Astronomische Waarneemtechnieken (Astronomical Observing Techniques) 11th Lecture: 1 December 2008 + Core or centre I(v)I(v)Line Δv_1 (absorption) Continuum Line (emission) Frequency v (a) Full width at half maximum Δv_1 (b) $\Delta v_2 \leftarrow$ $-I_{v_0}$ I(v)I(v) I_c Ic V₀ ν

Based on "Observational Astrophysics" (Springer) by P. Lena, F. Lebrun & F. Mignard, 2nd edition – Chapter 5; and other sources

Content:

- 1. Spectral Line Formation
- 2. Information in Spectroscopy
- 3. General features of Spectrometers
- 4. Diffractive components
- 5. Spectrometer concepts
- 6. Radio spectrometers



Formation of Spectral Lines

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

At the microscopic level the transition between two energetic states E_1 , E_2 requires the emission or absorption of a photon of frequency ν .

$$v_0 = \frac{E_2 - E_1}{h}$$

At the macroscopic level the received intensity is the sum over many such transitions, and can be described by the transfer equation:

$$I(v) = \int_0^\infty S(v, x) e^{-\tau(v, x)} dx$$

where S(v,x) is he source function describing the emission at point x and τ is the optical depth between 0 and x, and κ the local absorption coefficient:

$$\tau(\nu, x) = \int_0^x \kappa(\nu, \xi) d\xi$$

Excitation Processes (1)

• Electronic transitions due to the change of the principal quantum numbers of the electronic states (\rightarrow visible). n = 2, ²P

• 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 $n = 1, {}^{2}S$ 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 $I(\rightarrow near-far-IR)$.

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

Excitation Processes (2)

• Nuclear lines due to nuclear excititations or electron-positron annihilation ($\rightarrow MeV range$)

• Transitions in solids (ices) due to vibrations \rightarrow phonons (\rightarrow near-far-

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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	$\rm H_2$ 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	$^{12}\mathrm{C}$ line at 15.11 keV
Annihilations	$\gtrsim 10^4$	γ-rays	Positronium line at 511 keV

I = 1/2F=2ine structure splitting J = 3/2hyperfine structure splitting J = 1/2F = 0

J = 1/2

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

Information in Spectroscopy

Three General Types of Spectra

Continuous spectrum

Emission line spectrum

Absorption line spectrum

Qualitative Features of a Spectrum (1)

The line profile is characterized by:

- the FWHM ΔA
- the center wavelength or line position Λ_0
- the flanks
- the symmetry of the flanks
- the wings



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:

 $\Delta v = v_0 \left(1 - \frac{\left(1 - \frac{v_{\parallel}^2}{c^2}\right)^{1/2}}{1 - \frac{v_{\parallel}}{c}} \right) \approx v_0 \frac{v_{\parallel}}{c} \quad \Rightarrow \text{Doppler imaging}$



• (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 $\pm \Delta v$ with :

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

• Einstein effect: a strong gravitational fields causes a redshift of the light: $\Delta V \left(\begin{array}{cc} & 2GM \end{array} \right)^{1/2} \, GM$

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

Qualitative Features of a Spectrum (2)

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



Measuring the Spectral Line Intensity

The most common methods are:

- by numerical integration of the line profile: $\int_{0}^{\infty} [I(v) I_{c}] dv = f(N)$
- by fitting a Gaussian $\phi_G(v) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{(v-v_0)^2}{2\sigma^2}\right]$ if the line profile is determined by Doppler broadening, natural broadening or the instrumental profile ("unresolved line") [see below].
- by fitting a Lorentzian $\phi_L(v) = \frac{1}{2\pi} \frac{\Delta v_L}{(v-v_0)^2 + (\Delta v_L/2)^2}$ if the line profile is given by collisions, where $\Delta v_L = 1/\pi r$, with r the mean time between collisions. It represents homogeneous broadening in which all atoms interact in the same way within the line frequency range.
- by fitting a Voigt profile $\phi_V(v) = \phi_G(v) * \phi_L(v)$ which is a convolution of

Gaussian and Lorentzian profile (= most general case).

General Features of Spectrometers

Spectral Resolution (1)

The spectral resolution or spectral resolving power is defined as:

$$R = \frac{\lambda}{\Delta \lambda}$$

 $\Delta \lambda$ is called a spectral resolution element.

