## Spectroscopy – I. Gratings and Prisms

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## 1 Historical Notes

Some important milestones:

- 1637 Descartes explained the origin of the rainbow.
- 1666 Newton's classic experiments on the nature of colour.
- 1752 Melvil discovered the yellow "D lines" emitted by sodium vapour.
- 1802 Wollaston discovered dark lines in the spectrum of the Sun.
- 1814 Fraunhofer used a small theodolite telescope to examine stellar spectra and found similar lines as in the solar spectrum. He catalogued the features as A, B, C, ... etc, some of which persist to the present the sodium "D" lines, the "G" band (CN cyanogen).



• 1859 The famous Kirchhoff – Bunsen experiments established that a heated surface emits a continuous (Planck or "black body") spectrum; a heated low pressure gas emits an emission spectrum with discrete lines at wavelengths characteristic of the gas; and a cool low pressure gas in front of a hot source absorbs at those same characteristic wavelengths.



Figure 1: Summary of the Kirchhoff-Bunsen experiments.

The latter, of course is how we simplistically view stars – the heated interior provides a continuous Planck spectrum and the cooler **photosphere** does the line absorbing.

Recall that we looked at the radiation laws of Planck, Wien and Stefan-Boltzmann with regard to determining stellar temperatures ...



Figure 2: Planck curves for black-body radiation.

Astronomical examples of emission-line spectra would be the spectrum of a planetary nebula – or the spectrum of the corona of the Sun during a total eclipse. An example of a continuous spectrum might be a star with a helium atmosphere which was too cool to show helium lines (e.g a DC white dwarf).

Until well into the 20th century, astronomical spectroscopy was done with prisms, first with objective–prisms and later with more complex spectrographs mounted often at Cassegrain or Prime focus. Prisms have a number of disadvantages:

- Dispersion is not linear, increasing towards shorter wavelengths.
- Prism dispersion is not very high often two or three prisms were used in tandem to increase this.
- Glass absorbs ultraviolet light quartz or other UV transmitting glasses are necessary.
- Light losses occur at both surfaces (more if more than one prism is used) and in the glass.

• A solid glass prism must be kept at a constant temperature to avoid problems.

Until about 1930, use was made of diffraction gratings ruled on speculum metal. Rowland and later Michelson constructed excellent gratings on flat or concave surfaces for solar work. The early gratings had two major problems:

- In the process of ruling gratings at thousands of lines per cm, the diamond became worn so that the shape of the grooves or lines became less sharp and the production of large homogeneous gratings was difficult.
- Because gratings produce several orders, they were rather wasteful of light.

In the 1930's two developments made gratings much more attractive:

- Vacuum deposition of aluminium made it far easier to rule homogeneous gratings
- The aluminium surfaces allowed grooves to be ruled which were steeper on one side than the other and to do this with accurately maintained shape. "Blazing" allows the grating efficiency to be peaked at a selected wavelength region.

Nowadays, a number of different techniques are available – such as electron-beam etching and the production of holographic and "volume-phase" holographic gratings – which allow greater efficiency and flexibility. "Aberration-free" gratings and curved gratings – to obviate the need for focussing optics – can also be made.

## 2 Basics

Spectroscopy involves the use of some dispersive element (a prism or diffraction grating) to spread light out in wavelength so that we can examine and analyse the flux distribution as a function of wavelength or frequency.

There are various detailed ways of doing this – in astronomy we use a number of approaches which might be described in the following loose categories:

- Wide-field spectroscopy (or "slitless spectroscopy") using an objective-prism or grism
- Long-slit spectroscopy typically Cassegrain-focus spectroscopy.
- **Multi-object spectroscopy** which may be achieved using optical fibres placed in the focal plane of the telescope
- Area spectroscopy which can be achieved, for example, with a Fabry—Perot interferometer.
- Integral Field Spectroscopy "area" spectroscopy using lenslets, fibre optics, image slicers, or combinations of these.

## 2.1 Dispersion

If light of different wavelengths is deviated by a grating or prism through different angles,  $\theta$ , the rate of change of  $\theta$  with wavelength,  $d\theta/d\lambda$  is the **angular dispersion**.

If the deviated light is brought to a focus by a camera of focal length, f, the **linear dispersion**,  $f \ d\theta/d\lambda$ , measures the scale of the focussed spectrum.

