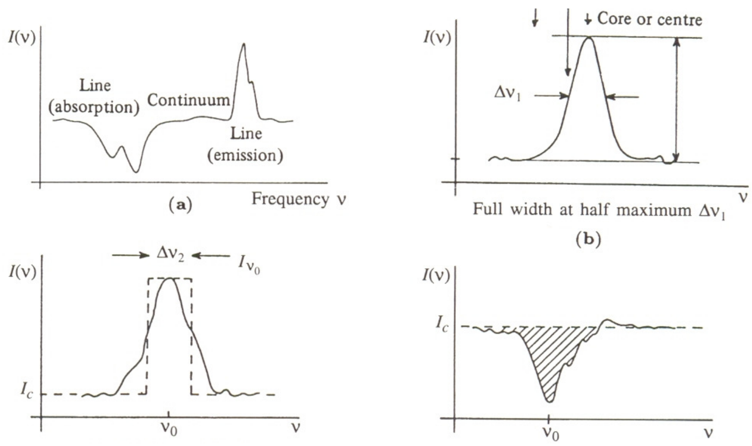
Astronomische Waarneemtechnieken (Astronomical Observing Techniques)

9th Lecture: 16 November 2011



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

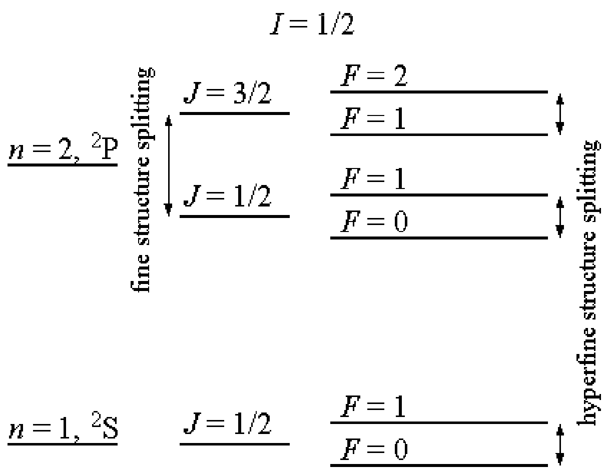
FORMATION OF SPECTRAL LINES

Formation of Spectral Lines

Macroscopically, the received radiation can be characterized by the specific intensity $I(\nu,\theta)$ at frequency ν and direction θ and polarization.

Microscopically, the transition between two energetic states E_1, E_2 requires the emission or absorption of a photon of frequency: $\nu_0 = \frac{E_2 - E_1}{h}$

Energy levels could be due to splitting at several fundamental levels:



$$E(J) = \hbar^2 \frac{J(J+1)}{2I}$$

Excitation Processes

• Electronic transitions due to the change of the principal quantum numbers of the electronic states (→ *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 (→ *near-far-IR*).

• Nuclear lines due to nuclear excititations or electron-positron annihilation (→ *MeV range*)

• Transitions in solids (ices) due to vibrations → phonons (→ *near-far-IR*).

* rotational transitions are generally weaker and often coupled to vibrational transitions → 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 μm
Atomic fine structure	1–10^{-3}	Infrared	Ne II line at 12.8 μm
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

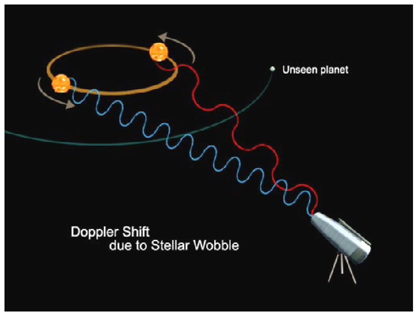
Absorption line spectrum

Physical Processes causing a Line-Shift

• Doppler effect: the emitter is in motion relative to the observer with a relative line-of-sight velocity component $v_{||}$. The resulting frequency shift is:

$$\Delta \nu = \nu_0 \left(1 - \frac{\left(1 - \frac{v_{||}^2}{c^2}\right)^{1/2}}{1 - \frac{v_{||}}{c}} \right) \approx \nu_0 \frac{v_{||}}{c}$$

→ Doppler imaging



• (normal) Zeeman effect: magnetic field splits line in three components (the linearly polarized π component at ν_0 and the two elliptically polarized σ components at ±Δν with :

$$\Delta \nu = \frac{eB}{4\pi m_e} = 1.4 \cdot 10^{10} B$$

• Einstein effect: a strong gravitational fields causes a redshift of the light:

$$\frac{\Delta \nu}{\nu} = \left(1 - \frac{2GM}{Rc^2}\right)^{1/2} - 1 \approx \frac{GM}{Rc^2}$$

GENERAL PRINCIPLE OF A SPECTROMETER

The Basic Priciple

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)

