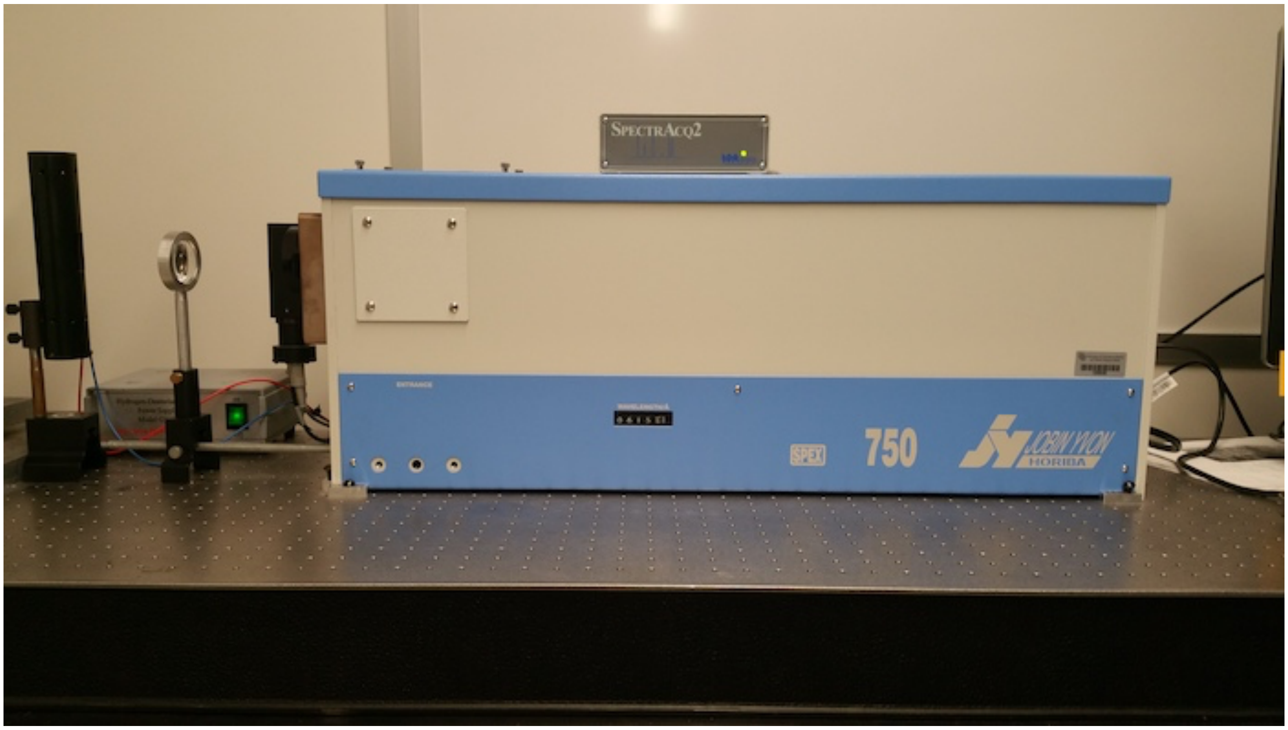
Modeling a Grating Monochromator Spectrometer

Randall Tagg 23-Nov-2021 Latest revision 30-Nov-2021

The Horiba / Jobin-Yvon monochromator



> **Figure 1** Monochromator sitting on optical table with light source, imaging lens, and detector on the left and computer interface on top of the monochromator.

For a general introduction to grating monochomator spectrometers, see:

[https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/size_spectrum.pdf (https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/size_spectrum.pdf)](https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/size_spectrum.pdf)

The apparatus you will use in this experiment is Jobin-Yvon 750S spectrometer with scanning grating.

