

# Chapter 7

## Spectroscopy

Astronomical spectroscopy started with the detection of the absorption lines in the solar spectrum by Fraunhofer at the beginning of the 19th century. Without understanding the nature of these lines he named the strongest of them with letters. Only about 50 years later it was recognized by Kirchhoff and Bunsen that some of these lines are due to atoms in the solar atmosphere. Fraunhofer's letters survived into the modern scientific jargon:

|                | A                           | B                           | C          | a                           | D    | E    | b    | F         | G          | H     |
|----------------|-----------------------------|-----------------------------|------------|-----------------------------|------|------|------|-----------|------------|-------|
| ident.         | O <sub>2</sub> <sup>a</sup> | O <sub>2</sub> <sup>a</sup> | H $\alpha$ | O <sub>2</sub> <sup>a</sup> | Na I | Fe I | Mg I | H $\beta$ | H $\gamma$ | Ca II |
| $\lambda$ [nm] | 759                         | 687                         | 656        | 628                         | 589  | 527  | 517  | 481       | 434        | 397   |

<sup>a</sup>: absorptions from the Earth's atmosphere

Spectroscopy often allows a detailed physical characterization of the observed stars and astrophysical plasmas. It is a long and interesting history from the initial analysis of stellar and nebular spectra to modern astronomical spectroscopy. Most important applications of spectroscopy are:

- determination of temperature, surface gravity, abundances, and many other parameters of stars. Most basic are the stellar spectral types

$$O - B - A - F - G - K - M$$

which define a temperature sequence from hot to cold stars.

- the measurement of Doppler shift for spectral lines due to the relative motion of the target or / and for distant objects due to the cosmological expansion

$$\frac{\Delta\lambda}{\lambda} = \frac{v_{\text{rad}}}{c} \quad \text{for } v_{\text{rad}} \ll c \quad \text{or/and} \quad \frac{\Delta\lambda}{\lambda} = z$$

respectively,

- the determination of temperatures, particle densities, abundances and other parameters of gaseous nebula from emission lines,
- the determination of column densities, abundances, temperatures and other parameters of the absorbing gas located between a light source and the observer.

Spectroscopy is a cornerstone for astrophysical studies providing detailed information on essentially all targets. Often a target is only well studied if its spectral properties are known.

## 7.1 Science requirements

Spectroscopy provides the wavelength dependence of the intensity  $I(\lambda)$  of the target. Thereby the key parameters are:

- the spectral resolution  $R = \lambda/\Delta\lambda$ ,
- the spectral coverage  $[\lambda_{\min}, \lambda_{\max}]$ .

The spectral resolution and coverage should be optimized for each particular science case. The resolution should be good enough to measure accurately a spectral feature. This means that the investigated spectral feature can be separated from other structures in the spectrum from the source, the background or the instrument so that its strengths or shape can be determined with sufficient precision. The spectral coverage should be optimized so that all important spectral features can be covered within a minimum of telescope time. Depending on the science needs one can combine the spectral information with spatial information  $I(x, \lambda)$  or  $I(x, y, \lambda)$ . Another possibility is to measure the temporal variability of the spectrum  $I(\lambda, t)$ .

The science goal defines which spectral quantities of a target have to be measured:

- *Rough spectral characterization*;  
in many cases even a coarse spectrum allows a quite good characterization of the object type.
- *Spectral dependence of the flux*;  
this requires a broad wavelength coverage and an accurate calibration of the spectral efficiency of the instrument.
- *Equivalent width*;  
equivalent width measurements are relative measurements of the attenuation of a spectral continuum by an absorption providing information on the abundance of the absorbing species.
- *Emission line strengths*;  
emission line diagnostic is based on the strength of the lines which should be measured absolutely, or relative to another well-known emission like H I lines.
- *Line profile structures*;  
useful for studies on the radial velocity structure or radiative transfer effects in an object. Depending on the scientific aim one has to select the appropriate spectral resolution to resolve sufficiently the line profile.
- *Doppler shift measurements*;  
requires an appropriate precision of the radial velocity calibration and suitable spectral features to measure radial velocity shifts.
- *Spatially resolved spectroscopy*;  
this combines spectroscopic measurements with spatial information and is most useful for the investigation of the structure of extended objects or to disentangle blended objects.
- *Time resolved spectroscopy*;  
for the investigation of the temporal variability of spectral features for the study of variable objects.

## 7.2 Spectrographs

Only X-ray and  $\gamma$ -ray detectors have sufficient energy resolution to provide a spectrum of the incoming radiation directly. At longer wavelengths a spectrograph is necessary. Spectrographs which disperse the light are based on the following concept:

- an entrance aperture at the focal plane of the telescope,
- a dispersive element (e.g. grating, prism, etc.) in a collimated beam section,
- a camera optics which focusses the dispersed beam onto the detector so that the different wavelengths from a point are imaged along a line.

A different type of spectrometer is the Fourier transform spectrometer which measures the interference pattern of an interferometer, where the path length of one arm is variable. The observed constructive and destructive interferences can be converted to a wavelength spectrum using Fourier transformation. This type of spectrometer has only special application in Astronomy.

### 7.2.1 Basic equations for grating spectrographs

A grating oriented perpendicular to the incoming beam produces for a given wavelength  $\lambda$  constructive interferences for the angles  $\theta$  according to:

$$\sin \theta_m = \frac{m \cdot \lambda}{a}, \quad (7.1)$$

where  $a$  is the periodic separation between the grating lines and  $m$  an integer number for the interference order. One should be aware that an overlap of the different orders ( $m - 1$ ,  $m$ ,  $m + 1$ , etc.) can occur.