Usually, however, the inverse of this, the **reciprocal linear dispersion** is quoted – normally in  $\mathring{A}/mm$ .

## 2.2 Resolving power

If a spectrograph can just resolve two lines near wavelength  $\lambda$  with a separation of  $\delta\lambda$ , the resolving power is defined as

# $\frac{\lambda}{\delta\lambda}$

a pure number. So, a Cassegrain spectrograph might typically have a resolution of 1Å at 4000Å and therefore a resolving power of 4000. An echelle spectrograph would have a resolution of less than 0.01Å at the same wavelength – and therefore a resolving power greater than 40000. Usually, the resolution or resolving power will be set by the detector (e.g. the pixel size of the CCD).

## 3 Objective-Prism Spectroscopy

Perhaps the simplest form of astronomical spectroscopy is the objective prism. Unsurprisingly, this is a very thin prism that sits in front of a telescope objective – often in front of the corrector plate of a Schmidt telescope (to get "wide field" results).

First, recall the dispersion of a prism:



Figure 3: Schematic objective-prism "plate".

Since we can write the **angular dispersion of the prism**:

$$\frac{d\zeta}{d\lambda} = \frac{d\zeta}{dn}\frac{dn}{d\lambda}$$

where n is the refractive index of the prism and  $\zeta$  is the emergent angles of the various wavelengths. The first quantity can be evaluated geometrically, the second depends on the prism material.

From the figure, Snell's law of refraction gives:

$$n = \frac{\sin \zeta}{\sin \zeta_0}$$

so that (taking  $\zeta_0$  as a constant):

$$\frac{d\zeta}{dn} = \frac{\sin\,\zeta_0}{\cos\,\zeta}$$

In the **minimum deviation** condition, the refracted ray inside the prism makes equal angles with the two prism faces, so  $\xi_0 = \zeta$  and  $\xi = \zeta_0$  (when used in a spectrograph, prisms are usually set close to minimum deviation because otherwise any slight divergence or convergence of the incident beam leads to astimatism in the image).

In this case, because of the symmetry, equal deviations occur at both prism faces, so the total rate of change is doubled and:

$$\frac{d\zeta}{dn} = \frac{2 \sin \zeta_0}{\cos \zeta} = \frac{2 \sin (\alpha/2)}{\cos \zeta}$$

where  $\alpha$  is the prism apex angle. For small  $\alpha$ , it is clear that  $\zeta$  is close to zero, so  $\cos\zeta$  is close to unity and the angular dispersion is proportional to the apex angle.

The Anglo-Australian Observatory (AAO) Schmidt has two objective prisms; one with an apex angle of 44 arcminutes, the other with an angle of 135 arcmin. The 44 arcmin prism gives a reciprocal linear dispersion of about 2400 Å/mm, so the 135 arcmin prism gives about three times the dispersion (~ 800 Å/mm) and two prisms can be used with the apexes mounted together or opposed to give four or two times the dispersion of the 44 arcmin prism.



Fig. 12.1. Differences in the appearance of spectra are apparent in lowdispersion spectra made with an objective prism. One may note emission lines in two of these spectra. (Stellar spectra obtained with the Burrell Schmidt-type telescope of the Warner and Swasey Observatory of Case Western Reserve University.)

Figure 4: Objective-prism plate from the Warner & Swasey Observatory Schmidt.

Objective prism data are still very useful because with a wide field many hundreds or thousands of (low dispersion) spectra can be obtained at the same time. This makes them very useful for survey work, especially, for example, for :

- objects with unusual spectra such as very hot or cool stars
- objects with strong emission lines such as emission–line galaxies or quasars.

A couple of examples are shown on the next pages.

Some important objective prism catalogues:

- the Harvard Draper catalogue (early 20th century) contains spectral types for more than 250000 stars ("HD stars"), mostly classified by Annie Cannon during 1911–1915. This has been an invaluable source catalogue.
- The Michigan Spectral Catalogue is a revision of the HD catalogue which includes luminosity classification and much important additional material, largely carried out by Nancy Houk and her collaborators.



Figure 5: Annie Cannon (1863 – 1941).

