Design considerations for grating spectrometer

1. Preliminary optical design

As with most spectrographs the idea is to achieve high throughput, dispersion, optical performance, stability and yet be produced for as low a cost as possible. We note for example the exciting new designs afforded by single mode fibres (e.g., Feger et al. 2014 and Crepp et al. 2016) and their feeding by adaptive optics systems (e.g., Jovanovic et al. 2017), the highly promising work of fibre manipulation of a multi-mode fibre (e.g., Calcines et al. 2018, Anagnos et al. 2018), the potential for high resolution integral field spectroscopy (e.g., Lovis et al. 2016) and in general the promise of astrophotonic spectrographs (e.g., Gatkine et al. 2019). Some of these suffer from relatively low throughput and/or wavelength coverage due to the properties of single mode fibres and problems of efficiently coupling light into a single mode fibre; so there remain a variety of technical hurdles to overcome prior to turn-key utilisation. Nonetheless, these devices and concepts provide great promise and will likely help to make it appropriate and feasible to have a high resolution spectrograph in space (e.g., Plavchan et al. 2018). Our currently preferred methodology for achieving efficient focal reduction is through tapering of the input fibre from the telescope as proven by Choochalerm et al. (2020).

One of the key issues for high precision spectrographs is that they must be stable on all timescales which might be of interest for astronomical phenomena. When considering exoplanets this might be from hours to hundreds of years (e.g., Feng et al. 2020). Both simultaneously calibrated spectrographs such as HARPS and Iodine stablised spectrographs such as HIRES work on the premise that the optical arrangement should be as stable as possible. So in the case of common user spectrographs like HIRES, a bespoke calibration procedure is required to ensure that each night begins and ends with ThAr lines falling on exactly the same position on the detector. HARPS achieves this with extreme temperature and pressure control along with complete isolation of the spectrograph from any human interaction.

There are many different successful designs available for us to develop from. We seek to benefit from these and in particular we take inspiration from the HARPS (Pepe et al. 2000) and PFS (Crane et al. 2006) instruments due to their exquisite performance over more than a decade of operation. Both of these designs are themselves derived from several similar previous instruments and so have considerable heritage. Given that we have a laboratory available some distance from any telescope, a fibre feed like HARPS was desirable. On the other hand, the small size and re-use of optical components provided by a double-pass design was particularly appealing from the PFS design. We first develop some insight into the critical design parameters for the spectrograph.

1.0.1. Finite image size and resolution

Based on an input image size of diameter h and a collimator lens with focal distance f_c and radius S, the light rays coming from the edge of the image will not be parallel to the ones from the center of the image and offset by a small angle $\delta\alpha$

$$\delta\alpha = \frac{h}{f_c} \tag{1}$$

where we assumed that $\tan \delta\alpha \sim \delta\alpha$. This small angle will then propagate into generating a finite size of the final image. The condition on the required dispersion of an element (grating or prism) is that a light ray of minimal wavelength to be resolved has to be deflected an angle ϵ, equal or larger than this $\delta\alpha$. A refocussing lens or camera will only affect the physical size of the image but will not contribute in separating images of different wavelengths further.

Let us compute this angle for an arbitrary echelle grating working at some blaze wavelength (the wavelength at which the incoming angle is equal to the outgoing angle, also called Littrow condition). Based on the grating equation for a general incoming and outgoing ray and where d is the distance between the repetitive grooves or facets in the diffraction grating

$$d(\sin\theta_{\rm in} + \sin\theta_{\rm out}) \quad = \quad m\lambda_B \tag{2}$$

Gratings are usually most efficient when working in the Littrow configuration. That is, the incident rays are perpendicular to the facets of the grating. In this situation there is always an integer number of wavelengths that are exactly reflected back with $\theta_{\rm in} = \theta_{\rm out}$ which we call *blaze wavelengths* ($\lambda_{\rm B}$). The dispersion around these blaze wavelengths can be treated as a small perturbation, so the properties of the dispersion around λ_B will define the performance of the spectrometer in terms of its resolving power. For a $\lambda_{\rm B}$ and a slightly different $\lambda_{\rm B} + \delta\lambda$, one can write

$$d(\sin\theta_{\rm B} + \sin\theta_{\rm B}) \quad = \quad m\lambda_B \tag{3}$$

$$d(\sin\theta_{\rm B} + \sin(\theta_{\rm B} + \epsilon)) \quad = \quad m(\lambda_{\rm B} + \delta\lambda) \tag{4}$$

Expanding in powers of small ϵ around $\theta_{\rm B}$ the difference between (3) and (4) leads to

$$\epsilon = \frac{m\,\delta\lambda_{\rm B}}{d\,\cos\theta_{\rm B}} \tag{5}$$

where m is the diffraction order, $\lambda_{\rm B}$ is the central blaze wavelength and θ_B is the blaze angle of the grating. To distinguish $\lambda_{\rm B}$ from $\lambda_{\rm B} + \delta\lambda$, the small angle ϵ must equal the one caused by the finite size of the input image, leading to the condition

$$\epsilon = \delta\alpha \tag{6}$$

By substituting the relations for $\delta\alpha$ in Eq.(1) and for ϵ in Eq.(5), we get

$$\frac{h}{f_c} = \frac{m\,\delta\lambda_{\rm B}}{d\,\cos\theta_{\rm B}} \tag{7}$$

This expression can now be re-arranged to find out the size of the first collimating lens (and therefore the size of the grating) by applying three definitions,

- **Resolving power** R is an adimensional number defined as $R = \lambda/\delta\lambda$, and quantifies how well a spectrometer can discriminate wavelengths. A high resolution spectrometer for stellar studies and exoplanet searches should have need a resolving power $> 5 \times 10^4$ ($R > 10^5$ desirable). Moderate resolutions between $1000 - 20000$ are typically sufficient for spectral classification and cosmological studies, and anything below 1000 is considered low-resolution.