The angular dispersion  $d\theta/d\lambda$  of the grating follows from differentiation (determine first  $d\lambda/d\theta$ ):

$$\frac{d\theta}{d\lambda} = \frac{m}{a \cos \theta}.$$

The angular width  $W_\theta$  of a monochromatic interference peak is broad for few grating lines and it becomes narrower as the number of illuminated grating lines  $N$  increases like

$$W_\theta = \frac{\lambda}{Na \cos \theta}.$$

This width can also be expressed in a wavelength width  $\Delta\lambda$

$$\Delta\lambda = W_\theta \frac{d\lambda}{d\theta} = \frac{\lambda}{Na \cos \theta} \cdot \frac{a \cos \theta}{m} = \frac{\lambda}{Nm},$$

or a resolving power  $R$  for a more general characterization of the diffraction limited resolution of the grating

$$R = \frac{\lambda}{\Delta\lambda} = Nm. \quad (7.2)$$

This formula indicates that the resolving power depends only on the number of illuminated grating lines and the dispersion order.

Gratings, in particular reflective gratings, are often inclined with respect to the incoming beam by an angle  $i$  which is the angle of the grating normal to the incoming beam. The angle  $\theta$  is then defined by the interference order  $m$  and the zero order. In this case Equation (7.1) includes the term  $\sin i$  for the grating inclination:

$$\sin \theta = \frac{m \cdot \lambda}{a} - \sin i. \quad (7.3)$$

This is called the grating equation. The resolving power is larger for inclined gratings because more lines are illuminated for a given beam diameter

$$R = \frac{\lambda}{\Delta\lambda} = \frac{N m}{\cos i}. \quad (7.4)$$

The grating equation describes also how one can change the central wavelength and the wavelength range for a given deflection angle  $\theta$  by changing the tilt angle  $i$ . The following list gives the dependence of spectrum parameters on grating properties:

- the resolving power  $R$  depends only on the number of illuminated lines and the diffraction order
- $R$  increases if the number of lines per mm of the grating are enhanced for a given beam (=pupil) diameter
- $R$  can be enhanced for a given grating by a larger illuminating beam (larger pupil) or by tilting the grating so that the illuminated lines increase like  $N_i = N_{i=0}/\cos i$
- $R$  is substantially larger for higher diffraction orders  $R \propto m$  (there is the restriction that overlap of grating orders occur)
- the wavelength region for a given deflection angle can be selected by changing the inclination  $i$  of the grating.

### 7.2.2 Different types of gratings

**Simple gratings.** Typical grating have about 100 – 1000 rulings/mm. This yields for the first order diffraction spectrum and a collimated beam diameter (pupil diameter) of 1 cm a grating resolving power of  $R = 1000 - 10000$ . The first order spectrum can be contaminated by the second order spectrum with  $\lambda_{m=2} = \lambda_{m=1}/2$  or higher order spectra  $\lambda_{m \geq 3}$ . For ground based optical spectroscopy this happens for  $\lambda_{m=1} > 660$  nm, when second order light from above the UV-cutoff  $\lambda_{m=2} > 330$  nm sets in. The second order can be suppressed with a short wavelength cutoff filter. For example a BG430 filter cuts all light shortwards of about 430 nm, allowing first order spectroscopy from 430 nm to 860 nm without second order contamination.

The same grating can also be used in second order with twice the resolution of the first order. In this case one has to select for a given wavelength range the correct pass-band filter to avoid the contamination by other orders.

**Blazed gratings.** Simple gratings are not very efficient since the light is distributed to several grating orders. The efficiency of reflecting gratings can be improved by an optimized inclination of the reflecting surfaces so that they reflect the light preferentially in the direction of the aimed interference order. Thus the grating efficiency is optimized for one particular wavelength or diffraction angle  $\theta_b$ , the so-called blaze angle.

**Echelle gratings.** An extreme case of the blazed grating is the echelle grating. It is strongly inclined with respect to incoming beam and more importantly it is optimized (blazed) for high order diffraction directions, say  $m = 10 - 100$ . With this type of grating the resolving power can be strongly enhanced even if the grating is quite coarse. For example a beam of 2 cm diameter illuminating an echelle grating with 20 lines / mm, inclined by  $i = 60^\circ$  ( $1/\cos i = 2$ ) will see effectively 800 grating lines, which produce for  $m \approx 50$  a spectral resolving power of  $R = 40'000$ . Of course for such a grating the free spectral range, without overlap by neighboring pixels, is only small and of the order  $\Delta\lambda \approx \lambda/m$ . Narrow band filters are required to select one particular order.

A more elegant solution is a **cross dispersion** with a second low order grating or a prism perpendicular to the dispersion of the echelle grating. In this way the individual orders are displaced with respect to each other and many orders of the echelle grating can be placed on a rectangular imaging detector.

**Transmission gratings and grisms.** The principles of transmission gratings are essentially the same as for reflecting gratings. One interesting variation of the transmission grating is the grisms. Grisms are a combination of a prism with a grating so that the spectrum is produced in the straight-through direction. The advantage of this concept is that they can be inserted in the collimated beam of an imaging camera. The same instrument serves then as imager and spectrograph.

### 7.2.3 Spectrograph apertures

The spectrograph aperture is typically matched to either the seeing limited resolution or the diffraction limited resolution of the telescope.

**Slit aperture.** A widely used aperture type for spectrographs is the slit aperture. The slit orientation is perpendicular to the spectrograph dispersion direction. Thus the slit is imaged onto the detector and any narrow wavelength dependence of the intensity produce a dark or bright line in the resulting spectrum. Therefore one speaks of emission and absorption lines when quasi-monochromatic absorptions or emissions of atoms or molecules are observed.