Survey Name (1)	Type <sup>a</sup> (2)	Area (deg. <sup>2</sup> ) (3)	Number of objects (4)	Density (# / deg. <sup>2</sup> ) (5)	Completeness <sup>b</sup> Limit (m <sub>B</sub> ) (6)	Ref. (7)
Kiso	С	5100	8162	1.60	16.0	2
Montreal	С	4400	469	0.11	14.8	3
Markarian	UV	15000	1500	0.10	15.2	4
Tololo	L	1225	201	0.16	2	5
UM	L	667	349	0.52	(16.9)	6
Wasilewski	L	825	96	0.18	(15.2)	7
POX	L	82	23	0.28	(16.0)	8
ESO - Ha	L	400	113	0.28		9
UCM	L	471	263	0.56	(~16.5)	10
Hamburg	L	1248	196	0.16		11
Marseille	L	46.5	92	1.98	(~16.0)	12
Case	UV + L	1440	1551	0.94	16.0	13
SBS	$\mathbf{U}\mathbf{V} + \mathbf{L}$	~990	~1300	1.31	(~17.0)	14
KISS - red	L	62.2	1128	18.14	(18.1)	15
KISS - blue	L	116.6	223	1.91	(18.2)	15

Table 1. Partial List of Previous Schmidt/Objective-Prism Surveys

C = Color Selected; UV = UV Excess Selected; L = Line Selected

<sup>b</sup>Values in parentheses are median apparent magnitudes for that survey, not a completeness limit.

Figure 6:



Figure 7: Direct frame from the Hamburg objective-prism survey.



Figure 8: Same field through the objective-prism. Note the bright emission features in the central object.



Figure 9: Scan of the above (central) object.



Figure 10: Kitt Peak National Observatory (KPNO) in the USA is using the Burrell Schmidt with initially a 2k x 2k CCD and later a 2k x 4k chip to search for active and star–forming galaxies in the KPNO International Spectrosopic Survey (KISS). This figure is a direct image of a field and the figure below is the objective–prism image of the same field.



Figure 11: See caption to above figure. Note the emission features marked.

### 4 Diffraction Gratings

We have already seen the effect of the diffraction of light by a circular aperture (Telescopes–I lecture) – the formation of the **Airy disk** and diffraction rings – and the resulting limits on resolution related to wavelength and the size of the telescope mirror.

If we have a single narrow slit – rather than a circular aperture – we see a central band of light with fainter lines on either side, analogous to the Airy disk and diffraction rings.

#### 4.1 Young's experiment – double-slit interference

In the case of two parallel slits, we get the additional effect of interference patterns. This is the classical experiment (1803) by Thomas Young which first demonstrated the wave nature of light (even though Young didn't actually use two "slits")



Figure 12: Geometry for double-slit interference

With the assumption that the distance between slits and screen is much larger than the separation of the two slits (D >> d), we can write the condition for constructive interference (bright lines on the screen) as:

$$m \ \lambda \ \simeq \ d \ sin \ heta$$

where m = 0 (central band;  $\theta = 0$ ), 1, 2, 3,....

and for destructive interference:

$$(m + \frac{1}{2}) \lambda \simeq d \sin \theta$$

The intensity of the "bands" produced by single-slit diffraction looks like:



Figure 13: Intensity patter produced by single slit diffraction.

– essentially the same as the cross section of intensity produced by a circular aperture (the Airy disk and rings).

The intensity of the double-slit pattern is the interference pattern convolved with the single-slit diffraction pattern:



Figure 14: Intensity patter produced by double slit interference and diffraction.

#### 4.2 Multiple-slit interference.

Increasing the number of (evenly-spaced) slits has the effect (amongst others) of narrowing the width of the bright interference fringes:



Figure 37.13 Multiple-slit interference patterns. Note that as the number of slits is increased, the primary maxima become narrower but remain fixed in position. Furthermore, the number of secondary maxima increases as the number of slits is increased. The decrease in intensity of the maxima, as indicated by the dashed lines, is due to the phenomenon of diffraction, which is discussed in Chapter 38.

Figure 15: Multiple-slit interference (evenly spaced slits).

The interference phenomena discussed in this section are normally presented for the case of monochromatic light (and are usually demonstrated using laser light). If the monochromatic light were replaced by "white" light, instead of a narrow band at the points of constructive interference, we would see a spectrum of light (because  $m\lambda = d \sin \theta$ , slightly different  $\lambda$  results in slightly different  $\theta$ ).