- **Opening angle** a. The beam input of the telescope is usually specified by its opening angle a. The tangent of this opening angle is the ratio between the radius of the collimator S and its focal length f_1 ($\tan a = S/f_1$). Using this definition and substituting for $\delta\lambda$ Eq. (7) becomes

$$S = Rh \tan a \, \frac{d \cos\theta_i}{m\,\lambda_B}\,. \tag{8}$$

- **Numerical aperture** N of an optic or fibre is defined as $N = n \sin a$, where n is the refractive index of the medium after the fibre. For vacuum applications $n \sim 1$, so the tangent of the opening angle a can be written in terms of N as

$$\tan a = \frac{N}{\sqrt{1-N^2}} \tag{9}$$

We can now write S as a function of the design parameters (R and N), obtaining

$$S = Rh \frac{N}{\sqrt{1-N^2}} \, \frac{d \cos\theta_i}{m\,\lambda_B} \tag{10}$$

For most practical cases, e.g., a typical fibre with N$\sim$0.22 one can simplify to

$$S = Rh\,N \, \frac{d \cos\theta_i}{m\,\lambda_B} \tag{11}$$

In an astronomical spectrograph the resolution is estimated from the FWHM of the instrumental profile, which in our case is the image of the entrance slit (or fibre). For a Gaussian profile, the FWHM is 2.35 σ, where σ is the square of the variance of the profile. For a box shaped profile of size h, its variance is $\sigma^2 = \frac{h^2}{12}$, so the effective h is to be used is $2.35/(\sqrt{12}h_r) = 0.67 h_r$, where h_r is the width of the slit (or fibre). By numerical substitution of the parameters for the HARPS spectrometer ($R \sim 10^5$, $\lambda_B = 550$ nm, $m = 100$, $\theta_B = 75$ deg, $d = 1/32$ mm) one obtains a beam diameter of $2S \sim 20$ cm, which matches the specifications listed in the instrument description [1].

1.0.2. Invariant grating relation

One more relation can be derived that is useful for spectrometer design. The right factor on the right-hand-side of (11) depends only on grating parameters. For example, we would like to know the diffraction order at which we need to work given some groove density and wavelength. In Littrow conditions, the diffraction order m can be derived from eq. (3) as

$$m = \frac{2\,d\ \sin\theta_B}{\lambda_B} \tag{12}$$

which we can substitute in Eq. (11) to obtain

$$2S = \frac{0.67\,h_r R\,N}{\tan\theta_B} \tag{13}$$

[1] http://www.eso.org/sci/facilities/lasilla/instruments/harps/inst/description.html

Table 1: Beam diameter, grating length and ruled area requirements for several representative grating parameters. Given that resolutions over 50 000 are always needed, the ruled area (cost and complexity scale with this) can be dramatically reduced by reducing the input image by fibre reformatting. The first line of the table is given in bold and are the effective sizes of the HARPS grating mosaic which is comprised of two gratings mosaiced together to give a total area of 84×21.4 cm.

Resolution	Fibre diameter	Numerical apperture	Blaze angle	Beam diameter	Grating length	Ruled Area
R	h_r	NA	θ_B	$2S$	l	A_r
[$\lambda/\delta\lambda$]	[μm]	[$-$]	[deg]	[cm]	[cm]	[cm^2]
10^5	**50**	**0.22**	**75**	**19.7**	**76.0**	**1498**
10^5	10	0.22	75	4.0	15.2	60.8
10^5	50	0.22	63	37.5	82.4	3088
10^5	10	0.22	63	7.6	16.5	125
10^5	50	0.22	45	73.7	104.2	7679
10^5	10	0.22	45	14.7	20.8	306.3

where the $2S$ is the diameter of the first colilmator lens (and diameter of the beam). Note that the dependence on the groove separation and wavelength have both disappeared. This means that there are always an infinite number of combinations of groove density, wavelength and working diffraction order that can achieve the same resolution for a given beam size. For example, we can work at low groove density (eg. 32 lines/mm) and high diffraction order (say m=100) or at a low diffraction order (m=1 and high groove density (3200 lines/mm) and still achieve the same resolving power. $2S$ is the diameter of the collimator, which is the deprojected size of the grating for a given angle θ_B. Assuming a rectangular grating, its height (along the grooves) is $2S$ and its length is l. Using trigonometry, one finds that the length l is related to the blaze angle and the beam diameter by $l\cos\theta_B = 2S$, which leads to

$$l = \frac{0.67\, h_r\, R\, N}{\sin\theta_B} \tag{14}$$

so the total ruled area A_r is

$$A_r = l2S = (0.67\, h_r\, R\, N)^2\, \frac{\cos\theta_B}{\sin^2\theta_B} \tag{15}$$

Table 1 shows the required grating sizes for some example spectrometers (eg. HARPS-like). Classic echelles work with low groove densities to obtain many overlaping orders (which is another design issue not discussed here) but the actual resolution has nothing to do with that, as it could be achieved with higher groove densities working at lower diffraction orders.