Basic equations for astronomical spectroscopy with a diffraction grating

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1. Interference condition

As shown in Figure 1, the path difference between interfering rays AB and A'B' is $a(\sin\alpha + \sin\beta)$ where a is the spacing between the repeated element in the grating from which reflection (or refraction) occurs.

The interference condition is fulfilled when the path difference is equal to multiples, m, of the wavelength of the illuminating light. This gives rise to the *grating equation*:

$$m\rho\lambda = \sin\alpha + \sin\beta$$

where $\rho = 1/a$ is the ruling density, m is the spectral order and λ is the wavelength of light.

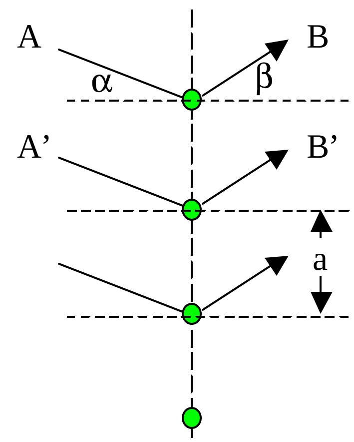

Figure 1: Interference of light by a diffraction grating. Although this is considered here as a transmission grating, the same principle applies to a reflection grating with suitable care taken with the sign of the angles.

2. Dispersion

By differentiating with respect to the output angle we obtain the *angular dispersion*

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

The *linear dispersion* is then

$$\frac{d\lambda}{dx} = \frac{d\lambda}{d\beta}\frac{d\beta}{dx} = \frac{\cos\beta}{m\rho f_2}$$

since $f_2 d\beta = dx$ where f_2 is the focal length of the camera (see Figure 2).

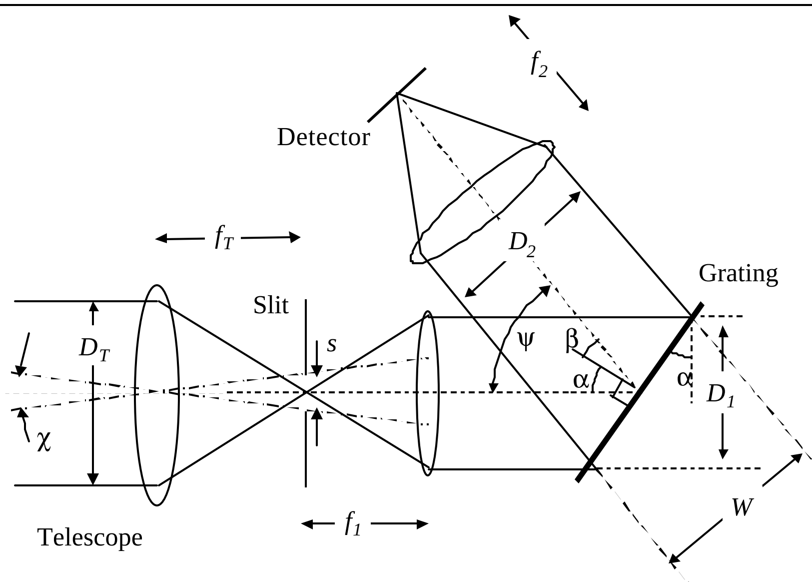

Figure 2. Illustration of the principle of a generic grating spectrograph showing the definition of quantities used in the text. To be consistent with the grating equation, α and β have the same sign if they are on the same side of the grating normal.

3. Resolving power

In standard textbooks, the *resolving power*, $R = l/\Delta l$ (where Δl is the resolution in wavelength), is usually described as being given by the total number of lines in the grating multiplied by the spectral order, hence

$$R_* = m\boldsymbol{r}W$$

(sometimes this is called the *spectral resolution* which can lead to confusion with Δl). But in practice, the resolving power is determined by the width of the image of the slit, *s*, projected on the detector, *s*'.