Since a diffraction grating is essentially nothing more than a multiple-slit interference system (with "lines", grooves or steps instead of slits), it produces a series of spectra as described above. The resolution of the grating is determined by the number of lines on the grating, as well as the "order" (m) of the spectrum.

#### 4.3 "Classical" Gratings

Diffraction gratings have been in use in astronomical spectroscopy for many decades. These have typically been of the transmission or surface reflecting (SR) types and generally consist of parallel lines "ruled" on a reflecting surface or small "steps" on a reflecting or transmitting surface (for an example of the latter, see the section on grisms later). Nowadays, gratings are often produced by photolithographic ("holographic") etching, electron-beam etching and other methods which give higher accuracy than the classical "ruling" methods (i.e. actually scoring with a diamond tool).



Figure 16: Photomicrograph of grating surface



Figure 17: Photomicrograph of grating surface



Figure 18: HUGE diffraction grating.



Figure 19: Diffraction grating of surface reflecting type. Note that the reflected rays will come from all of the hundreds of "lines" on the grating (the "lines" extend into the page). The grating sketched is a "blazed" grating or echellette.

In the figure, constructive interference at wavelength  $\lambda$  occurs when the path difference between two beams is equal to an integral number of wavelengths, so:

$$m \lambda = d(\sin \alpha \pm \sin \beta)$$

and the  $\pm$  is a result of the fact that the sign of  $\beta$  depends on which side of the normal, the reflected ray lies. In the case shown above, clearly:

$$m \lambda = d(\sin \alpha - \sin \beta)$$

where m is the order of the maxima, d is the spacing of the grating lines and  $\beta$  is the angle at which the mth order is formed (the angle of diffraction).

The angles  $\alpha$  and  $\beta$  are both measured relative to the **grating normal**. (Watch out for the sign of the angles, the angles are both positive when measured on the same side of the normal). Note that reference is sometimes made to the **blaze normal** – the perpendicular to the surface of the tilted "steps" on the grating.

The separation of the grating lines, d, is called the **grating constant**. If this is in mm, 1/d gives the number of lines/mm which is what is usually quoted for any grating.

Note that, because the reflected light rays are parallel, some optical element – a lens in the simplest case – is required to focus the beam to an image – the spectrum. In a spectrograph, there is usually some folded Schmidt-type camera to do this. (It is also possible to construct non-planar gratings which will act as the focussing element as well as the disperser).

#### 4.3.1 Grating dispersion

Given the grating equation:

$$m \lambda = d(\sin \alpha \pm \sin \beta)$$

and the fact that the angle of incidence,  $\alpha$ , is constant, then differentiating the grating equation gives the **angular dispersion** of the grating:

$$\frac{\Delta\beta}{\Delta\lambda} = \frac{m}{d\cos\beta}$$

This expression is fundamental to understanding how gratings work and we will return to it. Clearly, the dispersion is

- proportional to the order, m; the second order has twice the dispersion of the first.
- inversely proportional to the line separation, d; the more lines/mm, the greater the dispersion.

In addition, the occurrence of  $\cos \beta$  in the denominator means that in any order, the dispersion will be smallest on the normal but, provided  $\beta$  stays small,  $\cos \beta$  will be close to unity and the **dispersion will be close to linear** – an advantage of gratings.

#### 4.3.2 Grating orders

In the previous figure, only one value of m (=1) is shown. Of course, other values, or orders, (m = 2, 3, 4, ...) are always there at the same time.



Figure 20: Schematic diffraction grating, showing m=0, m=1 and m=2. Higher orders will exist.



Figure 21: Grating orders m = -1, 0, 1.

As m increases, the angle  $\beta$  increases (for a fixed incident angle,  $\alpha$ ). Since dispersion is given by:

$$\frac{\Delta \beta}{\Delta \lambda} = \frac{m}{d \cos \beta}$$

as  $\beta$  increases with m,  $\cos \beta$  will decrease and the dispersion will increase. It is easy to see that order 2 will have twice the dispersion of order 1; order 3 will have three times the dispersion of order 1 – and so on. (But note that the amount of light will be less in the higher orders – see the section on Young's experiment).

