N and the line/continuum increases with increasing resolution:



Model spectra of C_2H_2 at 900K and HCN at 600K (assumed Doppler broadening ~ 4 km/s) at different spectrograph resolutions (figure provided by F. Lahuis).

**DISPERSERS:
GRATINGS
AND FILTERS**

General Principle of a Grating

Use a device that introduces an optical path difference = $f\{\text{angle to the surface}\}$

The condition for constructive interference is given by the **grating equation**:

$$m\lambda = a \cdot (\sin \alpha \pm \sin \beta)$$

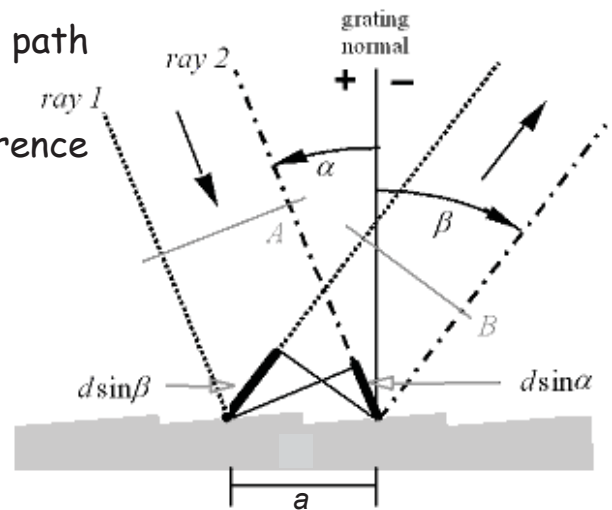
m = order of diffraction

λ = wavelength

a = distance between equally spaced grooves

α = angle of incoming beam

β = angle of reflected beam



Gratings are usually operated in a **collimated beam** at the pupil.

The **maximum resolution** is given by $R = mN$ where N is the number of

(illuminated) periods (grooves), and the **angular dispersion** is $d\theta/d\lambda \sim \frac{m}{a}$.

Blaze Angle

Generally, the energy of the beam diffracted by a periodic structure is uniformly distributed over the different orders m .

If we observe only one arbitrary order this is very inefficient.

For **blazed gratings** the *directions of constructive interference and specular reflection coincide*:

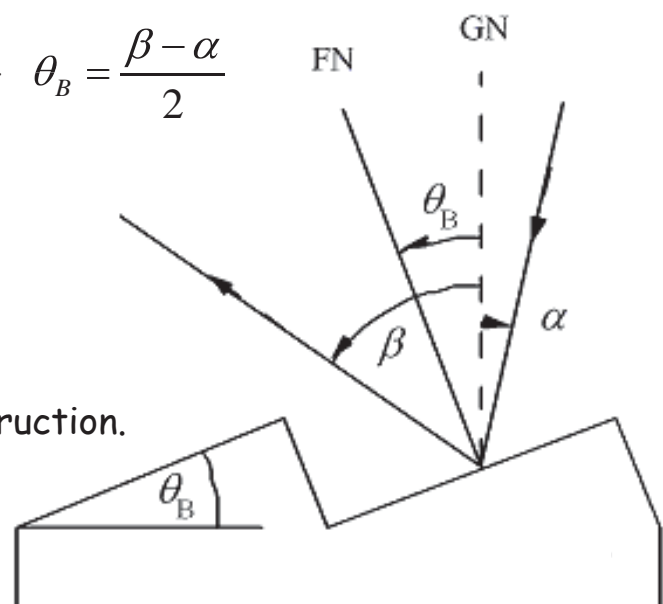
$$\alpha + \beta = 2(\alpha + \theta_B) \Rightarrow \theta_B = \frac{\beta - \alpha}{2}$$

Advantage:

- High efficiency

Disadvantage:

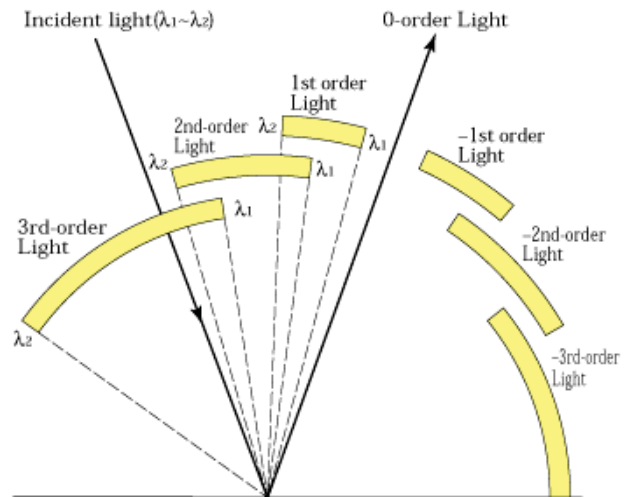
- Blaze angle θ_B (and hence blaze wavelength λ_B) are fixed by construction.



Free Spectral Range ...



A light bulb seen through a transmissive grating, showing three diffracted orders. $m = 0$ corresponds to direct transmission; colors with increasing wavelengths (from blue to red) are diffracted at increasing angles. Source: Wikipedia



Different diffraction orders overlap with each other:

$$m\lambda = a(\sin \alpha + \sin \beta) = (m+1)\lambda'$$

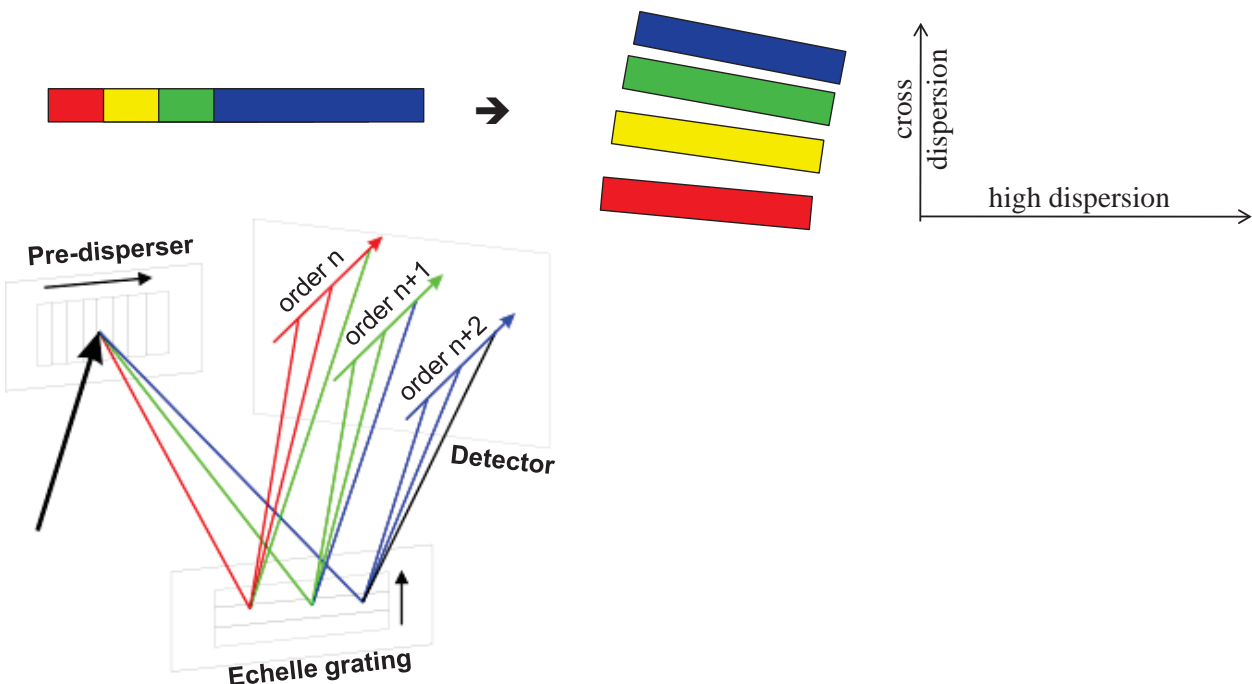
The **free spectral range** is the largest wavelength range for a given order that does not overlap the same range in an adjacent order.

$$\Delta\lambda_{free} = \lambda - \lambda' = \frac{\lambda'}{m}$$

...and Cross-Dispersion

To spatially separate the orders and avoid overlap, an additional optical element will be needed:

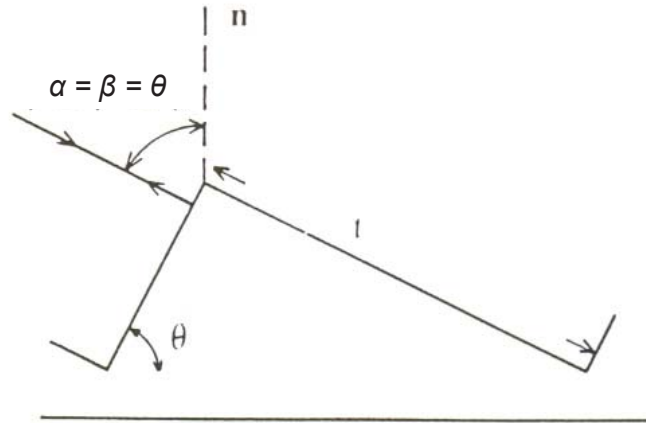
A low-dispersion prism/grating with a dispersion direction **perpendicular** to that of the high-dispersion grating



Echelle Gratings

To get high dispersion $d\theta/d\lambda \sim \frac{m}{a}$ one could *either* increase the groove density, *or* use large groove periods ($a \gg \lambda$) and a large angle of incidence, and operate at a very *high order of diffraction* ($m \gg 50$).

If $\alpha = \beta = \theta \rightarrow$ Littrow configuration



In Littrow configuration the grating equation becomes: $m\lambda_B = 2a \sin \Theta$

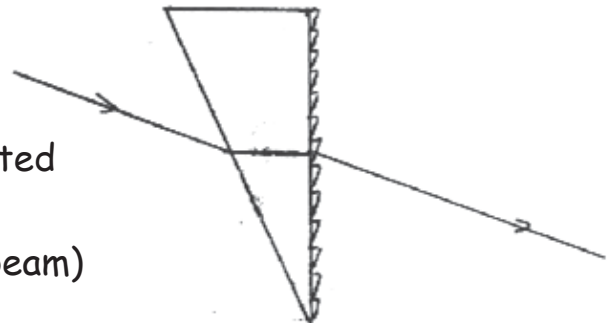
Grisms

Grism = transmission *GR*ating + *pr*ISM

For a given wavelength and diffraction order the refraction of grating and prism may compensate each other and the *optical axis remains (almost) unchanged*.

Advantages:

- ideal to bring in and out of a collimated beam ("filter wheel")
- reduces coma (if in non-collimated beam)



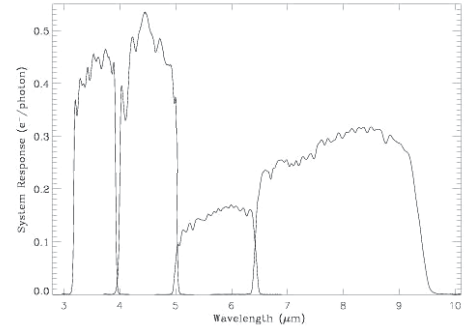
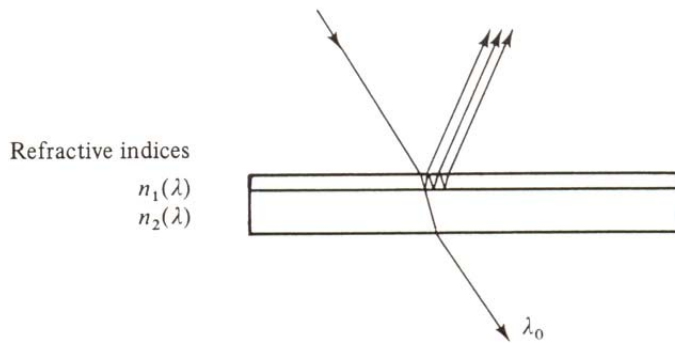
Disadvantage:

- difficult to manufacture (either by replication and gluing or by direct ruling).
- can be quite "bulky" (\leftarrow filter wheel)

Interference (Transmission) Filters

Principle: interference layers deposited on a substrate.