Before going further, it is useful to consider the invariance of Etendue in optical systems (note that fibres and some other optical systems do not conserve Etendue but systems made from normal optics – mirrors and lenses - do). This is normally stated as

$$n\Omega A = \text{constant}$$

where Ω is the solid angle of radiation incident at a surface of area A in a medium with refractive index *n*. For our purposes, we may set $n = 1$ (since we only consider optics in air or vacuum) and consider a one-dimensional analogue:

$$\boldsymbol{w}a = \boldsymbol{w}'a' = \text{constant}$$

where $\boldsymbol{w}$ and a are the opening angle of the beam and the aperture dimension respectively. To determine the width of the image of the slit formed on the detector, we use conservation of Etendue, $s\boldsymbol{q} = s'\boldsymbol{q}'$, where the angles at the slit and detector are $\boldsymbol{q} = D_1/f_1$ and $\boldsymbol{q}' = D_2/f_2$ (Figure 3), so

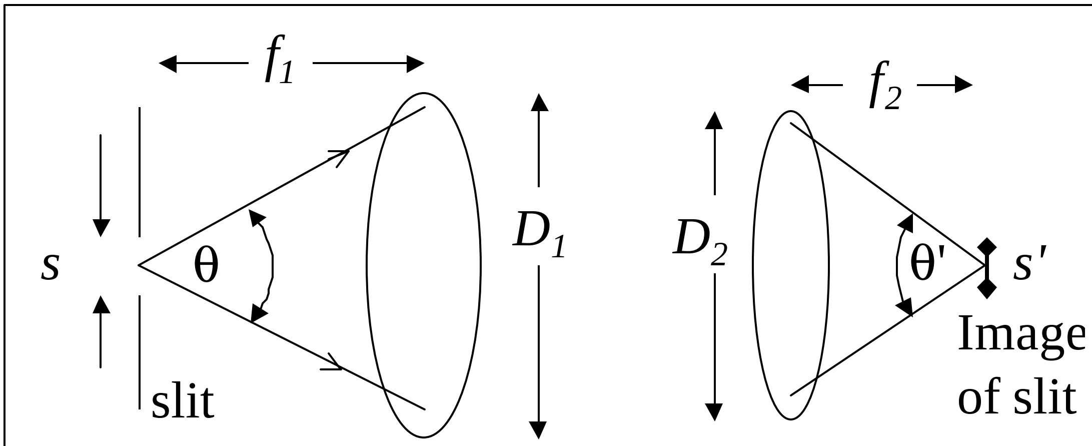

Figure 3: Projection of the slit (left) onto the detector (right).

$$s' = s\frac{\theta}{\theta'} = s\frac{F_2}{F_1}$$

where the collimator and camera focal ratios are $F_i = {f_i}/{D_i}$ for $i = 1,2$ respectively.

We now express the width of the image of the slit in wavelength units to determine the *spectral resolution* of the spectrograph

$$\Delta\lambda = \left(\frac{d\lambda}{dx}\right)s' = \frac{\cos\beta}{m\rho f_2}s\left(\frac{F_2}{F_1}\right) = \frac{sD_1\cos\beta}{m\rho D_2 f_1}$$

The length of the intersection between the collimated beam and the plane of the grating (not necessarily the actual physical length of the grating) is

$$W = \frac{D_2}{\cos\beta}$$

so

$$\Delta\lambda = \frac{s}{m\rho F_1 W}$$

The resolving power, defined as $R = \lambda/\Delta\lambda$, is then

$$R = \frac{m\rho\lambda F_1 W}{s}$$

Note that this is independent of the details of the camera. This expression is useful for a laboratory experiment since it is expressed in terms of the parameters of the experimental setup: the collimator focal ratio, F_1, the grating parameters, ρ and m, the effective grating length, W, and the physical slit width, s. Note that this expression may also be given in terms of the incident and diffracted ray angles at the grating by substituting for $m\rho\lambda$ from the grating equation and for the grating length using the previous expression for W.

For astronomy, it is more useful to express the resolving power in terms of the angular slit width (projected on the sky), χ, and the telescope aperture diameter, D_T. For this we note that

$$s = \chi f_T$$

and

$$\frac{f_T}{D_T} = \frac{f_1}{D_1} = F_T = F_1$$

since the spectrograph is directly beam-fed from the telescope (i.e. no reformatting with fibres is involved). Note that even if the slit is reimaged, the expression below still holds, due to the conservation of Etendue in the reimaging optics.