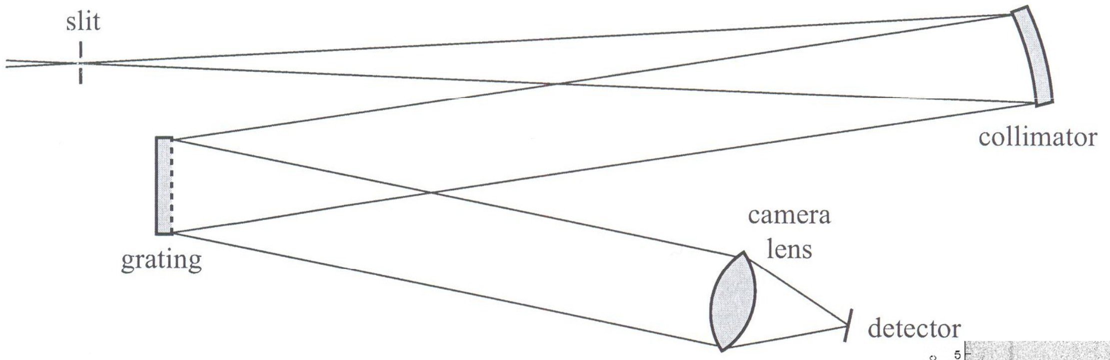
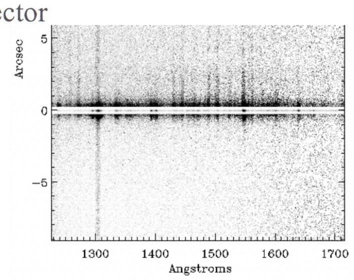


Fig. 1.— The essential components of an astronomical spectrograph.



Characteristics of a Spectrometer

- the spectral resolution or spectral resolving power is: $R = \frac{\lambda}{\Delta\lambda}$
  Δλ is called a spectral resolution element.

- the instrumental profile P(ν) broadens a theoretically infinitely narrow line $I_0(\nu) = \delta(\nu - \nu_0)$ to the observed line width:

  $$I(\nu) = P(\nu) * I_0(\nu)$$

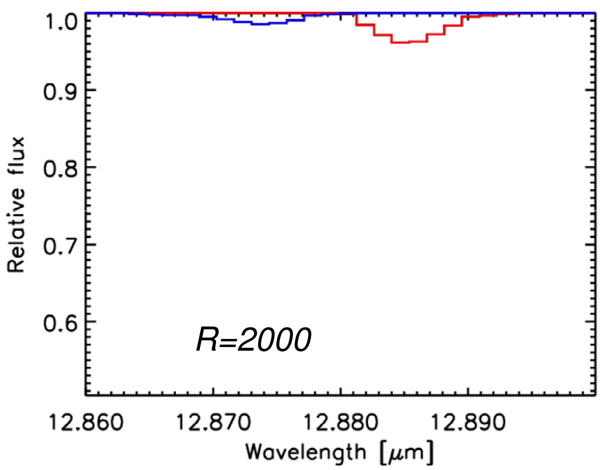
  Usually the instrumental profile determines the spectral resolution element, which is typically Nyquist-sampled.

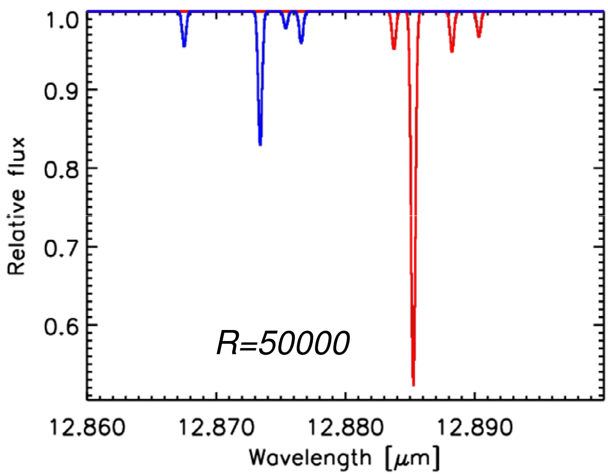
- the beam étendue determines the light gathering power of the instrument. Larger étendues require larger dispersive elements (A) or highly inclined beams (Ω).

- 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{angle to the surface}

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

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

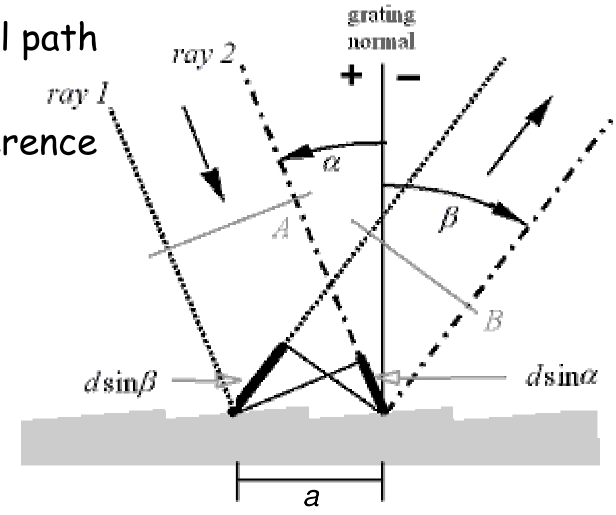
m = order of diffraction

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*:

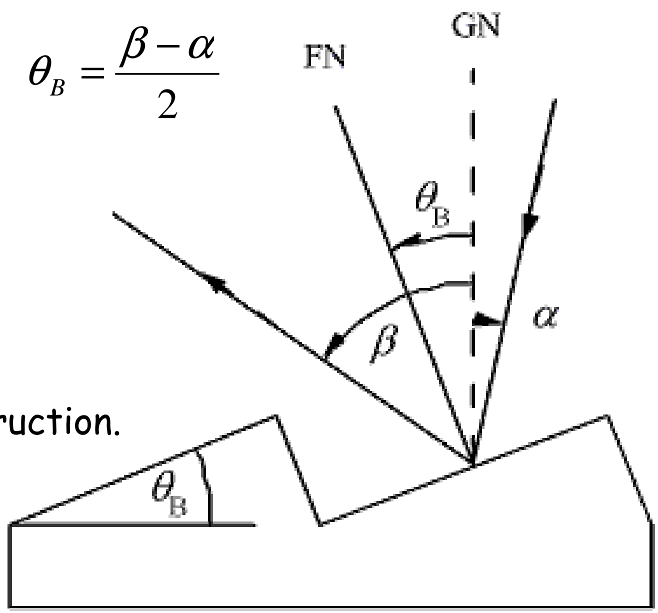
$$\alpha + \beta = 2(\alpha + \theta_B) \;\Rightarrow\; \theta_B = \frac{\beta - \alpha}{2}$$

Advantage:

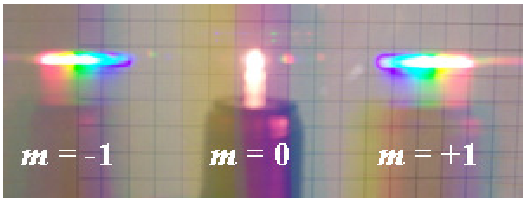
- High efficiency

Disadvantage:

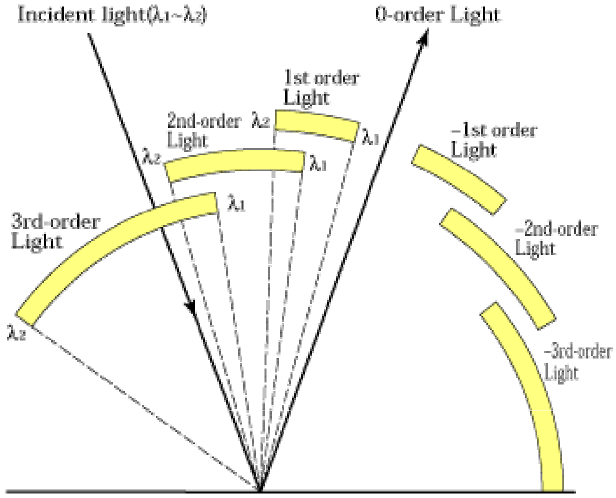
- Blaze angle Θ_B (and hence blaze wavelength Λ_B) are fixed by construction.



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:

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

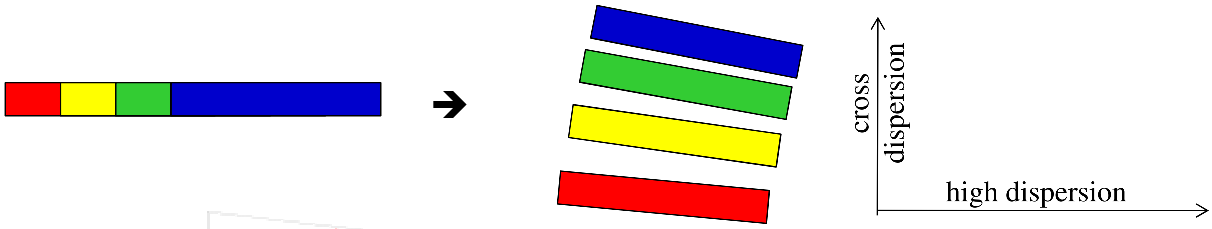
The free spectral range is the largest wavelength range for a given order that does not overlap the same range in an adjacent order.

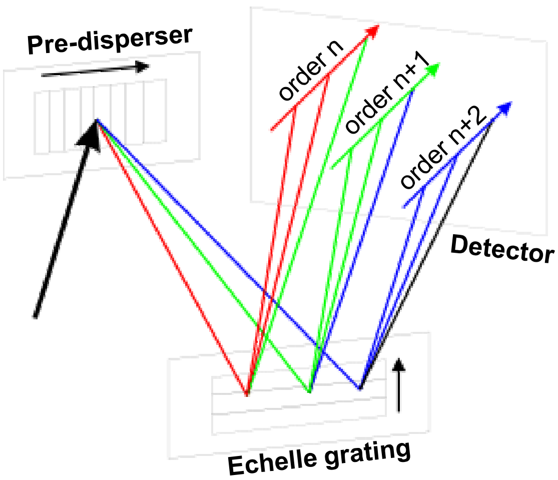
$$\Delta\lambda_{free} = \lambda - \lambda' = \frac{\lambda'}{m}$$

…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

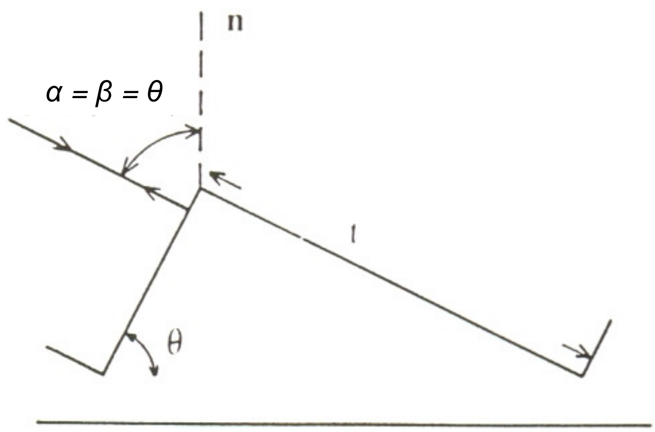




Echelle Gratings

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 >> λ) and a large angle of incidence, and operate at a very high order of diffraction (m >~50).