Even in the case of low orders, the orders begin to overlap – even if restricted to just the visible region of the spectrum:



Figure 22: Two spectral lines seen at different orders. At zero order, there is no dispersion. As m increases, the lines are separated by increasing dispersion, until they overlap other orders.

If we could see the whole spectrum (radio to  $\gamma$ -ray), then every order would completely overlap with every other order. In reality, of course, many effects limit what we can see/measure. For example, the atmosphere will eliminate most photons at shorter wavelengths than about 340nm – as well as large regions of the infrared spectrum; detectors will only register certain wavelength regions (CCDs are typically useful from about 350 to 1100nm; and so on.

# Still, it is very important to think about order overlap when actually using a spectrograph !

#### 4.3.3 Free spectral range

The grating equation

$$m \lambda = d(\sin \alpha \pm \sin \beta)$$

shows that, for a given incident angle,  $\alpha$ , there is not a unique solution, because

$$m \lambda = 2 m \frac{\lambda}{2} = 3 m \frac{\lambda}{3}$$
....

so that, for example, spectral flux at 400nm in order 2 will overlap flux at 800nm in order 1. In practice, therefore, we often use filters to effect **order separation** – or make use of the limited response of the detector (or the atmospheric ultraviolet cut-off) to do the same thing.

The order overlap also introduces the concept of free spectral range.



Figure 23:

Free spectral range can be defined as the largest wavelength range in a given order which does not overlap the same interval in an adjacent order.

Note that the term "free spectral range" is used elsewhere with rather different meanings (e.g. in order separation in Fabry-Perot spectroscopy; in cavity (resonance) modes; etc.)

#### 4.3.4 Blaze and efficiency

A grating is most efficient when the rays emerge as if by direct reflection from the grating facets, or close to it – this is known as the **blaze condition**. For a "flat" grating, order zero is most efficient – but useless for spectroscopy because there is no dispersion in that order. Thus the grating facets (reflecting elements) are tilted (as shown in most of the grating diagrams here) so that the blaze condition is satisfied for a higher order, usually 1 or 2.



Figure 24: Illustration of blaze angle. (Note that in this sketch – representing a grating manufactured by Edmund Optical – the grating is "ruled" on an epoxy layer deposited on a glass substrate and then aluminised.)

A grating is usually described as being blazed for a certain wavelength – that is, the blaze angle adopted gives maximum reflection efficiency at that wavelength for example, a grating might be blazed at 600nm in the first order. Note that it follows from the grating equation that such a grating is blazed at 300nm in the second order (and so on ....)



Figure 25: Examples of blazed grating efficiencies – also from the Edmund Optical web page. Note the fall-off in efficiency away from the blaze wavelength.

#### 4.4 Echelle gratings

Whilst grating spectra are linear, they are also long and thin, so increasing the dispersion reduces the spectral range, for a given size of detector. Long thin photographic plates could be bent to fit a curved focal plane, but the advent of flat,  $\sim$  square (high-efficiency) detectors makes this impossible.

The grating angular dispersion equation

$$\frac{\Delta\beta}{\Delta\lambda} = \frac{m}{d\cos\beta}$$

indicates another solution. The **echelle** grating can be rather coarse compared to an ordinary grating – a series of "steps" rather than lines – but achieves high dispersion by operating in high orders, typically  $m \sim 100$ .

(As *m* becomes large, both  $\beta$  and the dispersion will change little – hence one obtains almost completely overlapping orders of very similar dispersion and the orders need to be separated. We will see how this can be done later).



Figure 26: Littrow mode for an echelle grating. 'GN' is the grating normal, 'FN' the facet normal or blaze angle.

Echelles are typically operated in (or near) **Littrow mode** where  $\alpha = \beta = \theta$ .

#### 4.5 Volume Phase Holographic (VPH) Gratings

VPH gratings are currently the "cool dudes" in astronomy. They work by Bragg diffraction – analogous to the way crystals diffract X-rays:



Figure 27: Bragg diffraction.

The Bragg equation for constructive interference is:

$$m \lambda = 2 d \sin \theta$$

Where d is now the spacing between the crystal planes. When this equation is met and when the angle of incidence equals the angle of diffraction, we have the **Bragg condition**.