*Slit width:* Usually the slit width can be changed but then the spectral resolution or the resulting width of unresolved lines will change accordingly. For seeing limited observations the following choices can usually be made for the slit width:

- Narrow slits for high spectral resolution; they are usually matched to the “best seeing” conditions expected which is about 0.5 – 1.0 arcsec.
- Wide slits for spectrophotometric observations; they are wide enough (5 – 10 arcsec) so that essentially no light is lost on the aperture.
- intermediate slit widths which allow an adjustment to the seeing conditions. The selected slit width is often 1 – 1.5 times the seeing for a good compromise between spectral resolution, throughput, and background rejection.

*Slit orientation:* The orientation of the slit is another parameter which can in some case be chosen. Changing the slit orientation is usually achieved with a rotation of the entire spectrograph, since the slit orientation should remain perpendicular to the spectrograph dispersion direction. The rotation of an instrument may introduce mechanical flexures in the spectrograph which require a spectroscopic re-calibration in the same spectrograph position.

Standard slit orientations and consideration for the selection of a slit orientation are:

- The slit along the line through zenith and target (paralactic angle =  $0^\circ$ ) is an obvious orientation for Alt-Az telescopes because then the instrument is fixed with respect to the telescope. An additional advantage is that the atmospheric dispersion is along the slit and the danger that one section of the spectrum is less well transmitted through the slit is minimized.
- A North-South slit direction is useful for equatorial telescopes, because the spectrograph is then fixed with respect to the telescope. For observations near the meridian the North-South direction coincides with the zenith direction so that slit losses due to atmospheric dispersion are minimized.
- A particular slit orientation may be chosen due to particular reasons:
  - a slit orientation in order to avoid light of a nearby bright source “falling” into the spectrograph,
  - a slit orientation which allows to place a second target onto the slit for simultaneous spectroscopy of two sources,
  - a slit orientation best suited for simultaneous measurement of the sky spectrum for the background correction,
  - the orientation best suited for long slit spectroscopy of an extended target where all points along the slit can be investigated spectroscopically.

**No aperture.** Having no aperture in the focal plane provides spectroscopy of each point in the aperture. The problem is of course that the spectra of neighboring points (in the dispersion direction) overlap. Also the sky background from the whole aperture is passing through the system and is dispersed causing a high background which is harmful for weak targets. Good applications for “aperture-free spectroscopy” are:

- Low resolution survey of bright targets in uncrowded fields; if the spectra are short and the number of bright targets small then the spectra of the different objects do not overlap.
- High resolution spectral imaging of targets with narrow emission lines: if the emission line target is compact and the emission lines well separated spectrally, then one can obtain “monochromatic” images for various emission lines simultaneously.

**Entrance lens for a fiber.** Often the entrance aperture of a spectrograph is a lens in the focal plane of the telescope which focusses the light into an optical fiber. The spectrograph can then be mounted in a laboratory near the telescope. Very stable fiber spectrographs of this kind can be built which are suited for high precision radial velocity measurements.

If multiple fibers are placed in the focal plane then one can obtain multi-object spectroscopy. The fiber outputs are placed in a line configuration in the entrance aperture of a spectrograph (like a slit with multiple sources.)

**Custom made masks.** Science programs may require very specific apertures. For example for the spectroscopy of a strongly distorted lensed galaxy one may use an arc-like aperture in the focal plane in order to investigate the object spectroscopically. Such an aperture can be made with a laser cutting machine. Some observatories offer the possibility to cut special spectrograph apertures using the detector images taken with the imaging mode of the same instrument.

Using custom made masks with multiple apertures is another way to take multi-object spectroscopy.

## 7.3 Examples for spectrographs

### 7.3.1 The classical spectrograph from Boller & Chivens.

The Boller & Chivens (B&C) spectrograph was a kind of standard reflective grating spectrograph available at many astronomical observatories between 1970 and 1990.

This type of spectrograph consists of the following components:

- insertable reflection prism for the input of the light from internal calibration lamps,
- a slit entrance aperture, where the slit width can be changed between 5 and 1200  $\mu\text{m}$ ,
- optimization optics (field lens, spectrum widener),
- order separation filters which can be exchanged remotely,
- shutter,
- collimator mirror,
- exposure meter mirror and sensor which allows to monitor the flux,
- a tiltable grating, which can be exchanged manually with other gratings,
- Hartmann mask for spectrograph focus measurements,
- camera optics,
- focal plane with detectors.

In addition a slit viewing optics or camera is required. With the slit viewing camera the positioning of the star on the slit can be monitored and adjusted if required with a handset for the telescope drive motors.

With the Boller & Chivens spectrograph one can select the spectral range and spectral resolution by the following means:

- different gratings can be selected
- different grating orders can be selected with the order separating filters
- the spectral range can be adjusted by changing the tilt angle of the grating.

Every change in the configuration requires a new set of calibration measurements (flat-fields, flux and wavelength calibration).

A typical set of gratings for the B&C spectrograph has the following parameters:

| grating<br>1/mm | blaze (nm)<br>(order) | dispersion<br>nm / mm | dispersion<br>nm / pixel <sup>a</sup> | coverage<br>nm <sup>a</sup> |
|-----------------|-----------------------|-----------------------|---------------------------------------|-----------------------------|
| 300             | 500                   | 22.1                  | 0.53                                  | 544                         |
| 600             | 500                   | 11.7                  | 0.28                                  | 287                         |
| 600             | 750                   | 11.7                  | 0.28                                  | 287                         |
| 600             | 625(2)                | 5.8                   | 0.14                                  | 143                         |
| 600             | 625(3)                | 3.8                   | 0.09                                  | 94                          |
| 1200            | 400                   | 5.8                   | 0.14                                  | 143                         |
| 1200            | 500                   | 5.8                   | 0.14                                  | 143                         |
| 1200            | 750                   | 5.8                   | 0.14                                  | 143                         |

<sup>a</sup>: for a 1024 x 1024 pixel CCD camera with pixel size 24  $\mu\text{m}$

The B&C spectrograph allows medium resolution spectroscopy with a 2 pixel resolution from 1 nm with a very broad spectral coverage of 500 nm down to a resolution of 0.2 nm with a small coverage of 100 nm.