If α = β = θ → Littrow configuration

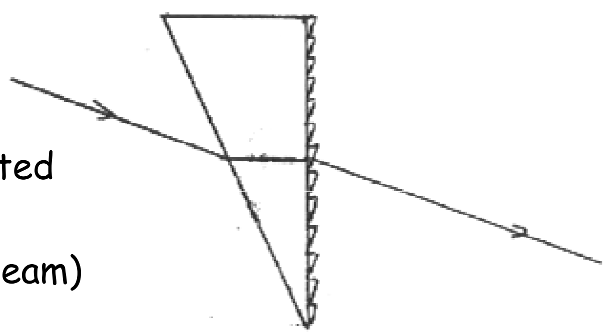


In Littrow configuration the grating equation becomes: $m\lambda_B = 2a \sin \Theta$

Grisms

Grism = transmission GRating + prISM

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:

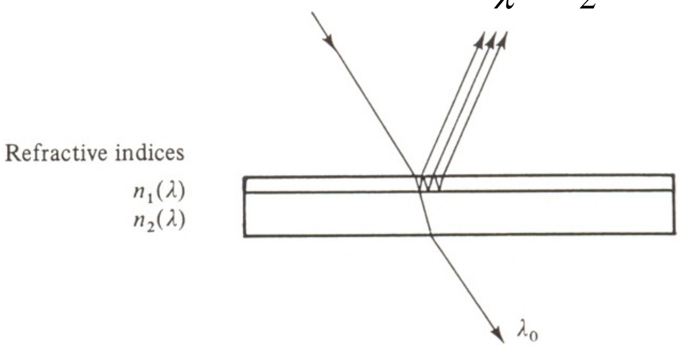
• difficult to manufacture (either by replication and gluing or by direct ruling.

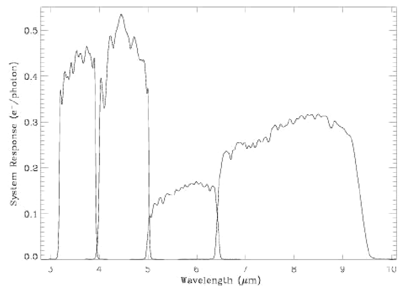
• can be quite "bulky" (← filter wheel)

Interference (Transmission) Filters

Principle: interference layers deposited on a substrate.

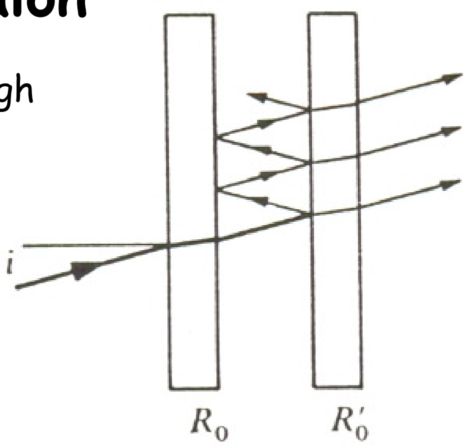
The transmission is maximal where $\frac{2n_1 d}{\lambda} + \frac{\pi}{2} = 2k\pi$





- spectral resolution typically R ~ few - 1000
- needs often multiple interference layers
- filters are often tilted with respect to the optical axis to avoid reflections → 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.

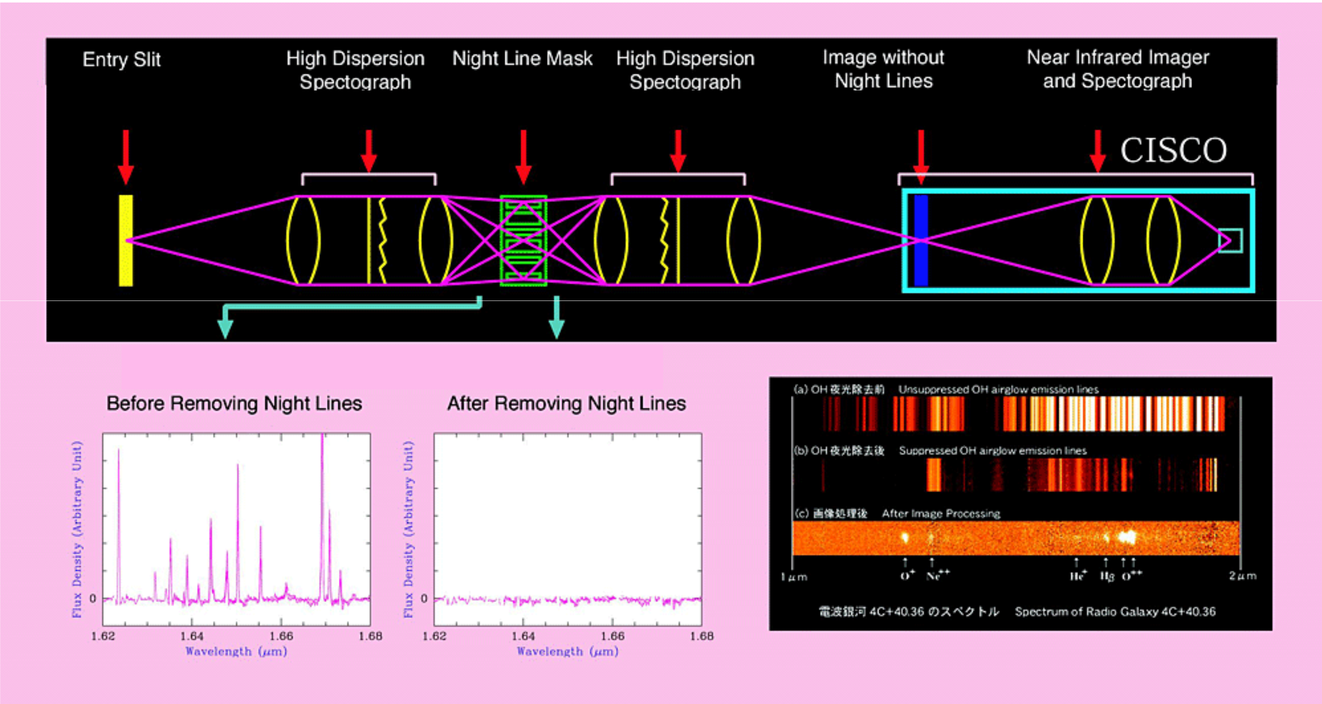
The performance of a Fabry-Perot is characterized by:

1. The finesse $F = \frac{\pi\sqrt{r}}{1-r}$,
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

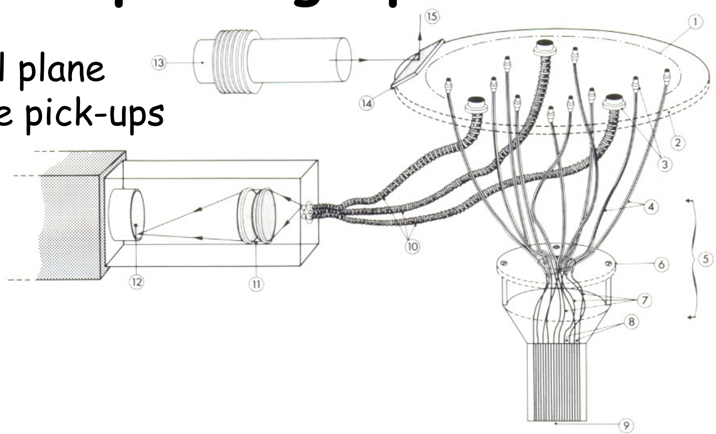
OHS filter out the wavelengths of atmospheric OH lines, which contribute the major part of the near-IR background.



http://subarutelescope.org/Introduction/instrument/img/OHS_concept.gif

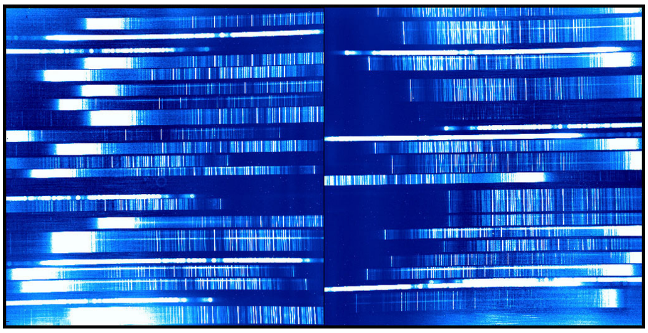
Multi-Object Spectrographs

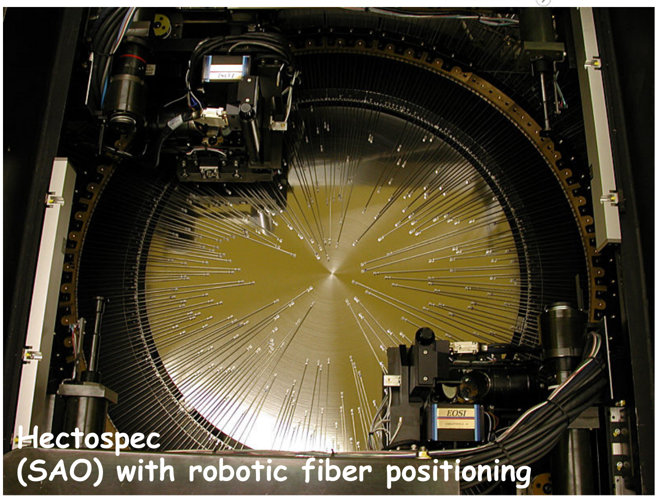
Use numerous "slits" in the focal plane simultaneously → multiple source pick-ups using fibers or mirrors.



Needs different slit masks for different fields.