The transmission is maximal where $\frac{2n_1d}{\lambda} + \frac{\pi}{2} = 2k\pi$



- spectral resolution typically $R \sim \text{few} - 1000$
- needs often multiple **interference layers**
- filters are often tilted with respect to the optical axis to avoid reflections \rightarrow shift of λ_0
- wavelengths farther from λ_0 (for which the above equation is also satisfied) need a blocking or **absorbing filter**.

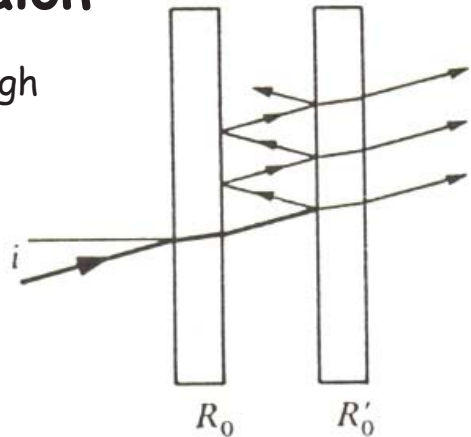
Fabry-Perot Etalon

Two parallel plates (**Fabry-Perot etalon**) of high reflectivity r and transmission $t = 1 - r$.

The transmission is:

$$I = I_0 \left(\frac{r}{1-r} \right)^2 \left[1 + \frac{4r}{(1-r)^2} \sin^2(2\pi dk \cos i) \right]^{-1}$$

and has transmission peaks where $k = \frac{m}{2d}$



Here, m is the **order** of the interferometer, d is the **separation** of the plates, and $\Delta k = 1/2d$ the **free spectral range**.

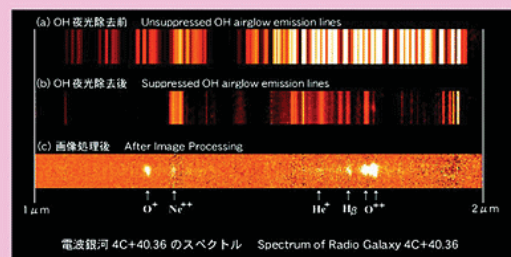
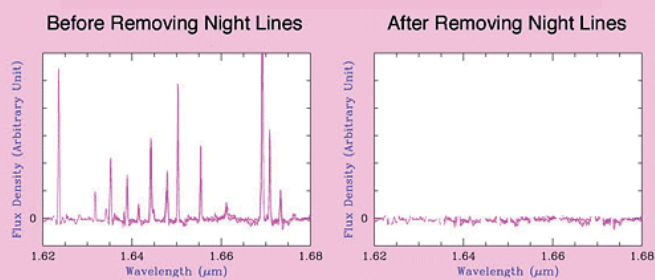
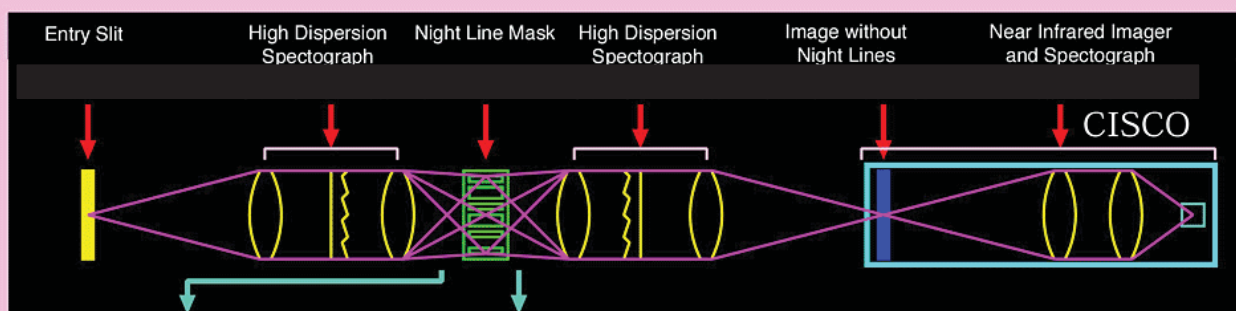
The performance of a Fabry-Perot is characterized by:

1. The **fineness** $F = \frac{\pi\sqrt{r}}{1-r}$,
2. The **resolution** $R = \frac{k}{\Delta k} = mF$, and
3. The **maximum throughput** $U = 2\pi \frac{S}{R}$ (S = illuminated area of the etalon).