In the VPH grating, a photo-sensitive material – often Dichromated Gelatin (DCG) – has a "volume" grating printed in it holographically. Effectively, a 3D set of lines is "ruled" in the gelatin, though actually no lines are visible; the diffraction effect is achieved by a fringe structure created by sinusoidal modulation of the refractive index. The gelatin is first deposited on a flat glass plate, then the grating is "printed", then another glass plate covers the gelatin, so that the DCG is sandwiched between two glass plates which protects it (DCG is hygroscopic) and provides a rigid support.

Dichromated Gelatin is capable of a relatively wide range of refractive index modulation and can record fringe structure of up to ~ 6000 lines/mm over a depth of around 20  $\mu$ m. DCG has good clarity and low scattering from about 300 nm to over 1800nm.

The energy distribution of the diffracted light is controlled by Bragg diffraction, so the angle of incidence, the grating depth and the intensity of the refractive index modulation determine the output energy as a function of wavelength - that is, how much light goes into each order. Thus gratings can easily be manufactured to different specifications.







Figure 29: Possible VPH grating configurations. For example, A: Transmission grating with fringes perpendicular to the grating surface –  $\alpha = \beta$  for the Bragg condition; D: Reflection grating.



Figure 30: A Volume Phase Holographic Grating.

VPH gratings can have very high efficiences (something which we are always pursuing in lowlight-level astronomy). They typically perform better than SR gratings – especially in higher orders – but also perform well away from the wavelength they were designed to work at. This is sometimes called the "**super-blaze**", though it is not related to "blaze" in the usual grating definition.



Figure 31: "Superblaze"

Another neat idea is that it is possible to "multiplex" VPH gratings, effectively producing more than one set of fringe planes in a given grating



Figure 32: Results from a NOAO multiplexed VPH grating.

VPH gratings have a number of advantages over more conventional gratings:

- The diffraction efficiency tends to be high often above 80%, and sometimes close to 100%.
- The efficiency is governed by Bragg diffraction, so remains high when the grating is rotated to different angles (wavelength regions).
- Because the diffracting region is sandwiched between glass plates, it is robust the outer grating surfaces can be safely cleaned and given "anti-reflection" coatings to improve throughput.
- Grating "customisation" is relatively easy each grating is an original rather than a copy of an expensively ruled master.
- Transmission and reflection geometries are possible.

### 4.6 Summary

To summarise, gratings have the advantage that:

- they can have high dispersions;
- the dispersion is close to linear;
- they can be reflective and therefore have good efficiency, especially in the ultraviolet,
- although the light can distribute over several orders, they can be "blazed" to have peak efficiency over a selected wavelength range. (This usually means having a selection of gratings avalable, suitable for different wavelength ranges and dispersions).

### 5 Grisms

A dispersive element formed by combining a transmission grating and a prism is called a **Car-penter's prism** or, more commonly a **grism** (grating-prism). These are useful in spectrographs that require in-line presentation of the spectrum – the light deviation caused by the diffraction of the grating is balanced by the refracting effect of the prism.

Because the dispersive effects of the grating and prism are superimposed, the dispersion of a grism is not linear.

The figure shows the usual configuration; a right-angle prism has the grating on the hypotenuse face. Light is incident normally on the back face of the prism, is refracted at the prism/grating interface and diffracted at the grating/air interface



Figure 33: Grating-prism or **grism**. GN is the grating normal; Z is the zero-order of the prism; A is the vertex angle of the prism; D is the deviation angle between Z and in-line diffraction; and  $\theta$  is the blaze (groove) angle of the grating.

The grating equation for the grism is:

$$m \lambda = d (n \sin \alpha + \sin \beta)$$

where n is the refractive index of the glass.

From the figure, we can see that for in-line diffraction we must have  $\alpha = -\beta$  (different signs because the angles are on opposite sides of the grating normal) and thus we must have:

$$\alpha = -\beta = \theta = A$$

So,

$$m \lambda = d (n - 1) \sin \theta$$

Thus the apex angle,  $A \ (= \theta)$ , which provides in-line diffraction for wavelength  $\lambda$ , in order m is given by:

$$\sin A = \frac{m \lambda}{d (n - 1)}$$

Thus a grism can be optimised for a particular job. Because of the in-line transmission, grisms can be easily moved in or out of the optical path and it is possible to use them in a "grism wheel" – just like optical transmission filters in photometry.