Thus the *resolving power* is

$$R = \frac{m\rho\lambda W}{\chi D_T}$$

Note that $R \le R_*$, the resolving power obtained with a finite slit width is always less than the theoretical maximum which may be obtained with a infinitely narrow slit. This condition is maintained for wavelengths satisfying

$$\lambda < \lambda_* = \chi D_T$$

Thus, long-wavelength applications may approach the theoretical limit; in which case they are said to be *diffraction-limited*. If so, the resolving power is independent of the slit width and it becomes relatively straightforward for the spectrograph to be used with different telescopes. For a non-diffraction-limited spectrograph, the resolving power obtained would depend on the aperture of the telescope to which it was fitted.

Note also that the resolving power (when not diffraction-limited) is inversely proportional to the telescope aperture diameter. To maintain the same resolving power requires a proportional scaling up in W which implies that the spectrograph should scale in direct proportion to the telescope.

4. Practical example

Consider a spectrograph with the following parameters:

$$m = 1,\ \rho = 1200/\mathrm{mm},\ \chi = 0.5\,\mathrm{arcsec},\ D_T = 8\mathrm{m}, D_1 = 100\mathrm{mm},\ \lambda = 500\mathrm{nm}$$

If the grating tilt is $\alpha = 20^\circ$ then, from the grating equation, $\beta = \arcsin(m\rho\lambda - \sin\alpha) = 15^\circ$. Thus the illuminated grating length is $W = D_1/\cos\beta = 104\mathrm{mm}$ and the resolving power is $R = 1560$. This compares with the diffraction-limited case where $R_* = 124800$. Only at wavelengths longer than $\lambda_* = 19\mu\mathrm{m}$ will the spectrograph be diffraction limited.

Note that, in this example, the angle between the axes of the collimator and camera, $\Psi = \boldsymbol{a} - \boldsymbol{b} = 5^\circ$ (remember the sign convention for these angles), which is probably impractical.

5. Anamorphism

The ratio s'/s is the magnification of the spectrograph in the dispersion direction only. In the direction along the slit the magnification is, in general, different. This gives rise to an *anamorphic magnification.* To see this, we need to consider the shape of the beam exiting from the grating. If the grating was a mirror (or was used in zero order, $m = 0$) , naturally the output and input beams would have the same circular shape.

From Figure 1, we can seen that the width of the output beam, as seen at the input aperture of the camera, in the direction perpendicular to the slit (the dispersion direction) is

$$D_2 = W \cos \boldsymbol{b}$$

but the width in the direction parallel to the slit is

$$D_1 = W \cos \boldsymbol{a}$$

Hence the anamorphic factor (Figure 4) is

$$A = \frac{D_2}{D_1} = \frac{\cos \boldsymbol{b}}{\cos \boldsymbol{a}}$$

By conservation of Etendue, this also means that magnification in the two directions is also different. We have already seen that the magnification in the dispersion direction is

$$M_l = \frac{s'}{s} = \frac{F_2}{F_1} = \frac{f_2 D_1}{f_1 D_2}$$

but in the along-slit direction, it is simply

$$M_x = \frac{f_2}{f_1}$$

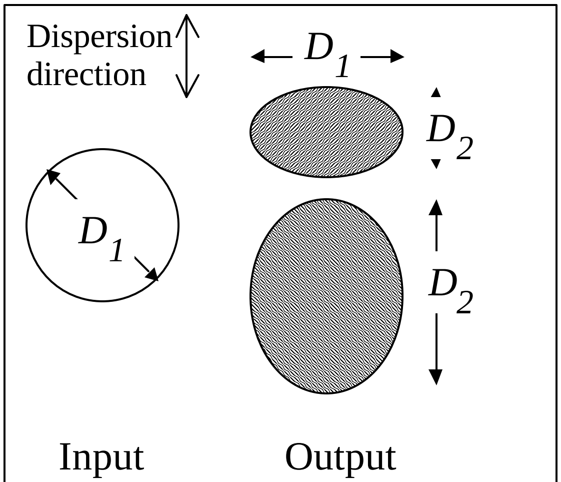

Figure 4: Anamorphism in the beam shapes. Two examples are shown for the output beam shape. Top: for the *normal to collimator* configuration. Bottom: for the *normal to camera* configuration.