[https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/750si.pdf (https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/750si.pdf)](https://www.horiba.com/fileadmin/uploads/Scientific/Documents/OSD/750si.pdf)

This is based on the M-series spectometers:

[https://www.horiba.com/fileadmin/uploads/Scientific/Documents/Mono/mseries-v3.pdf (https://www.horiba.com/fileadmin/uploads/Scientific/Documents/Mono/mseries-v3.pdf)](https://www.horiba.com/fileadmin/uploads/Scientific/Documents/Mono/mseries-v3.pdf)

The spectrograph is operated using software called SynerJY. (Scroll down at the following link.)

https://www.horiba.com/en_en/products/detail/action/show/Product/spectroscopy-software-1628/ (https://www.horiba.com/en_en/products/detail/action/show/Product/spectroscopy-software-1628/)

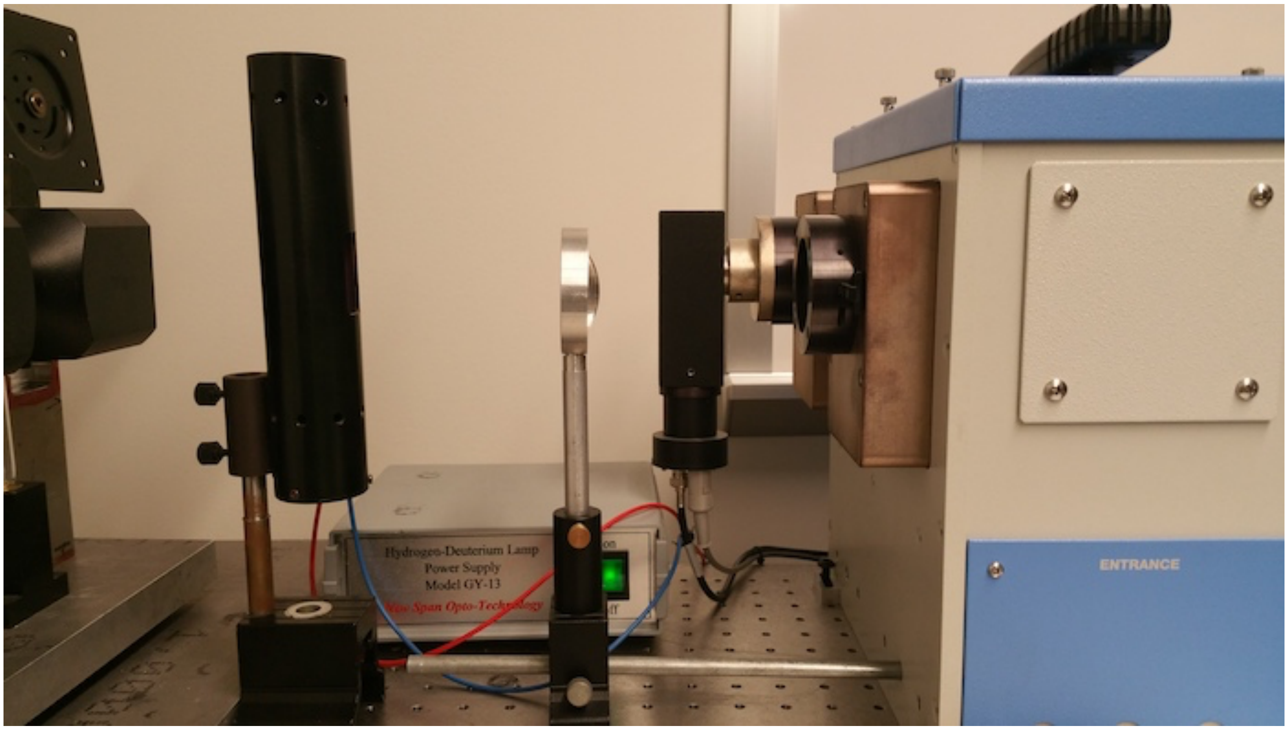


Figure 2 Foreground: a light source (a narrow vertical discharge lamp) is imaged by a convex lens onto the entrance slit of the monochrometer. Background: a photomultiplier tube light detector is attached to the exit aperture of the monochrometer. This photomultiplier uses a built-in high-voltage power supply controlled by the computer interface box and the photomultiplier output is sent to an analog-to-digital converter in the same computer interface. The interface is shown sitting on top of the monochromator in Figure 1.