The typical resolution that can be achieved depends on the type of spectrometer: Spectrometer Begion Typical

Spectrometer	Region	Typical resolution
Interference filter	Visible, IR	$10^2 - 10^3$
Grating	IR, visible, UV	$10^3 - 10^6$
Bragg crystal	X-ray	10^{3}
Atomic resonance	Visible, UV	10^{7}
Fabry–Perot	Visible, IR	$10^4 - 10^6$
Fourier transform	Visible, IR	$10^4 - 10^6$
Heterodyne	Radiofrequencies	$> 10^{6}$
	IR, submillimetre	$>10^{5}$
Bolometer	X-ray	10^{2}
Scintillator	γ-ray	10^{3}

Spectral Resolution (2)

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 a resolutions of R=2000 (left) and R=50000 (right). Figure provided by F. Lahuis.

Other Characteristics of Spectrometers

• the instrumental profile $P(\nu)$ broadens a theoretically infinitely

narrow line $I_0(v) = \delta(v - v_0)$ to the observed line width:

$$I(v) = P(v) * I_0(v)$$

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

$$t(v) = \frac{I_{exit}(v)}{I_{entry}(v)}$$

Diffractive Components

Interference Filters

 $n_1(\lambda)$

 $n_2(\lambda)$

Refractive indices Principle: maximum transmission $\frac{2n_1d}{\lambda_0} + \frac{\pi}{2} = 2k\pi$ at Λ_0 where Destructive interference at $\Lambda_0 \pm \Delta \Lambda$.

Other wavelengths (for which the above equation is also satisfied) are absorbed by a blocking or absorbing filter. Note:

- spectral resolution R~few 1000
- often >10 interference layers
- filters are often tilted to avoid reflections \rightarrow shift of Λ_0 .

The opposite are neutral density filters, which provide wavelengthindependent attenuation.





Constructive interference occurs at: $a \cdot (\sin \alpha \pm \sin \beta) = m\lambda$

The maximum resolution is then given by: R = mN

(often limited by the pupil diameter)





A light bulb of a flashlight seen through a transmissive grating, showing three diffracted orders. The order m = 0corresponds to a direct transmission of light through the grating. In the first positive order (m = +1), colors with increasing wavelengths (from blue to red) are diffracted at increasing angles. Source: Wikipedia

Blazed Gratings

Generally, the energy of the beam diffracted by a periodic structure is uniformly distributed over the different orders m. If we observe only one order this is very inefficient.

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



Advantage:

•High efficiency

Disadvantage:

•Blaze angle $\boldsymbol{\Theta}_{B}$ (and hence blaze wavelength $\Lambda_{\rm B}$) are fixed by construction.

Echelle Gratings

Echelle gratings use:

- 1. a very high order of diffraction m
- 2. a large groove period a $\gg \Lambda$
- 3. a high angle of incidence (a = $\beta = \theta$) \rightarrow Littrow condition



 \rightarrow Echelle gratings achieve high resolution (R = mN) and high dispersion (~m/a).

Free Spectral Range and Cross Dispersion

The 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.

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

An additional element with a dispersion direction perpendicular to that of the grating will separate the orders and avoid spatial overlap.





Holographic and Immersion Gratings

Interference pattern of two laser beams \rightarrow expose on photoresist coating \rightarrow chemical etching \rightarrow holographic grating.

Advantage: little scattered light

Disadvantage: cannot be blazed due to sinusoidal groove profile \rightarrow low efficiency

Immersion gratings are reflection gratings in which light passes through a medium with high refractive index *n* before hitting the diffraction grating.

Advantages: n times higher resolution for same size, and: coarse grooves enable continuous wavelength coverage in crossdispersed mode.

Disadvantage: limited wavelength ranges

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 (amost) unchanged

Advantages:

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

Disadvantage:

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







Grating Production

Common techniques:

- Direct ruling
- Replication
- Etching

Above: MIT 'B' Engine. This ruling engine, now in operation at Newport, is shown with its cover removed.

Below: A large mosaic grating. A monolithic 214 x 840 mm replica mosaic grating was produced from two 214 x 415 mm submasters.

Source: NEWPORT Grating Handbook



Some Spectrometer Concepts

Single Slit Spectrometers



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 (1)

Multiple source pick-ups in the focal plane; light transport e.g. by fibers.

Advantage:

up to thousands of spectra simultaneously.

Disadvantages:

complex mechanism to position the fibers,

fiber transmission limits wavelength range,

compact objects



Multi-object Spectrographs (2)



Example: Hectospec (SAO) with robotic positioning of the fibers

Integral Field Spectrographs

Concept: 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.



Echelle Spectrographs (2)



3 mirror TMA collimator / camera



The high orders are close together and imaged simultaneously on the same array.

→ allows to "expand" a single-slit spectrum to a length many times the size of the detector.

 \rightarrow high resolution.