### 7.3.2 Spectroscopy with FORS

FORS (focal reducer and low dispersion spectrograph) is a multi-purpose, Cassegrain instrument at the VLT for imaging, spectroscopy, and polarimetry. It is based on successful previous instruments called EFOSC used at other ESO telescopes on La Silla, which are still available. These instruments are based on transmitting optics.

FORS consists of the following components:

- a box with calibration lamps,
- a focal plane aperture unit with 19 slitlets for multi-object spectroscopy, 9 longslit masks, and mask exchange unit holding up to 10 custom made masks cut by a laser,
- two remotely exchangeable F/15 collimators: a standard resolution (SR) collimator for 2 pixel resolution ( $15 \mu\text{m}$  pixels) of  $0.25''$  and high resolution (HR) collimator for a resolution of  $0.125''$  for the HR collimators,
- two grism wheels with in total 10 grisms,
- a shutter,
- a filter wheel with broad band imaging filters and two order separation filters (GG435, and OG590) for spectroscopy,
- camera optics,
- detector focal plane with two 2k x 4k CCD detectors,
- additional polarimetric components for polarimetry and spectropolarimetry.

Flatfield and wavelength calibration lamps are shining up to a telescope shutter at the location of the telescope mirror M3 and the diffusely reflected light is used for the calibration. Acquisition of targets is made with images taken in FORS imaging mode and using a movable sensor arm in the focal plane of the telescope for tracking with a guide star.

The standard FORS grisms provide a fixed wavelength range for an object located on the  $x = 0$  line (line perpendicular to dispersion direction). The covered wavelength range is shifted for the targets with an offset in  $x$ -direction. Slits can be made with an on-site laser cutting machine. With these slits one can select any point in the focal plane for spectroscopy. However one has to check whether the entire spectrum falls onto the detector. In addition one can take also slitless spectroscopy of all targets in the field, or of all targets in as particular section of the field.

Some standard FORS grisms have the following parameters

| Grism      | $\lambda_{\text{central}}$<br>nm | $\lambda_{\text{range}}$<br>nm | dispersion<br>nm/mm | $R^a$ | filter |
|------------|----------------------------------|--------------------------------|---------------------|-------|--------|
| GRIS_1200B | 435                              | 366–511                        | 2.4                 | 1420  |        |
| GRIS_1400V | 520                              | 456–586                        | 2.1                 | 2100  |        |
| GRIS_1200R | 650                              | 575–731                        | 2.5                 | 2140  | GG435  |
| GRIS_1028z | 860                              | 773–948                        | 2.8                 | 2560  | OG590  |
| GRIS_600B  | 465                              | 330–621                        | 5.0                 | 780   |        |
| GRIS_600RI | 678                              | 512–845                        | 5.5                 | 1000  | GG435  |
| GRIS_300V  | 590                              | 330–(660)                      | 11.2                | 440   |        |
| GRIS_300V  | 590                              | 445–(870)                      | 11.2                | 440   | GG435  |
| GRIS_150I  | 720                              | 330–(660)                      | 23.0                | 260   |        |
| GRIS_150I  | 720                              | 445–(870)                      | 23.0                | 260   | GG435  |
| GRIS_150I  | 720                              | 600–1100                       | 23.0                | 260   | OG590  |

<sup>a</sup>: resolving power  $\lambda/\Delta\lambda$  for a slit width of 1 arcsec



FORS is a very versatile instrument for faint objects since with grisms one can achieve an overall instrument efficiency of  $\approx 50\%$  (including telescope, spectrograph and detector). FORS can take low resolution spectroscopy of many targets (about 20) using different aperture mask. At the same time also intermediate resolution spectroscopy is possible for a more detailed characterization of brighter targets. The indicated resolving power  $R$  can be doubled by using only a  $0.5''$ -wide slit, if one can accept the light losses on the aperture.

### 7.3.3 HARPS - the high precision radial velocity spectrograph

HARPS is an echelle spectrograph at the 3.6m telescope optimized for high precision radial velocity (RV) measurements. The instrument is built to measure radial velocities to a precision of  $RV = \pm 1$  m/s that corresponds to a measuring precision of

$$\frac{\pm\Delta\lambda}{\lambda} = \frac{\pm\Delta v}{c} = \frac{\pm 1 \text{ m/s}}{300'000 \text{ km/s}} = \pm 3.3 \cdot 10^{-9}.$$

HARPS is a so-called fiber-fed echelle-spectrograph optimized for stability. The light of a star is focussed by the telescope onto an entrance lens of an optical fiber which guides the light to a laboratory. The spectrograph is located in a temperature controlled vacuum vessel to avoid drifts due to temperature and air pressure variations. Simultaneously a second fiber is illuminated with a Th-Ar spectral reference light source or sky background light. The signal from the target and the second fiber are recorded simultaneously on the same detector. The spectral range covered is 378 nm – 681 nm with a spectral resolving power of about  $R = \Delta\lambda/\lambda = 90'000$ .