Thus, as might expect from the conservation of Etendue, the ratio of magnification between the two directions is also given by the anamorphic factor since

$$\frac{M_x}{M_l} = \frac{D_2}{D_1} = A$$

There are two main configurations which may be used with blazed gratings, the *normal to camera* configuration in which the normal to the grating is pointed generally towards the camera, as illustrated in Figure 1. In this case $b < a$ so $A > 1$. The alternative is the *normal to collimator* configuration in which $b > a$ so $A < 1$. It is possible to satisfy the grating equation for the same wavelength and spectral order in either configuration but they are not equivalent when their detailed behaviour is examined. To do this, we need to consider the question of *blazing* the grating.

6. Blazing

The grating is most efficient when the rays emerge from the grating as if by direct reflection off the facets of which the grating is composed. This is known as the *blaze condition*. This can be understood by going back to the expression for the intensity from a diffraction grating consisting of N rulings (see e.g. *Fundamentals of Optics*, Jenkins & White):

$$I = \left(\frac{\sin^2 Nf}{\sin^2 f}\right)\left(\frac{\sin^2 q}{q^2}\right),$$

where $2f$ is the phase difference between the centre of adjacent rulings and q is the phase difference between the centre and edge of a single ruling. The second term in the expression is known as the *blaze function.* As can be seen from Figure 5, its effect is to modulate the interference pattern for a single wavelength. Unfortunately, the maximum, when $q = 0$, occurs for zero order, $m = 0$. For practical spectroscopy, we would like to shift the maximum of the blaze function to occur when, say, $m = 1$ for some useful wavelength. This can be done by profiling the grating surface so that each periodic unit adopts the shape shown in Figure 6. These facets are tilted at an angle g to the plane of the grating. The phase difference between centre and edge of the facet is then

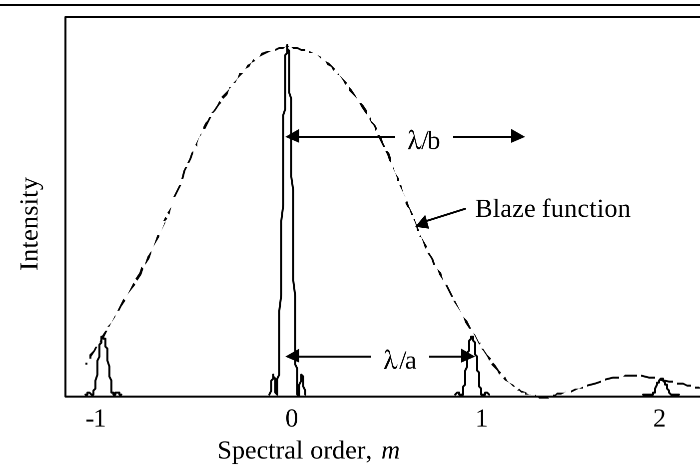

Figure 5: Illustrative plot of diffracted intensity at a single wavelength versus angle labeled by the spectral order.

$$\boldsymbol{q} = \frac{\boldsymbol{p}\cos \boldsymbol{g}}{\boldsymbol{r}\,\boldsymbol{l}}(\sin i - \sin r)$$

From Figure 6, it can be seen that

$$i = \boldsymbol{a} - \boldsymbol{g} \text{ and } r = \boldsymbol{g} - \boldsymbol{b}$$

(Recall the sign convention that $\boldsymbol{a}$ and $\boldsymbol{b}$ have the same sign if they are on the same side of the grating normal.) So the blaze peak condition ($\boldsymbol{q} = 0$) occurs when $i = r$, which is equivalent to simple reflection from the facets, and

$$\boldsymbol{a} + \boldsymbol{b} = 2\boldsymbol{g}$$

Making use of the identity,

$\sin x + \sin y = 2\sin\frac{x+y}{2}\cos\frac{x-y}{2}$, we can rewrite the grating equation at the blaze condition as