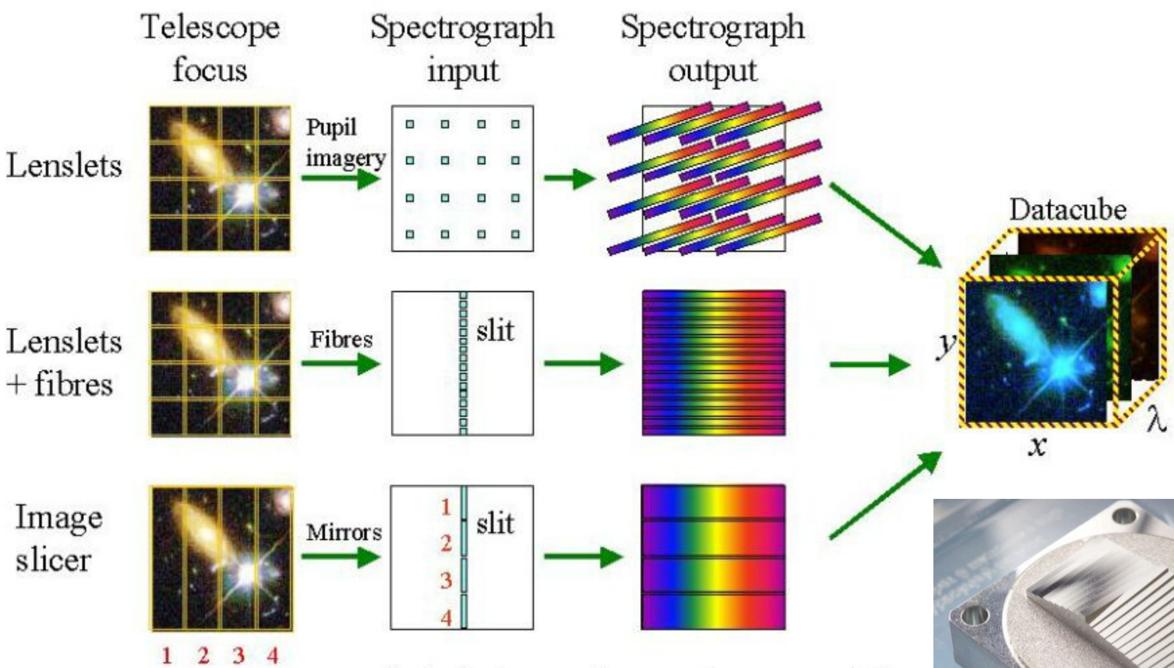
Align all spectra on the same detector:



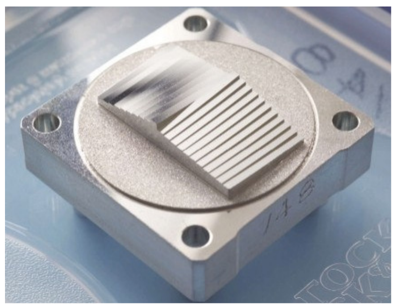


Integral Field Spectrographs

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.



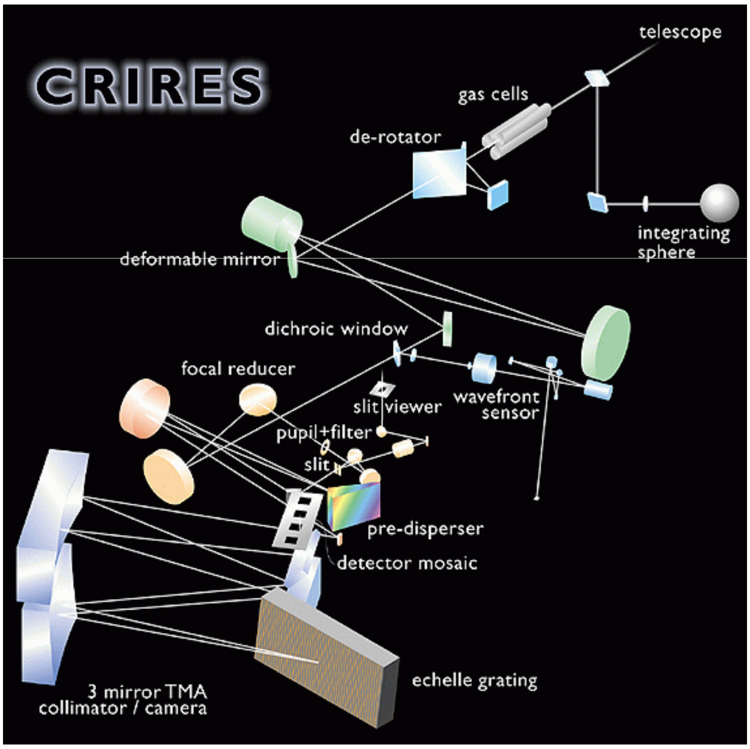
JWST-MIRI image slicer:

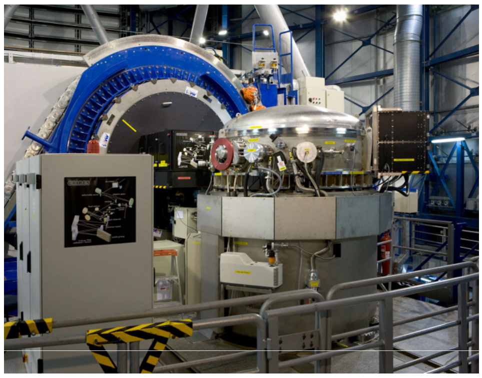


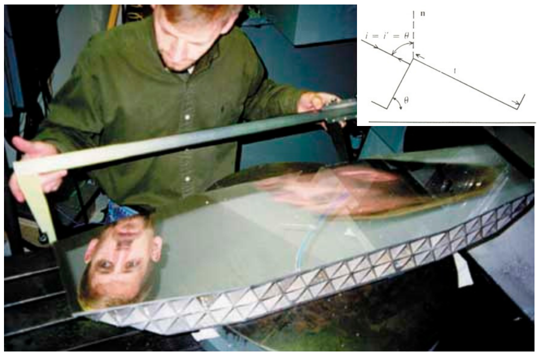
Echelle Spectrographs

Operation in high order → pre-disperser essential

Example: ESO's VLT instrument CRIRES:

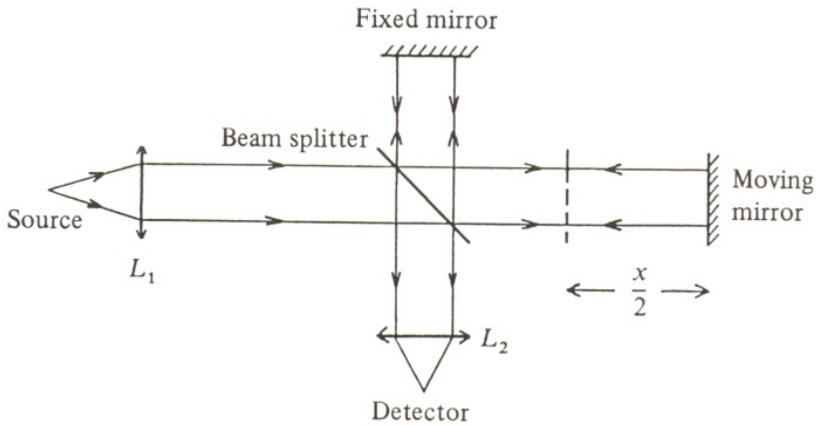






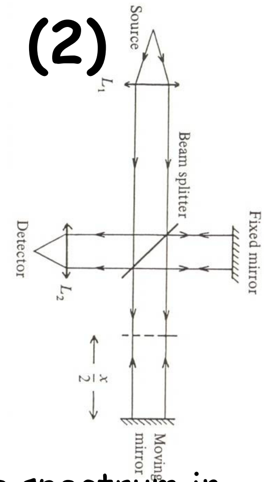
The ruled echelle grating of the SOFIA Facility Spectrometer AIRES. Two images of the engineer are seen reflected from the facets of the grooves that are at angles of 90 degrees from each other.

Fourier Transform Spectrometer (1)



- The FTS or Michelson interferometer is a <u>two-wave</u> interferometer (as opposed to a grating with *N* waves from *N* grooves).
- The signal is an interferogram. It is the Fourier transform of the spectrum of the object.
- For each setting of the spectrometer arm length (x) <u>all</u> spectral elements contribute to the signal ("spectral multiplexing").
- FTS are axisymmetric and particularly suited to observe extended sources.

Fourier Transform Spectrometer (2)



If x is the difference in path length the intensity of a monochromatic wave of intensity I_0 and wave number k is:

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

Then, a source with a spectral distribution $I_0(k)$ in the range $[k_1,k_2]$ has: $I(x)=\frac{1}{2}\int_{k_1}^{k_2} I_0(k)(1+\cos 2\pi kx)dk$

Moving the mirror in many small steps across x_m, the source spectrum in the frequency domain, $I_0(k)$, can be recovered via inverse Fourier transform: $I_0'(k)=FT\{I(x)-\langle I(x)\rangle\}=I_0(k)*\mathrm{sinc}(x_m k)$

Finite interval $[-x_m/2, +x_m/2]$ → resolution is degraded to $R=\frac{k_0}{\Delta k}=x_m k_0$

<u>Whole</u> integration time used for <u>each</u> spectral element – as compared to a Fabry-Perot spectrometer ➔ S/N gain of $G=\frac{\sqrt{M}}{2}$

(M is the number of spectral elements).

This is called the Fellgett (or multiplex) advantage.

Pros and Cons of the Different Types

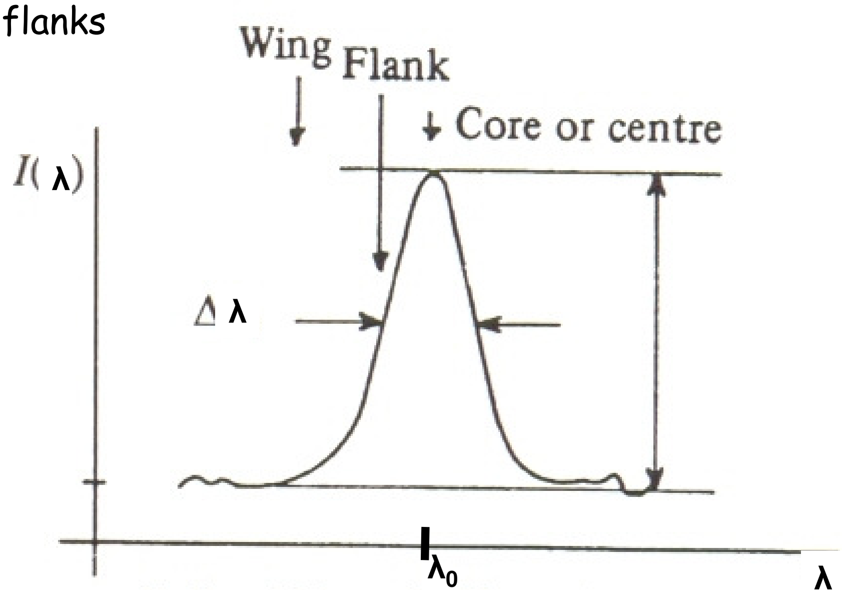
Spectrometer	Advantages	Disadvantages
Long-slit	• relatively simple → high throughput • easy to calibrate	• only one object at a time • inefficient use of detector space
Echelle	• high spectral resolution • efficient use of detector	• challenging grating/optics • limited instantaneous Δλ
Integral field	• instantaneous 2D info • ideal for resolved objects	• complex optics • single objects only
Multi-object	• up to thousands of spectra • ideal for spectral surveys	• complex mechanisms to select fields • fibre transmission limits Δλ • compact objects/regions only
Fabry-Perot	• ideal for large objects • high spectral resolution • more compact than FTS	• not practical for large Δλ • line and continuum observed at different times → calibration • needs pre-disperser
Fourier-transform (FTS)	• Fellgett advantage: $G=\sqrt{M}/2$ • good for extended sources	• requires low RN detectors • high resolution ⇔ wide interval • difficult in cryo instruments