The main components of HARPS are:

- one fiber head for the target at the Cassegrain focus of the ESO 3.6 m telescope,
- a second fiber input which can be fed by a ThAr emission line lamp, or alternative with the sky background spectrum using a fiber head in the focal plane offset by 2 arcmin from the target fiber,
- an echelle grating, 31.6 gr/mm with a blaze angle of  $75^\circ$  with dimensions of  $840 \times 214 \times 125$  mm,
- collimator mirror with a diameter of 730 mm ( $F = 1560$  mm), which is used in triple pass mode,
- cross disperser grism with 257 gr/mm,
- a mosaic of two  $2k \times 4k$  CCD detectors which record the echelle grating orders  $m = 89 - 161$  in a square image plane

The HARPS spectrograph achieves a spectral resolution ( $\approx 3$  pixels) of about  $\Delta\lambda = 0.005$  nm or  $50$  mÅ. With this one tries to measure wavelength shifts of the order  $10^{-5}$  Å. This is only possible if a large number, say  $> 10000$ , of narrow lines with a width of  $\approx 0.02$  nm are present in the spectrum. The measured wavelength shift corresponds to a physical shift of the spectrum of about 10 nm or  $\approx 1/1000$  of a detector pixel. It is obvious that such a measurement requires an extremely high stability for the instrument.

### 7.3.4 SINFONI - a 3d spectrograph

SINFONI is an integral field spectrograph for the near-IR region which can be used together with an AO system. It provides a spectrum for each point in the field of view. Characteristic parameters of this system are:

- 4 gratings for the J ( $1.25 \mu\text{m}$ ), H ( $1.6 \mu\text{m}$ ), K ( $2.2 \mu\text{m}$ ) and H+K spectral bands,
- spectral resolving power  $R = 2000, 3000, 4000$  in J, H, K, respectively and 1500 in H+K,
- an image slicer which splits a square field of view into 32 slices which are arranged into a kind of long slit configuration for spectral dispersion,
- selectable spatial resolutions of  $0.025''$ ,  $0.10''$ , or  $0.25''$  arcsec with corresponding field of views of  $0.8'' \times 0.8''$ ,  $3'' \times 3''$ , and  $8'' \times 8''$  respectively,
- a  $2k \times 2k$  infrared detector which provides 2000 spectra for the field of view covered.

The heart of the integral field spectrograph is its image slicer which converts the two-dimensional field-of-view into a one-dimensional long slit configuration. This slit is fed into a long-slit spectrograph to disperse the light of each pixel in the two-dimensional field-of-view at the same time. During the data reduction the two-dimensional spatial information is combined with the spectral information for each spatial point into a 3-dimensional data cube.

In SINFONI the image-slicer consists of two sets of plane mirrors. The first set, called "Small Slicer", consists of a stack of 32 mirrors which slice the image into 32 slitlets. The second set, called "Big Slicer", rearranges the fan of 32 slitlets to form a pseudo long-slit format.

SINFONI can be used for seeing limited observations. But the full power of SINFONI is achieved when it is used with the AO system. For the correction of the image deformation by the atmosphere one can use either a natural guide star near the target, the target itself if it is bright enough, or an artificial laser guide star.

## 7.4 Spectroscopic calibration and data reduction

### 7.4.1 Calibration measurements

The final data product for spectroscopy of an unresolved source is the intensity as function of wavelength  $I(\lambda)$ . The data reduction requires the determination of the efficiency of the system as function of wavelength and a mapping of the wavelength scale for the 2-dimensional count spectrum. The following spectroscopic calibration measurements are required for the data reduction:

- bias and dark frames,
- flat-field spectrum using a lamp with a continuous spectrum,
- wavelength calibration with a lamp producing a rich spectrum of narrow emission lines with well known wavelengths,
- a sky background spectrum useful for the correction for the sky contamination,
- observations of a spectrophotometric standard star for flux calibrated spectroscopy,
- if required a spectrum of a source without narrow spectral features for the identification and correction of absorptions lines from the Earth atmosphere.

**Bias or dark frames.** In spectroscopy the sky background is often very low because the signal is distributed over many pixels. For this reason an accurate read-out noise (fixed pattern) or dark current determination and subtraction may be important for faint sources. If read-out noise is a dominant noise source then one should consider carefully the options to reduce it with an optimized observing strategy:

- reduce as much as possible the number of read-outs,
- select the read-out mode with the lowest read-out noise,
- a lower spectral resolution (if scientifically acceptable) provides higher count rates,
- apply pixel binning in the read-out mode if possible: a  $2 \times 1$  or  $3 \times 1$  binning perpendicular to the dispersion direction does not reduce the spectral resolution.

**Spectroscopic flat-field.** The flat-field corrects for pixel-to-pixel efficiency variations of the detector. Typically, an even illumination of the spectrograph aperture with a continuum source (hot tungsten lamp) is made. This can be achieved with an internal lamp which illuminates a screen in front of the spectrograph or with an illuminated screen in the dome to which the telescope is pointing for calibrations.

One frequent problem with spectroscopic flat fields is that the artificial light source is not bright enough (not hot enough) for calibrations in the blue / near-UV part of the spectrum. In that case one can use for low resolution spectroscopy a twilight spectrum (solar spectrum) and evaluate the pixel to pixel efficiency differences by averaging along the slit direction.

**Wavelength calibration.** An exposure with an emission line calibration lamp is used for the wavelength calibration. The line spectrum should have sufficient emission lines with the following properties:

- distributed in a sufficient frequency over the whole wavelength range,
- enough lines should be free from blends for an accurate centroid measurement,
- the lines should not be saturated in the exposure.

Typically one should have about 10 suitable lines for low to medium resolution spectroscopy if one aims for a good wavelength precision of about a tenth of the spectral resolution. In an echelle spectrum each order should have about 10 calibration lines to achieve this.