ADVANCED SPECTROMETER CONCEPTS

OH Suppression Spectrographs

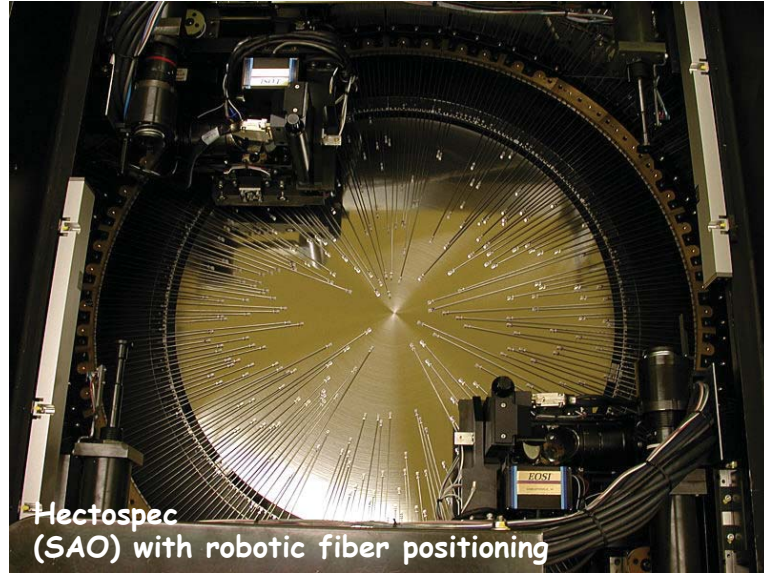
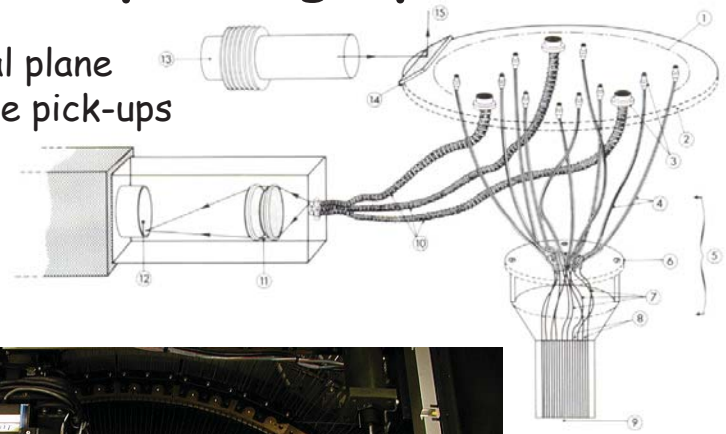
OHS filter out the wavelengths of atmospheric OH lines, which contribute the major part of the near-IR background.



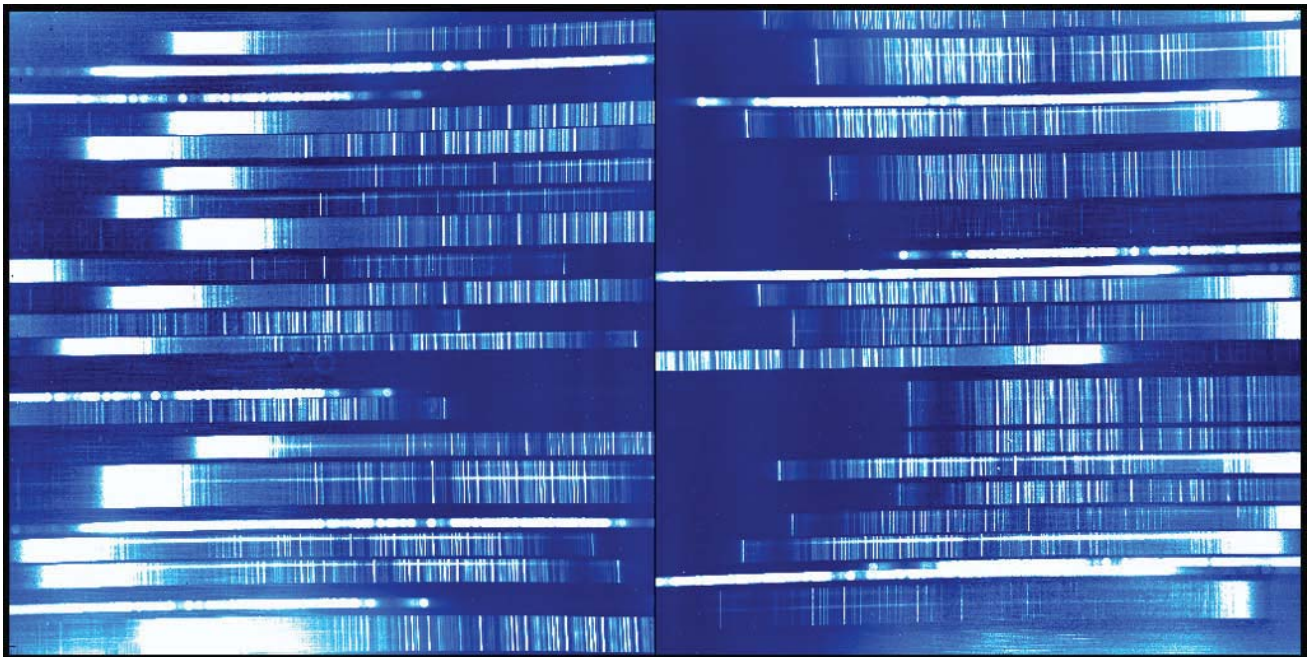
Multi-Object Spectrographs

Use numerous "slits" in the focal plane simultaneously → multiple source pick-ups using fibers or mirrors.

Needs different slit masks for different fields.