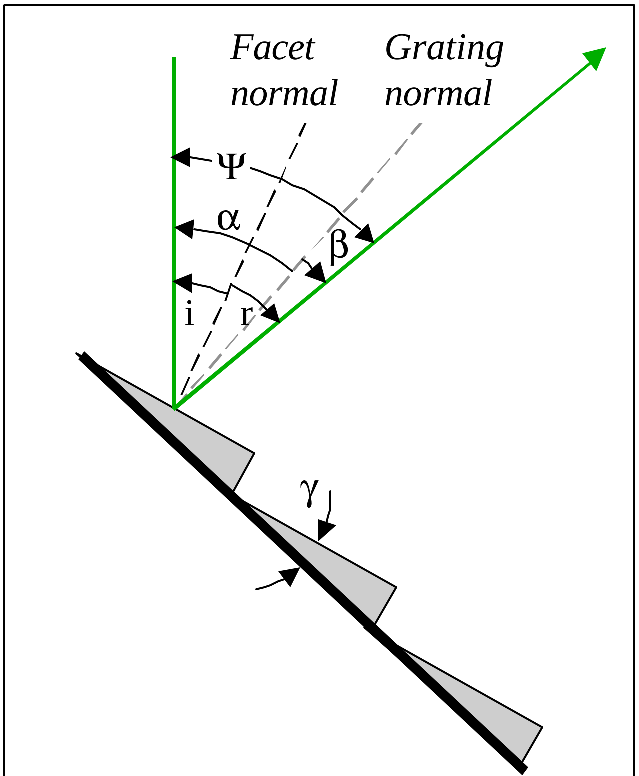

Figure 6: Illustration of blaze condition for reflection grating.

$$\boldsymbol{r} m \boldsymbol{l}_B = 2\sin \boldsymbol{g} \cos\frac{\Psi}{2}$$

since $\Psi = \boldsymbol{a} - \boldsymbol{b}$, where $\boldsymbol{l}_B$ is the wavelength for which the blaze condition is satisfied and Ψ is the collimator-camera angle which is fixed by the design of the spectrograph (Figure 1).

Figure 7 shows an idealised blaze function for a grating blazed at wavelength $\boldsymbol{l}_B$ in first order. It is useful to note (*Astronomical Optics*, Schroeder) that, in the ideal case, the efficiency of a grating drops to 40.5% of the maximum at wavelengths on either side of the blaze peak of (approximately)

$$\boldsymbol{l}_+ = \frac{2m\boldsymbol{l}_B}{2m-1} \text{ and } \boldsymbol{l}_- = \frac{2m\boldsymbol{l}_B}{2m+1}$$

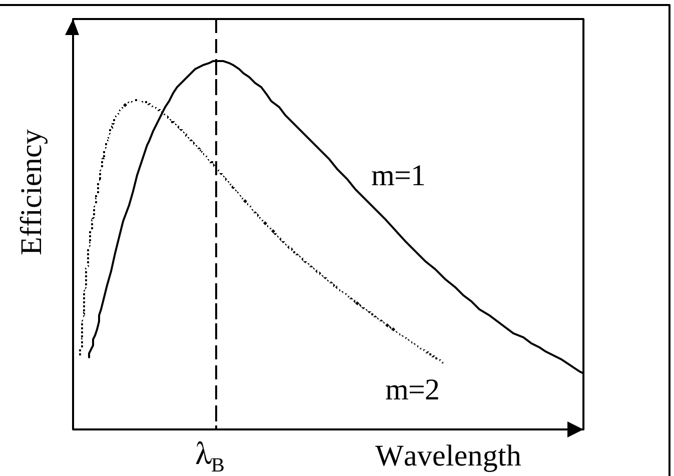

Figure 7: Typical relationship between efficiency and wavelength for a blazed diffraction grating.

and that the useful wavelength range, defined in this way, is

$$l_{+} - l_{-} = \frac{l_B}{m}$$

for large *m*. (This is very similar to the expression for the *free spectral range* which gives the wavelength range within a single order which may be obtained without being overlapped by light from different orders.)