SPECTRAL LINE ANALYSIS

Qualitative Features of a Spectrum (1)

The line profile is characterized by:

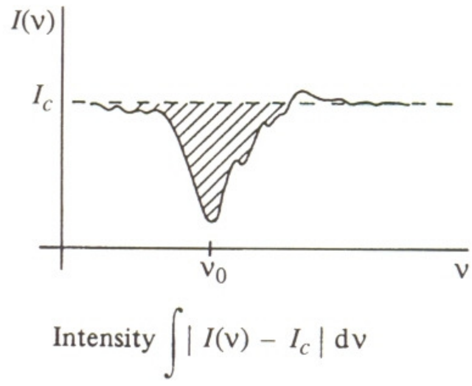
- the FWHM $\Delta\lambda$
- the center wavelength or line position λ_0
- the flanks
- the symmetry of the flanks
- the wings



Qualitative Features of a Spectrum (2)

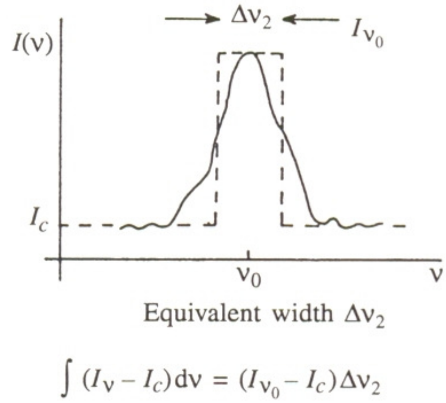
The line intensity describes the total power contained within the line and can be characterized by either:

• by the continuum-subtracted total line intensity I (= absolute measurement)



or

• by the equivalent width, which expresses the integrated line flux as a rectangular window of the continuum strength at that wavelength (= relative measurement).



Measuring Spectral Line Intensity

The most common methods are:

• by numerical integration of the line profile: $\int_{line} [I(\nu) - I_c] d\nu = f(N)$

• by fitting a Gaussian $\phi_G(\nu) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(\nu-\nu_0)^2}{2\sigma^2}\right]$ if the line profile is determined by Doppler broadening or the instrumental profile ("unresolved line") [see below].

• by fitting a Lorentzian $\phi_L(\nu) = \frac{1}{2\pi} \frac{\Delta\nu_L}{(\nu-\nu_0)^2 + (\Delta\nu_L/2)^2}$ if the line profile is given by collisions, where $\Delta\nu_L = 1/\pi\tau$, with τ the mean time between collisions.

• by fitting a Voigt profile $\phi_V(\nu) = \phi_G(\nu) * \phi_L(\nu)$ which is a convolution of Gaussian and Lorentzian profile (= most general case).

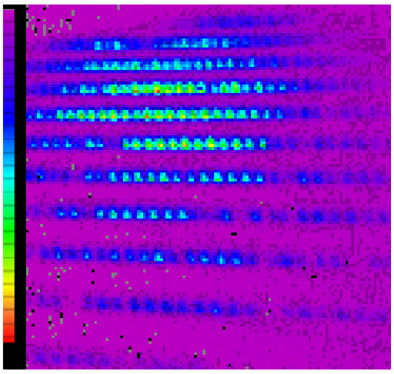
Optimal Extraction

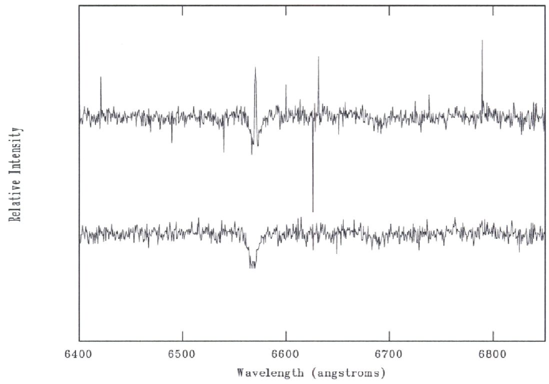
Extracting the spectral information from the dispersed light on a real detector is non-trivial:

Usually, spectral resolution elements cover more than one pixel → 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.