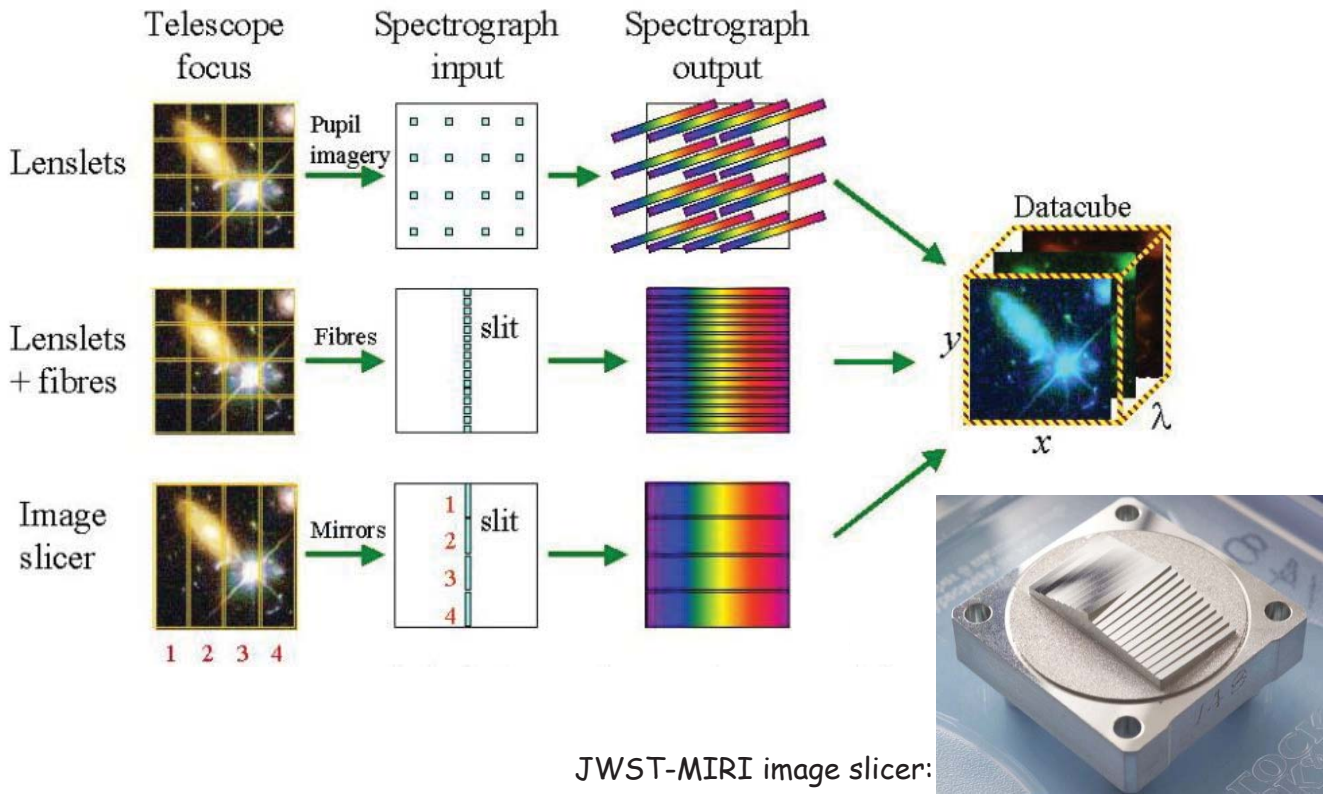


Data Products (2): MOS Spectra

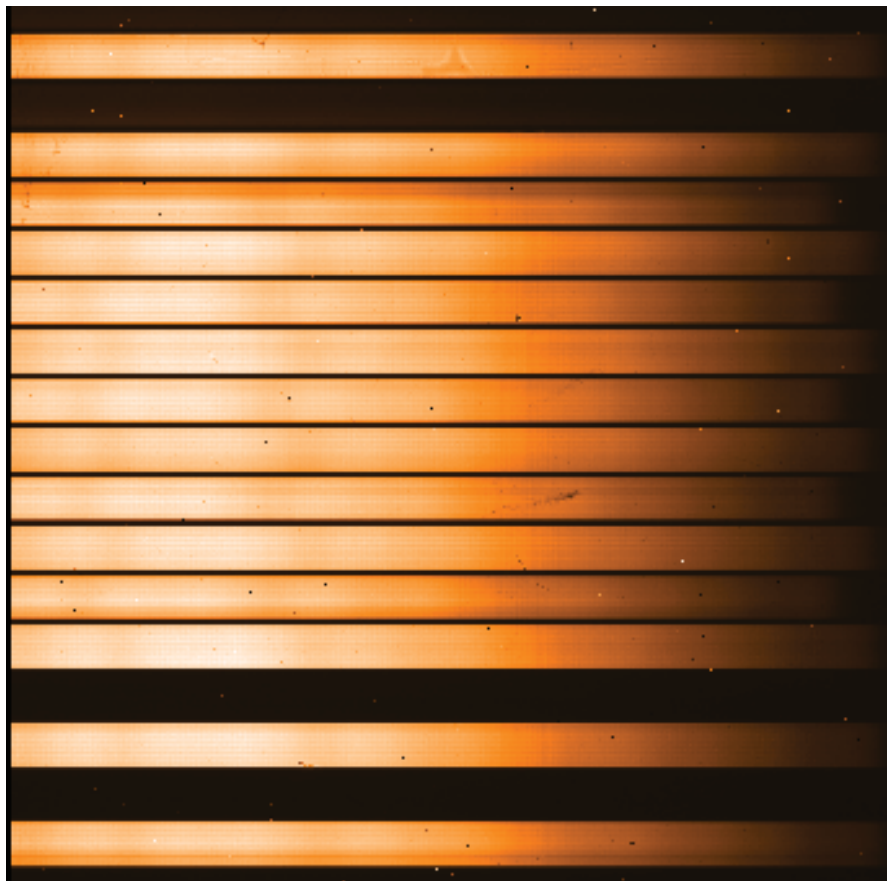


Integral Field Spectrographs

Cut an area on the sky in several adjacent slices or sub-portions, realign them optically into one long slice and treat it as a long slit spectrograph.