However, real gratings depart from this idealised situation, especially when different polarisation states are considered and when the facet size is comparable with l. Note also that the behaviour in higher orders is subject to the physical requirement that the sum of the blaze functions of all orders must not exceed unity. In practice, as indicated in Figure 7, the peak efficiency decreases with increasing order. The actual blaze profile which may be obtained is a complicated matter requiring consideration of Maxwell's equations and is beyond the scope of this paper.

For the *Littrow* configuration, $\Psi = 0$ (the incident and diffracted rays are parallel), so

$$m\,r\,l_B^L = 2\sin g$$

So the resolving power in the Littrow configuration (only) can be expressed as

$$R = \frac{2D_1 \tan g}{cD_T}$$

The relationship between non-Littrow and Littrow blaze conditions is

$$l_B = l_B^L \cos\frac{\Psi}{2}$$

Note that most catalogues of gratings give r, g and l_B^L only, so it is necessary to transform from the Littrow case to the actual geometry of the spectrograph. Furthermore the efficiency as a function of wavelength is usually given for a near-Littrow configuration ($\Psi \approx 0$). Generally the efficiency of a grating declines slightly with increasing Ψ.

7. Which configuration is best?

We are now in a position to analyse the difference between the *normal-to-camera* and *normal-to-collimator* configurations noted earlier.

It can be seen from Figure 8, that the two configurations can both satisfy the blaze condition since specular reflections are obtained from the groove facets. In fact, these two configurations are equivalent to using the same grating in positive and negative orders *but exchanged end-to-end*. To see this, the blaze wavelengths in the +1 and –1 orders are found to be

$$l_B^{+1} = 2\sin g \cos(\Psi/2)/\,r \qquad \text{and} \qquad l_B^{-1} = -2\sin g \cos(\Psi/2)/\,r$$

so $l_B^{+1} = -\,l_B^{-1}$ unless

$$\Psi \to 2p - \Psi \quad \text{or} \quad g \to -g$$

Both transformations are equivalent to turning the grating around end-to-end as illustrated in Figure 8.

So we have established that both configurations are indeed satisfactory in terms of satisfying the grating equation and the blaze condition. But they differ in the following respects:

The *normal-to-camera* configuration has a dilated beam on the grating so the increased value of *W* will result in a higher spectral resolution. At the same time, the beam