Fourier Transform Spectrometer (1)

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



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

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

A source with a spectral distribution $I_0(\sigma)$ in the range $[\sigma_1, \sigma_2]$ has:

$$I(x) = \frac{I_0}{2} \int_{\sigma_1}^{\sigma_2} I_0(\sigma) (1 + \cos 2\pi \sigma x) d\sigma$$

Fourier Transform Spectrometer (2)

The signal is an interferogram. It is the Fourier transform of the spectrum of the object.

 \rightarrow For each setting of the spectrometer arm length (value of x) all spectral elements contribute to the signal ("spectral multiplexing").

A FTS measures the temporal coherence of the signal.

The source spectrum $I_0(\sigma)$ (frequency domain) can be recovered via inverse Fourier transform $I'_0(\sigma) = FT[I(x) - \langle I(x) \rangle]$

with the mean value: $\langle I(x) \rangle = \frac{1}{2} \int_{\sigma_1}^{\sigma_2} I_0(\sigma) d\sigma$

For a finite interval in x [-x_m/2, +x_m/2] one gets $I'_0(\sigma) = I_0(\sigma) * \operatorname{sinc}(x_m \sigma)$ i.e. the recovered spectrum is degraded in resolution. The resolution is: $R = \frac{\sigma_0}{\Lambda \sigma} = x_m \sigma_0$

Fourier Transform Spectrometer (3)

Now: considering the maximum beam étendue beyond which the resolution would be degraded:

At the same resolution the thoughput of an FTS can be ~100-1000 higher than that of a grating spectrometer ("throughput advantage").

Notes: FTS (like FPS) are axisymmetric and particularly suited to observe extended sources.

Since the whole integration time is used for each spectral element as compared to a scanning monochromator - an FTS will produce a gain of $G = \frac{\sqrt{M}}{2}$ in the S/N of the resulting spectrum (where *M* is the number of spectral elements and the dominating noise is detector noise).

This is called the Fellgett advantage (or multiplex advantage).

Fourier Transform Spectrometer (4)

Example: the FTS of the CFHT mounted at the Cassegrain focus (Maillard & Michel 1982)



Fabry-Perot Spectrometer (1)

Combines the throughput advantage of he FTS (Q= 2π) with very high spectral resolution while being more compact.

Principle: two parallel plates (Fabry-Perot etalon) of high reflectivity r and transmission t = 1 - r.



and has transmission peaks when $\sigma = \frac{m}{2d}$

m is the order of the interferometer and $\Delta \sigma = 1/2d$ the free spectral interval.

Fabry-Perot Spectrometer (2)

An important quantity characterizing a FPS is the finesse $F = \frac{\pi \sqrt{r}}{1-r}$

since it determines the resolution $R = \frac{\sigma}{\Delta \sigma} = mF$

The maximum throughput of a FPS is given by $U = 2\pi \frac{S}{R}$ where S is the area of the etalon.

Advantages:

• simultaneous spectroscopic information over a large field *Disadvantages:*

- needs a pre-disperser to isolate a free spectral interval
- good for line spectroscopy, not practical for extended spectral range

Spectrometers

Radio

Multichannel Spectrometers

- 1. IF signal leaving the mixer
- 2. set of filters with bandpass B split the frequency band Δv in N= $\Delta v/B$ channels.
- Each filter is followed by a quadratic detector and a commutator comparing the signal with a calibration reference.

The resolution is given by: $R = \frac{V_0}{B}$ where B can be very narrow.

Multi-channel spectrometers can have up to 512 parallel channels.



Acousto-Optical Spectrometer

An AOS converts the frequencies to ultrasonic waves that disperse a monochromatic light beam onto an array of visible light detectors.



The acoustic wave can be created in a crystal ("Bragg-cell") and modulates the refractive index \rightarrow induces a phase grating. The angular dispersion is a measure of the IF-spectrum.

Autocorrelation Spectrometers

Reminder of lecture on Fourier transforms:

f(x)	Function
$\widetilde{f}(s) = FT\{f(x)\}$	Fourier transform of $f(x)$
$\left \widetilde{f}(s)\right ^2$	Spectral density or power spectrum of $f(x)$
$\left \widetilde{f}(s)\right ^2 = f(x) \otimes f(x)$	Wiener - Khinchine (autocorrelation) theorem
$k(x) = \int_{-\infty}^{+\infty} f(u)f(u+x)du$	Autocorrelation

Principle of the autocorrelator:

Spectrum I(v) is the Fourier transform of the autocorrelation of x(t), a time-dependent IF signal \rightarrow digitize x(t) and compute the autocorrelation function R(t) = spectrum of x(t)