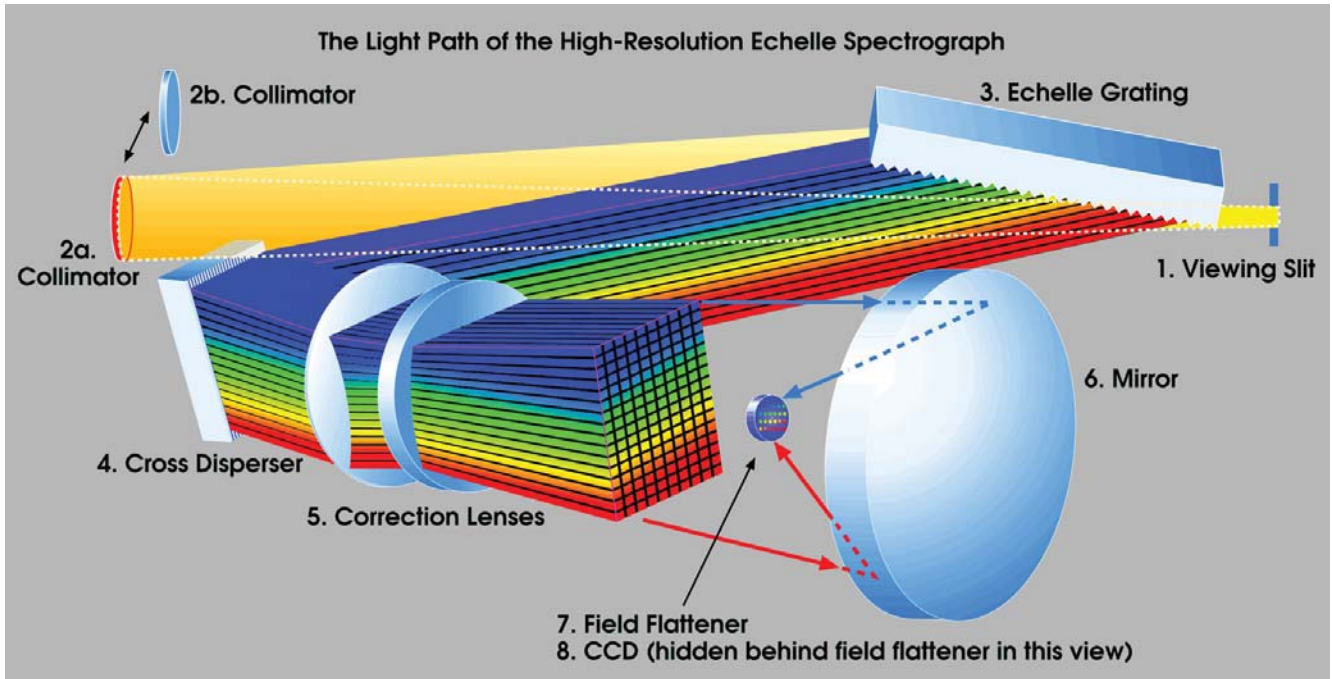


Data Products (3): IFU Spectra



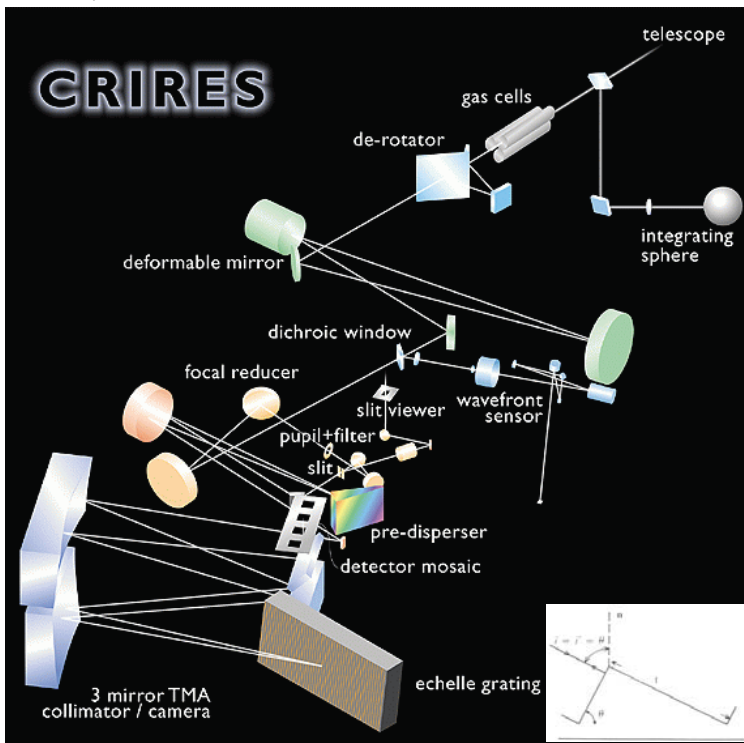
Echelle Spectrographs

Operation in high order → pre-disperser essential



Echelle Spectrographs (2)

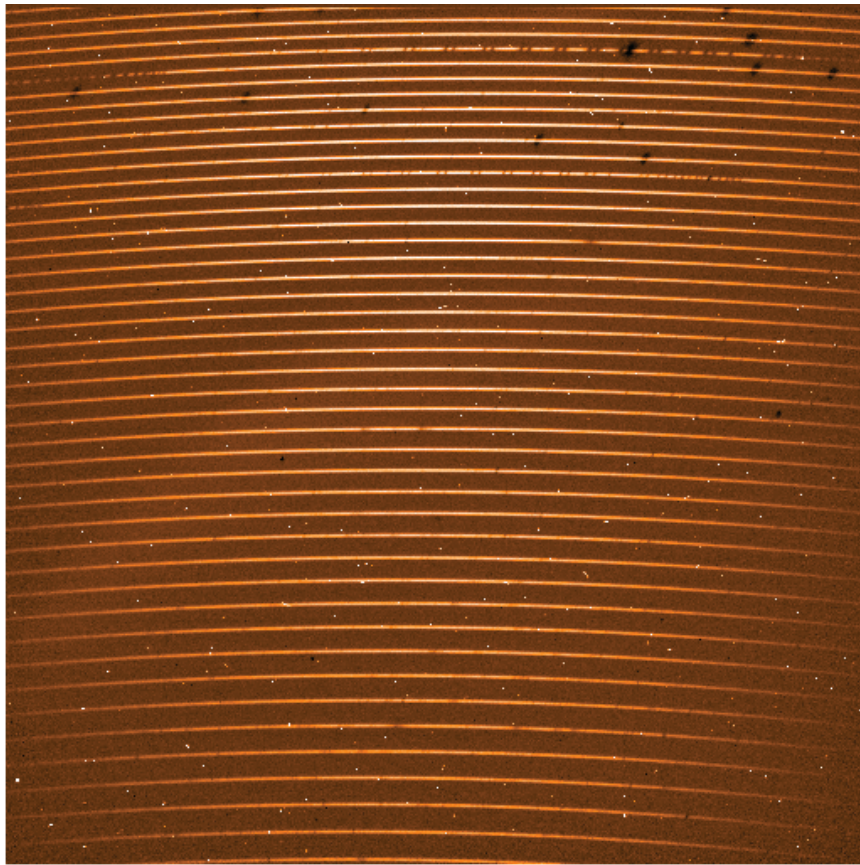
Example: ESO's VLT instrument CRIRES:



The ruled echelle grating of the SOFIA Facility Spectrometer ARIES. Two images of the engineer are seen reflected from the facets of the grooves that are at angles of 90 degrees from each other.