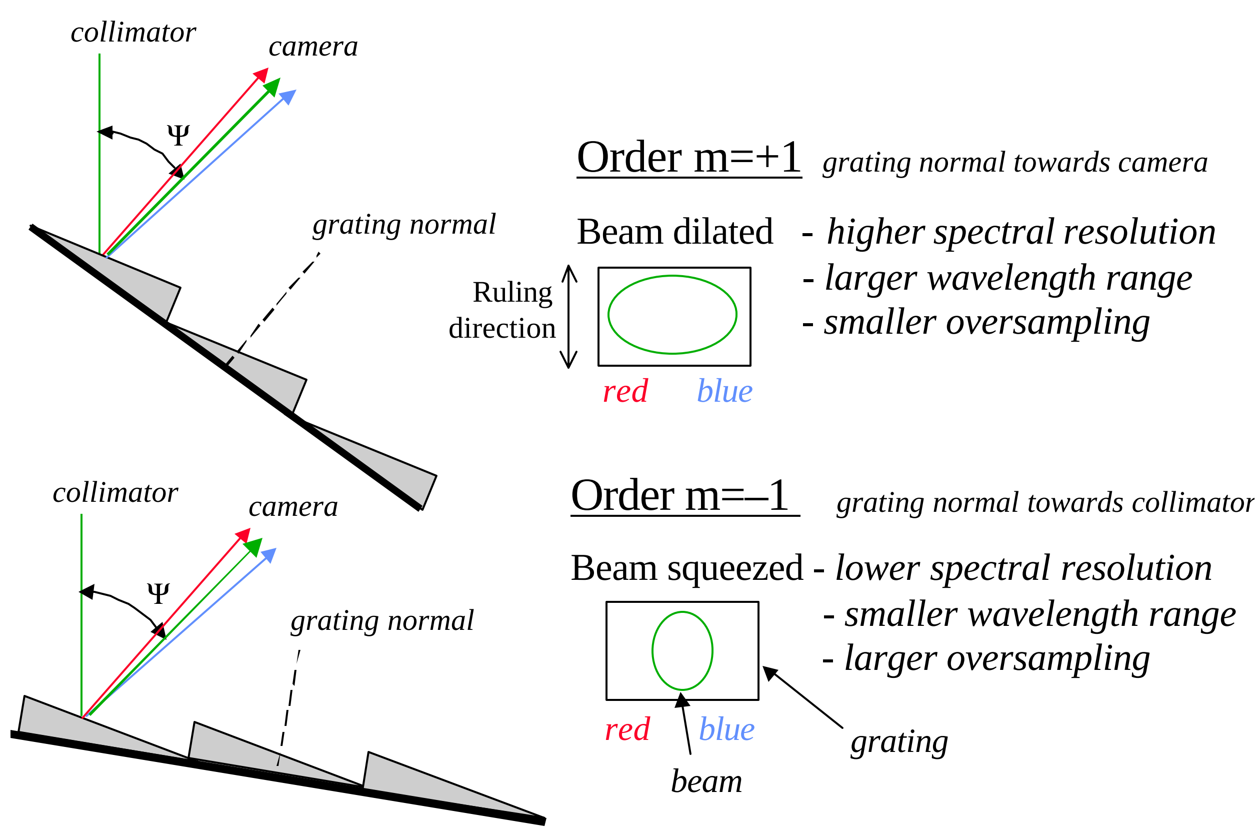

Figure 8: Illustration of the use of the same grating in the *normal to camera* (top) and normal to collimator (bottom) configurations.

anamorphism will result in a lower magnification in the dispersion direction. Thus the slit will project onto fewer detector pixels (s' is smaller). This will reduce the oversampling in the spectrum (generally a bad thing) but also increase the wavelength range that will fit on the detector at any one time (a good thing) since the linear dispersion is larger since β is smaller.

The *normal-to-collimator* configuration has a squashed beam on the grating leading to lower spectral resolution . The magnification is greater in the dispersion direction leading to higher (better) oversampling but a smaller simultaneous wavelength range since the linear dispersion if smaller.

Which configuration is best depends on the details of the spectrograph (for example the slit width and camera speed) and the requirements of the observation to be made. In most case, the normal-to-camera configuration is to be preferred but this may not always be the case. For this reason, many spectrographs have the capability to use their gratings in either configuration. However, don't forget to reverse the sense of the grating when changing configuration, otherwise you could find yourself working very far from blaze with a consequent large reduction in efficiency – this happens quite frequently!

8. Grisms

A grism is a combination of transmission grating and prism (Figure 9). Naturally, the grating equation applies to this situation but with the modification that the refractive index of the medium, n, (where we assume that the indices of the prism glass and the resin in which the grating is replicated are the same, $n = n_G = n_R$) must be included:

$$m\rho\lambda = n\sin\alpha + n'\sin\beta$$

Note that the ruling density, ρ, is defined in the plane of the grating, not the plane normal to the optical axis of the spectrograph. For the special case shown in Fig 9 where the input prism face and the facets are both normal to the optical axis, and where the external medium is air, $n'=1$, the most useful configuration is where $\delta = 0$, i.e. the light is undeviated, allowing the camera and collimator to be in line. Here $\beta = -\alpha$ so