For high precision radial velocity measurements one should in addition consider:

- mechanical flexures by a varying gravity vector can introduce shifts in the wavelength scale for instruments attached to a telescope. The effect can be reduced if wavelength calibration are taken for each scientific observation with the same instrument and telescope orientation.
- one should avoid any change in the instrument configuration (slit width, grating orientation, instrument rotation angle, etc.) during a run with high-precision measurements, because it may be necessary to redo the wavelength calibration,
- radial velocity standard stars should be observed with the same instrument setup in order to measure the offset of the wavelength calibration and to check the stability of the system,
- for echelle spectra it is important that there are enough calibration lines in each echelle order,
- sky emission lines and telluric absorptions can be very useful for checking the wavelength calibration.

Frequently used wavelength calibration lamps are:

- ThAr lamp for high resolution echelle spectra in the visual and near-IR,
- Halogen + N<sub>2</sub>O gas cell for the mid-infrared,
- Ne, He, Ar, or HgCd lamps for medium and low resolution spectra in the region 400 – 1000 nm.

One can combine the exposures of different lamps for the wavelength calibration.

**Sky background spectrum.** In many science applications it is important to carry out an accurate sky background subtraction. In long slit spectroscopy the sky spectrum can be extracted from detector regions located besides the target spectrum. It may be necessary to carry out separate wavelength calibrations for the sky spectrum, especially if the slit is not perfectly aligned with the detector pixel row (or columns).

If the sky spectrum is strong then an accurate background subtraction may be required, for example for the strong sky lines in the red or near-IR spectral region, or for spectroscopy in the thermal infrared region. In this case it can be useful to take pairs of spectra with the target offset along the slit. The subtraction of the two (dark corrected) images yields then a positive and negative target spectrum with the sky lines removed. This only works well if the strength of the sky lines does not vary between the two observations. Note that sky lines can show significant variations within an hour.

In multiple-object spectroscopy it is important to place a number of fibers or apertures on the clear sky for a sky background spectrum. If no sky spectrum can be obtained simultaneously with the target then a sky spectrum has to be taken before or after the target observations.

**Spectrophotometric calibrations.** We can distinguish two quality levels:

- absolute photometric flux calibration  $I(\lambda)$ ,
- relative, color calibration  $I(\lambda)/I_0$ .

For an absolute flux calibration one needs photometric conditions and observations of a spectrophotometric standard star with a wide slit for the calibration of the instrument efficiency. Also the science target has to be measured with a wide slit to ensure that no light is lost on the aperture. Often one needs then in addition a narrow slit spectrum of the target because the wavelength is not well determined if spectral data are only taken with a wide slit.

Color calibrated spectra are taken like flux calibrated spectra but they do not need photometric observing conditions.

*Zenith angle:* It is important for photometric calibration measurements to carry out the measurements for small zenith angles. For large zenith angles  $z > 45^\circ$  the airmass dependent atmospheric absorptions increase rapidly and the calibration accuracy will be reduced. Atmospheric dispersion may also introduce for (unappropriate) small aperture a wavelength dependent aperture throughput.

*Spectrophotometric standard stars:* There exist many lists of well measured spectrophotometric standards stars in the literature. Popular lists often use A-stars or hot white dwarfs as standard stars.

**Atmospheric line absorptions.** There are many telluric absorption lines in the red and infrared spectral region which can disturb the measurement of spectral features. The exact location and strength of these absorptions can be obtained with observations of an astronomical source without narrow spectral features. Good sources for this are fast rotating B stars or hot white dwarfs.

An accurate correction for telluric line absorption is possible with a high spectral resolution. Because telluric absorption lines are narrow they can often be easily distinguished from target features and a simple interpolation yields then a contamination free spectrum.

#### 7.4.2 Spectroscopic data reduction

Many aspects of the spectroscopic data reduction are identical to the photometric data reduction. An important difference is that the wavelength scale has to be determined for the final data product.

The standard steps for the reduction of spectroscopic data are:

- cosmic ray event rejection,
- bias or dark subtraction,
- bad pixel correction,
- flat-fielding,
- target and sky spectrum extraction,
- wavelength calibration,
- sky background subtraction and corrections for atmospheric absorptions,
- spectrophotometric calibration.

**Detector data reduction.** The correction for detector effects are almost identical to the case of photometric imaging data.

*Cosmic ray events:* Cosmic ray events are quite easy to recognize in spectroscopy since the structure of the spectroscopic signal on the detector is predictable.

*Bad pixels:* Dithering for bad pixel correction is often not feasible or too complicated in spectroscopy. But for bad pixels the same applies as for the cosmic ray events - the expected target signal can be inferred from adjacent pixel rows (same spectrum) or pixel

columns (same Gaussian intensity profile). Thus it is often possible to interpolate over bad pixels without risk that one introduces a spurious signal.

*Read out bias or dark subtraction:* The same applies as for the reduction of imaging photometry.

*Flat-fielding:* Spectroscopic flatfields often show a strong wavelength dependence in the intensity because the efficiency of the spectrograph and the illuminating lamp can depend strongly on wavelength. Thus, one may obtain flatfields where one half of the CCD where the blue part of the spectrum is registered, has 5000 counts, and the other (“red”) half 50'000 counts. In this case one should normalize the flat-field locally and consider in the analysis that the flat-fielding noise depends on the wavelength.

**Target and sky spectrum extraction.** The spectrum extraction converts the 2-dimensional data into 1-dimensional data. All registered photoelectrons corresponding to a given wavelength should be added to the same bin in the 1-dimensional spectrum.

The location of the spectrum can be determined from a spectrum of a bright point source, while a spectral lamp illumination yields the wavelengths of different locations in the aperture.

The extraction of the target spectrum is rather easy if the spectrum is well aligned with the pixel rows (or column), so that several pixels located perpendicular to the spectrum can just be added up for one spectral bin. One can (and should) check with an extraction of the lamp spectrum whether the spectral resolution is degraded by the extraction.

If the spectrum is not aligned with the pixels and is even curved then one needs a careful spectrum extraction. However this problem has often been solved and one should be able to find well tested software for this task.