Data Products (4): Echelle Spectra

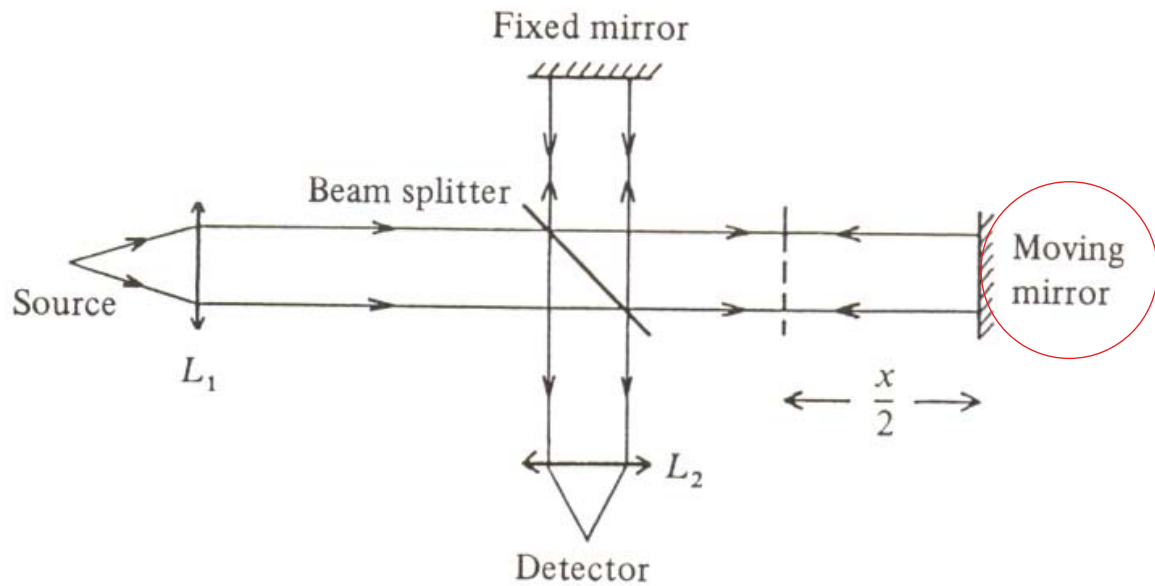
echelle spectrum of V454 Aur



The Fourier Transform Spectrometer (FTS)

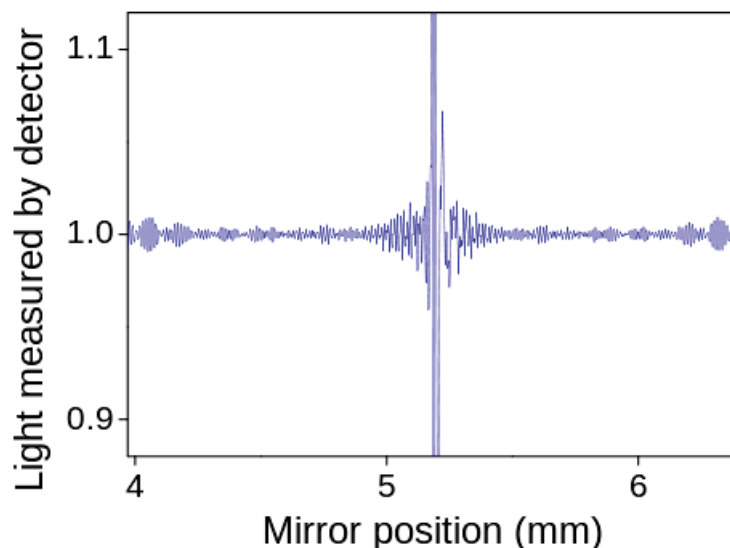
FTS - Principle

First, let's *assume* we only have a **single pixel detector**



- The FTS or **Michelson interferometer** is a two-wave interferometer (as opposed to a grating with N waves from N grooves).

FTS - Output Signal



- For each setting (travel distance) of the arm, the intensity will be recorded.
- The signal is an **interferogram**. It is the Fourier transform of the spectrum of the object.

FTS - Measured Intensity

The exit intensity $I(x)$ for a **monochromatic** input intensity I_0 (with wave number $k=1/\lambda$ and path length difference x) is:

$$I(x) = \frac{I_0}{2} (1 + \cos 2\pi kx)$$

A source with a **spectrum** $I_0(k)$ in the range $[k_1, k_2]$ produces a signal of:

$$I(x) = \frac{1}{2} \int_{k_1}^{k_2} I_0(k) (1 + \cos 2\pi kx) dk$$

Note that for each value of x , all spectral elements of the incident spectrum contribute to the signal = **spectral multiplexing**

FTS - Recovered Source Spectrum

The signal contains a mean value (offset) $\langle I(x) \rangle = \frac{1}{2} \int_{k_1}^{k_2} I_0(k) dk$ which can be subtracted. We then calculate the inverse Fourier Transform:

$$I'_0(k) = FT \{ I(x) - \langle I(x) \rangle \}$$

If $I(x)$ were known from $[-\infty, +\infty]$, I'_0 would be I_0 .

However, $I(x)$ is only measured over the **finite interval** $[-x_m/2, +x_m/2]$, hence: $I'_0(x) = I_0(x) \cdot \Pi\left(\frac{x}{x_m}\right)$

Or in frequency space: $I'_0(k) = I_0(k) * \text{sinc}(x_m k)$

*in other words: **the resolution has been degraded***

FTS - Spectral Resolution

The interferogram of a monochromatic source $I_0(k) = \delta(k - k_0)$ is the instrumental profile: $\text{sinc}(x_m k) * \delta(k - k_0)$

The first zero of the instrumental profile occurs at

$$k - k_0 = \pm \frac{1}{x_m}$$

(analogous to the Rayleigh criterion) the **spectral resolution** of an FTS is:

$$R = \frac{k_0}{\Delta k} = x_m k_0$$

FTS - Multiplex Advantage

Goal: get the source spectrum $I_0(k)$ within $[k_1, k_2]$ at resolution R within time T .