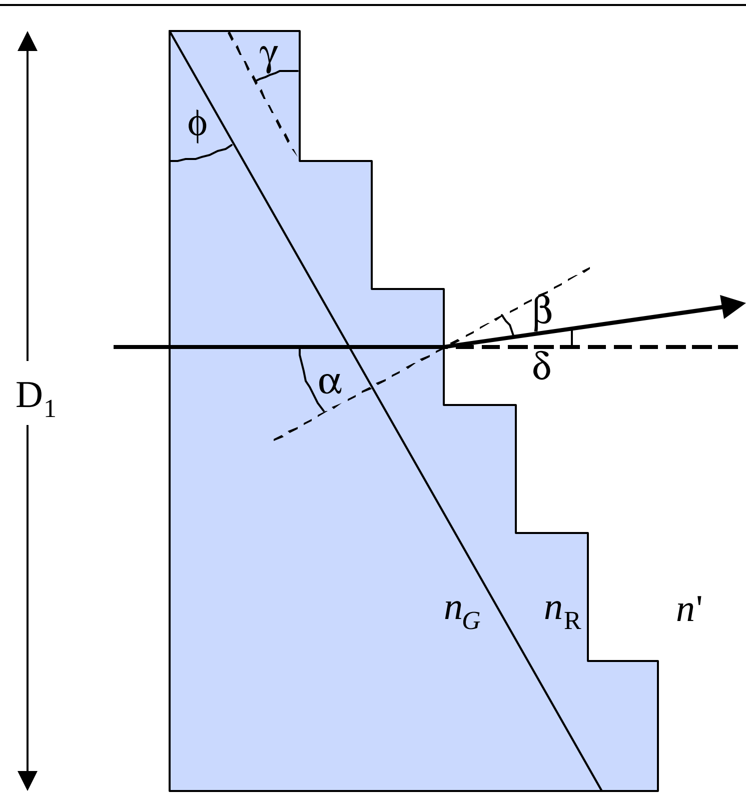

Figure 9: Typical configuration of a grism.

$$m\rho\lambda_U = (n-1)\sin\phi$$

Note that, for typical materials ($n = 1.5$), there is roughly a factor 4 difference in the blaze wavelength for the same grating used in reflection or as part of a grism!

The advantage of this configuration is that the monochromatic image of the target will appear at the same location as a direct image obtained with the grism removed.

This is also the blaze condition since the phase difference between the centre and edge of a facet is zero ($\theta = 0$), since rays emerging from the centre and edge of a facet pass through identical thickness' of glass and are parallel at all times. So we may set, for the special configuration described, $\lambda_B = \lambda_U$.

Working through the same equations as for the reflection grating, we find, as before, that

$$R = \frac{m\rho\lambda W}{\chi D_T}$$

Since the grating length is $W = D_1 / \cos\phi$, we can also express the resolving power as

$$R = \frac{(n-1)\tan\phi D_1}{\chi D_T}$$

Simple considerations of geometry show that the sizes of the input and output beams in the dispersion direction must be the same. Thus the anamorphic factor is unity. This allows grism-based spectrographs to use a smaller camera than that necessary for a spectrograph employing reflection gratings in a non-Littrow configuration. However, it should be noted that the efficiency of grisms with high ruling density, $\rho \geq 600/\mathrm{mm}$, is lower that the equivalent reflection grating due to groove shadowing and other effects.

It is also useful to consider the case where the facet groove angle ,γ , differs from the prism vertex angle, ϕ, and where the index of the resin and prism glass are different. Then the blaze wavelength is no longer the same as the undeviated wavelength.

$$m\rho\lambda_B \approx n_G \sin\phi + n_R \cos\gamma \sin\left\{\gamma - \arcsin\left(\frac{n_G}{n_R}\sin\phi\right)\right\} - \sin\gamma$$

If we set $\gamma = \phi$ (as shown in Figure 9), the expression simplifies to:

$$m\rho\lambda_B \approx (n_G - 1)\sin\phi + n_R \cos\phi \sin\left\{\phi - \arcsin\left(\frac{n_G}{n_R}\sin\phi\right)\right\} = m\rho(\lambda_U + \Delta\lambda_*)$$

To take an example actually encountered with LDSS-2, a grism with $\rho = 600/\mathrm{mm}$ and vertex angle $\phi = 30^{\circ}$ (equal to the facet groove angle) was replicated on a glass prism with index $n_G = 1.52$. This should have yielded a blaze wavelength $\lambda_B = \lambda_U = 433\mathrm{nm}$ if the resin and glass indices had been well matched. But at the first attempt, a resin with $n_R = 1.60$ was used. This caused the blaze to be shifted red-wards by $\Delta\lambda_* = 66\mathrm{nm}$ to 500nm so the grism was remade with a better choice of resin.

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