The width of the spectrum extraction depends on the science goals:

- a wide target extraction, including essentially 100 % of the target flux, for relative or absolute spectrophotometry,
- a narrow target extraction if the target is weak and one aims for the maximum S/N in the spectrum.

A more sophisticated extraction method weights the pixels according to the expected flux as determined from the averaged intensity profile. Since the method is more complicated also more care is required to verify the quality of the resulting spectra.

*Sky extraction:* The goal of the sky extraction is to obtain a sky spectrum which is well suited for the correction of the sky emission in the target spectrum. Therefore the sky spectrum should not be contaminated by light from the target. The sky spectrum has a higher S/N if a wider sky region is extracted. Of course one needs to rescale thereafter the strength of the sky spectrum to the strength in the target spectrum.

**Wavelength calibration.** A lamp line spectrum should be extracted in exactly the same way as the target spectrum and as the sky spectrum for the wavelength calibration. A wavelength calibration is only valid if nothing has been changed in the instrument setup between the calibration and the target observation. Usually the sky spectra need a separate wavelength calibration.

The extracted lamp spectrum is then used to define the conversion of pixel number into wavelength. This requires:

- an accurate determination of the centers of the spectral lines,

- a fit function  $\lambda_i(\text{pix}_i)$  using a higher order polynomial function or another suitable function so that one can convert the pixel spectrum  $f(\text{pix}_i)$  into a wavelength spectrum  $f(\lambda_i)$ ,
- a  $\lambda$ -rebinning into a spectrum with equal wavelength steps  $\Delta\lambda$  or  $\Delta\log\lambda$ .

There exist software packages which perform these calibration steps. Still a careful analysis of the resulting spectra is required. Important is an assessment of the precision of the wavelength calibration. The precision achieved routinely for the wavelength calibration is about a tenth of the spectral resolution. Achieving a higher precision in the wavelength calibration is possible but requires quite some investigations for optimizing the measuring and the data reduction process. Telluric absorption and emission lines often provide a good check for the wavelength calibration.

**Sky background subtraction and correction for telluric absorptions.** Subtraction of the sky background is straight forward if the sky spectrum is much weaker than the target. Different cases of sky subtraction are:

- weak sky spectrum continuum with a few strong, narrow lines; one may just ignore the lines or interpolate over the wavelength region affected by the line.
- quite a strong background continuum from scattered moon light; a narrow or optimum extraction may help because the effect of the sky spectrum is reduced and the subtraction yields a relatively good target spectrum. For flux calibration purposes one may then use a wide extraction.
- for the subtraction of strong, narrow sky lines one often needs to achieve a very good match of the sky lines in the target spectrum and the sky spectrum to obtain a corrected target spectrum without strong, narrow residuals. It can be helpful to extract a very narrow target spectrum and use the regions just beside the spectrum for the sky subtraction. Best results are obtained if the problem was already considered in the observing and calibration strategy.
- in the thermal infrared the background spectrum is often much stronger than the target spectrum; The sky spectrum should then be extracted from the same detector region as the target spectrum in order to take also the detector pixel noise into account. This is achieved by shifting the target spectrum on the detector between consecutive exposures. An alternative, although one which requires substantial telescope time, is a blank sky observation before or after the target observation.

**Correction for telluric absorptions.** For the correction of telluric absorptions one takes a flat comparison spectrum  $F_{\text{obs}}$  (e.g. a fast rotating B star spectrum) and constructs an absorption free spectrum  $F_{\text{corr}}$  by interpolating this spectrum for regions where telluric absorptions reduce the flux (taking intrinsic absorptions of the source into account). The normalized spectrum of the telluric absorptions is then obtained by the ratio  $F_{\text{tell}} = F_{\text{obs}}(\text{B star})/F_{\text{corr}}(\text{B star})$ . A target spectrum corrected for telluric absorptions is then obtained by

$$F_{\text{corr}} = F_{\text{obs}}/F_{\text{tell}}.$$

**Flux calibration.** The spectroscopic flux calibration must follow the same basic rules as a flux calibration of imaging data. The most important points are:

- a wide spectroscopic extraction so that all light is included in the final data from a measurement taken under photometric conditions for the determination of the spectroscopic efficiency curve of the instrument (telescope + spectrograph + detector),

- a correction of the spectrophotometric standard star for the sky transmission taking the airmass of the measurements into account. The sky transmission spectrum can be taken from the literature or be measured with two observations of the same standard star, one with small zenith angle or airmass  $\approx 1$  and one with large airmass  $\approx 2$ .
- a wide extraction of the target star taken with a wide slit under photometric conditions,
- a correction for the atmospheric extinction for the target star,
- from the measured flux ratio (target star)/(standard star) the absolute flux spectrum of the target can be derived.

*Sky transmission:* Accurate knowledge of the sky transmission is particularly important in the blue, near-UV spectral region where the atmospheric transmission is quite low. For the other wavelength the sky transmission shows little spectral dependence.

*Absolute spectrophotometric calibration and color calibration:* An absolute spectropolarimetric calibration requires photometric conditions during the observations. Spectroscopy is often taken for single targets without simultaneous measurements of other nearby targets. In this case one cannot check the photometric calibration with measurements of nearby stars.

*Filter convolution:* It is always useful to derive the flux in broad-band filters  $X$  with an integration of the reduced spectrum  $F(\lambda)$  weighted with the filter function  $T_x(\lambda)$  for a magnitude determination:

$$F_X = \int F(\lambda) T_X(\lambda) d\lambda.$$

Evaluating the same quantity for the spectrophotometric standard star can then be used as a check. The derived filter magnitude enables a comparison of the spectrophotometry to available imaging photometry.