The number of spectral elements shall be M , and the detector read noise σ_D shall dominate.

For a sequential scanning spectrometer with a **monochromator** (single element (pixel) detector*) the S/N is:

$$(S/N)_{\text{spec. elem.}}^{\text{sequential}} = \frac{I_0(k)(T/M)}{\sigma_D \sqrt{T/M}}$$

For a FTS the whole time T is used for *each* spectral element

$$(S/N)_{\text{spec. elem.}}^{\text{FTS}} = \frac{1}{2} \frac{I_0(k)T}{\sigma_D \sqrt{T}}$$

The multiplex gain is thus $G = \frac{\sqrt{M}}{2}$ (Fellgett advantage)

*mainly in the old days or at long IR wavelengths were only small detector formats are available.

FTS - Advantages and Disadvantages

- Multiplex advantage only applies to few pixel detectors
 - at O/NIR wavelength, gratings are preferred
 - at FIR wavelength, FTS are often preferred
- Optical simplicity of FTS provides high throughput
- FTS are superior if read noise dominates, but lose their advantages if photon shot noise dominates (thermal IR from the ground)
- FTS can be combined with imaging by placing a mosaic of detectors in the focal plane.

Pros and Cons of the Different Types

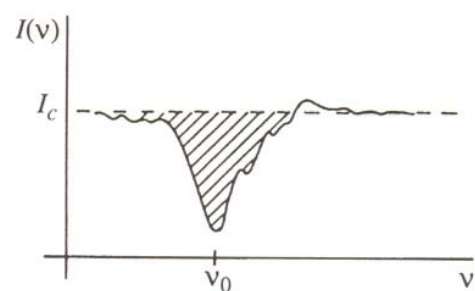
Spectrometer	Advantages	Disadvantages
Long-slit	<ul style="list-style-type: none"> • relatively simple → high throughput • easy to calibrate 	<ul style="list-style-type: none"> • only one object at a time • inefficient use of detector space
Echelle	<ul style="list-style-type: none"> • high spectral resolution • efficient use of detector 	<ul style="list-style-type: none"> • challenging grating/optics • limited instantaneous $\Delta\lambda$
Integral field	<ul style="list-style-type: none"> • instantaneous 2D info • ideal for resolved objects 	<ul style="list-style-type: none"> • complex optics • single objects only
Multi-object	<ul style="list-style-type: none"> • up to thousands of spectra • ideal for spectral surveys 	<ul style="list-style-type: none"> • complex mechanisms to select fields • fibre transmission limits $\Delta\lambda$ • compact objects/regions only
Fabry-Perot	<ul style="list-style-type: none"> • ideal for large objects • high spectral resolution • more compact than FTS 	<ul style="list-style-type: none"> • not practical for large $\Delta\lambda$ • line and continuum observed at different times → calibration • needs pre-disperser
Fourier-transform (FTS)	<ul style="list-style-type: none"> • Fellgett advantage: $G=\sqrt{M}/2$ • good for extended emission • high throughput 	<ul style="list-style-type: none"> • less gain with high background • high resolution \Leftrightarrow wide interval • difficult in cryo instruments

SPECTRAL LINE ANALYSIS

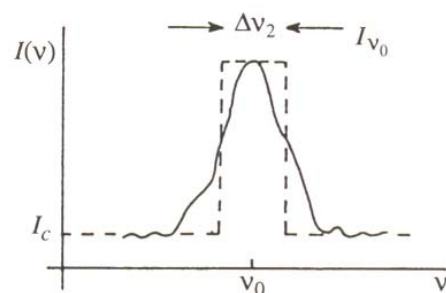
Line Intensity

The **line intensity** describes the total power contained within the line and **can be measured and/or characterized** by either:

- Fitting the line with a **Gauss** (Doppler, instrument), **Lorentzian** (collisions) or **Voigt** (both) profile
- Numerical integration $\int [I(\nu) - I_c] d\nu = f(N)$ over the continuum-subtracted **total line intensity** I (= absolute measurement)
- Calculating the **equivalent width**, which expresses the integrated line flux as a rectangular window of the continuum strength at that wavelength (= relative measurement).



$$\text{Intensity} \int |I(\nu) - I_c| d\nu$$



Equivalent width $\Delta\nu_2$

$$\int (I_\nu - I_c) d\nu = (I_{\nu_0} - I_c) \Delta\nu_2$$

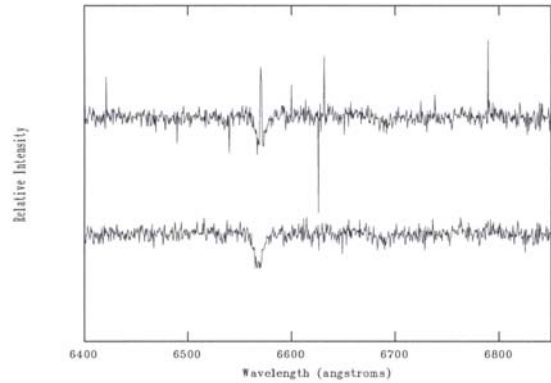
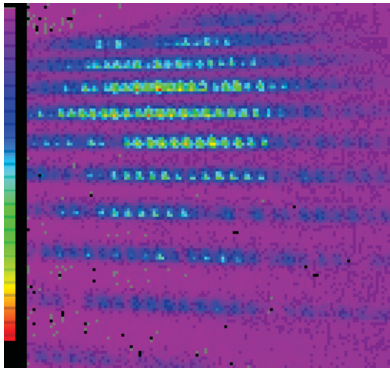
Optimal Extraction

Extracting the spectral information from the dispersed light on a real detector is non-trivial:

Usually, spectral resolution elements cover more than one pixel \rightarrow the information should be weighted according to the S/N per pixel:

$$S(\lambda) = \frac{\sum_i W_i(\lambda) \cdot (C_i(\lambda) - B(\lambda))}{\sum_i W_i(\lambda)}$$

where S is the summed signal, B is the background, and C is the detected signal per pixel i .



STIS spectrum of an O star (Massey et al. 2004):
top: standard extraction; bottom: optimal extraction.