This procedure is also very useful if “only” color calibrated spectroscopy was possible (e.g. due to clouds), because then the obtained spectra can be flux calibrated using filter photometry.



## 7.5 Measurements of spectral features

The relative or absolute flux in spectral features can be measured in the reduced spectrum by just integrating over the area enclosed. For this one needs to distinguish between different spectral features like:

- continuum of the target,
- spectral lines from the target,
- interstellar absorptions,
- uncorrected absorptions from the Earth atmosphere.

In order to disentangle accurately the different components it may be necessary to use a model of the emissions and absorptions.

*Flux modelling:* The best analysis of the measured spectrum can be achieved by modelling the spectrum, taking all the known properties of the source into account. Depending on the science goals the modelling can be simple or very complicated:

- *Simple:* a fit of a linear function, a power law, or Planck function for the slope of the continuum and Gaussian fits to spectral lines,
- *Sophisticated:* fits of detailed model spectra to the observed spectrum using a multi-dimensional optimization of the model parameters.

The first approach is certainly useful for a first characterization of the target. The second approach can provide detailed information on the target but it is often very time consuming and one needs to assess the scientific goals and merits of a more sophisticated analysis carefully.

### 7.5.1 Line center and line strength

For spectral lines the most basic characterization are the line center and the line strength. The line center can be measured in the following way:

- the wavelength of the flux maximum or flux minimum,
- the wavelength of the center of a Gaussian fit to the line,
- the wavelength of the median flux of the feature or any other well defined procedure.

One should determine barycentric wavelengths for measurements more accurate than  $|\pm \Delta\lambda/\lambda| < \pm 10^{-4}$ , corresponding to a radial velocity precision of  $RV < 30$  km/s.

*Radial velocity:* If the spectral feature is identified and the rest wavelength known then one can use the radial velocity  $RV$  to characterize the line center. However, first one needs to specify the zero point of the  $RV$  scale: examples are barycentric  $RV$ , or  $RV$  with respect to  $RV$  zero-point defined for the target.

*Multiple components:* Lines may consist of several components each with a different wavelength or  $RV$ . Depending on the science case one can then derive the center of each component or the center of the entire feature.

*Emission line strength:* The emission line flux is the measured flux in the spectrum which can be attributed to a particular line. Often emission lines are blended with other lines and one needs to disentangle the flux of different components. This can be achieved with a multiple line fit to the data. The emission line strength should be given as absolute flux or as relative flux with respect to a prominent standard line (e.g.  $H\beta = 100$  for visual spectra of photoionized nebulae). The precision of such a line measurement depends

- for weak lines on the uncertainties in the determination of the continuum level and the contamination by other lines,
- for strong lines on the photometric calibration (absolute or color calibration) of the spectrum.

*Equivalent width:* The equivalent width EW is the flux in an emission line or the strength of the attenuation of an absorption line with respect to the continuum level. The equivalent width gives the absorption line strength or emission line flux as wavelength width for the normalized continuum spectrum:

$$\text{EW} = \int \frac{I(\lambda)}{I_{\text{cont}}(\lambda)} d\lambda.$$

For absorption spectra the EW is given usually as a positive value with the units  $\text{\AA}$ . Equivalent widths of absorptions are very useful units since they provide the strength of an absorption feature from continuum normalized spectra (without flux calibration). Equivalent widths do not depend in principle on the spectral resolution, except for the fact that the continuum definition is less accurate for low resolution spectra, and the contamination by other lines is much more difficult to take properly into account.

### 7.5.2 Line structures

If the spectral resolution is high enough then the structure of lines can be resolved and characterized. The most basic parameter for the line structure is the line width; usually one indicates the full width a half maximum FWHM. The measured FWHM must consider the spectral resolution of the spectrograph, which can be determined from the width of the lines in the wavelength calibration spectrum, unresolved lines in an astrophysical target, sky emission lines or telluric absorption lines. For line widths not much larger than the spectrograph resolution one should use the relation:

$$(\text{FWHM}_{\text{line}})^2 = (\text{FWHM}_{\text{measured}})^2 - (\text{FWHM}_{\text{spectrograph}})^2$$

The spectrograph resolution is not critical for lines much wider, say  $> 4\times$ , than the spectrograph resolution.

If there are complicated, multi-component line structures then one can try to decompose the profile into several Gaussian components characterized each by the central wavelength or radial velocity and the width of the Gaussian fit.

**Generic line profiles.** For certain physical phenomena generic types of spectral lines are produced and the line structure yields already useful parameters for the interpretation. Examples are:

- for absorption lines in rapidly rotating stars the line width is a good measure of the projected rotational velocity  $v \sin i$ ,
- for emission lines from rotating disks the separation of the emission peaks measures the line of sight velocity of the disk rotation,
- the width of flat top emission lines from an optically thin emission from a spherically symmetric, expanding shell indicates the expansion velocity,
- in P-Cygni profiles the maximum velocity  $RV_{\text{max}}$  for the blue end of the absorption describes the outflow velocity,
- inverse P-Cygni profiles are produced by gas accreted by gravitating body.

### 7.5.3 Radial velocities

Spectra with many narrow absorption lines are well suited for high precision radial velocity measurements. The most accurate method is a cross-correlation of the target spectrum with a high S/N template spectrum of a RV standard object with the same or a similar spectrum. Since the same atomic transitions are present in all cool stars a spectrum from a solar type standard star is a good template spectrum for all cool stars of spectral type F, G, and K and even early type (elliptical) galaxies.

For the cross-correlation analysis it is important to use normalized spectra, and to introduce a logarithmic step width for the wavelength axis because a radial velocity shift corresponds to a multiplicative shift in the wavelength spectrum. One should not forget to discard all telluric absorption lines in the spectra in order to avoid erroneous results.