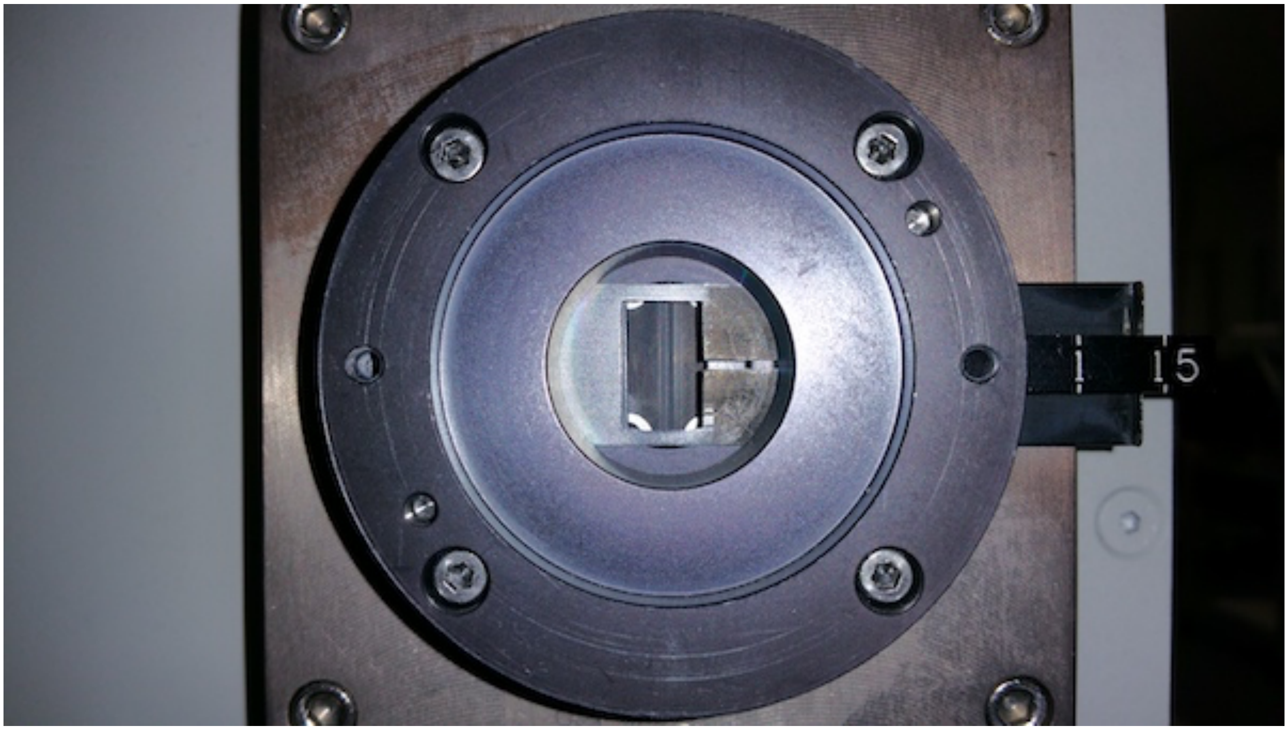


Figure 3 Entrance slit and its housing.

The monochromator data acquisition interface is described at:

https://www.horiba.com/cz/scientific/products/optical-spectroscopy/acquisition-controllers/details/spectracq2-224/ (https://www.horiba.com/cz/scientific/products/optical-spectroscopy/acquisition-controllers/details/spectracq2-224/)

The photomultiplier housing is described at:

https://static.horiba.com/fileadmin/Horiba/Products/Scientific/Optical_Components_and_OEM/Si Housings.pdf (https://static.horiba.com/fileadmin/Horiba/Products/Scientific/Optical_Components_and_OEM/S Housings.pdf)

The detector options are described at:

https://www.horiba.com/cz/scientific/products/optical-spectroscopy/detectors/single-channel/ (https://www.horiba.com/cz/scientific/products/optical-spectroscopy/detectors/single-channel/)

Monochromator optics: the Czerny-Turner configuration

At the entrance of spectrograph a slit is provided whose width is changeable in software over the range 3 μm-3000 μm . The external light source which is focused on the input slit is collimated by a concave spherical mirror onto a 110×100mm (width x height) grating with 1800 grooves per mm. The diffracted light is refocused by a second concave spherical mirror onto the external slit. The focal length of the mirrors is 0.75 m. See the optical system diagrams below.

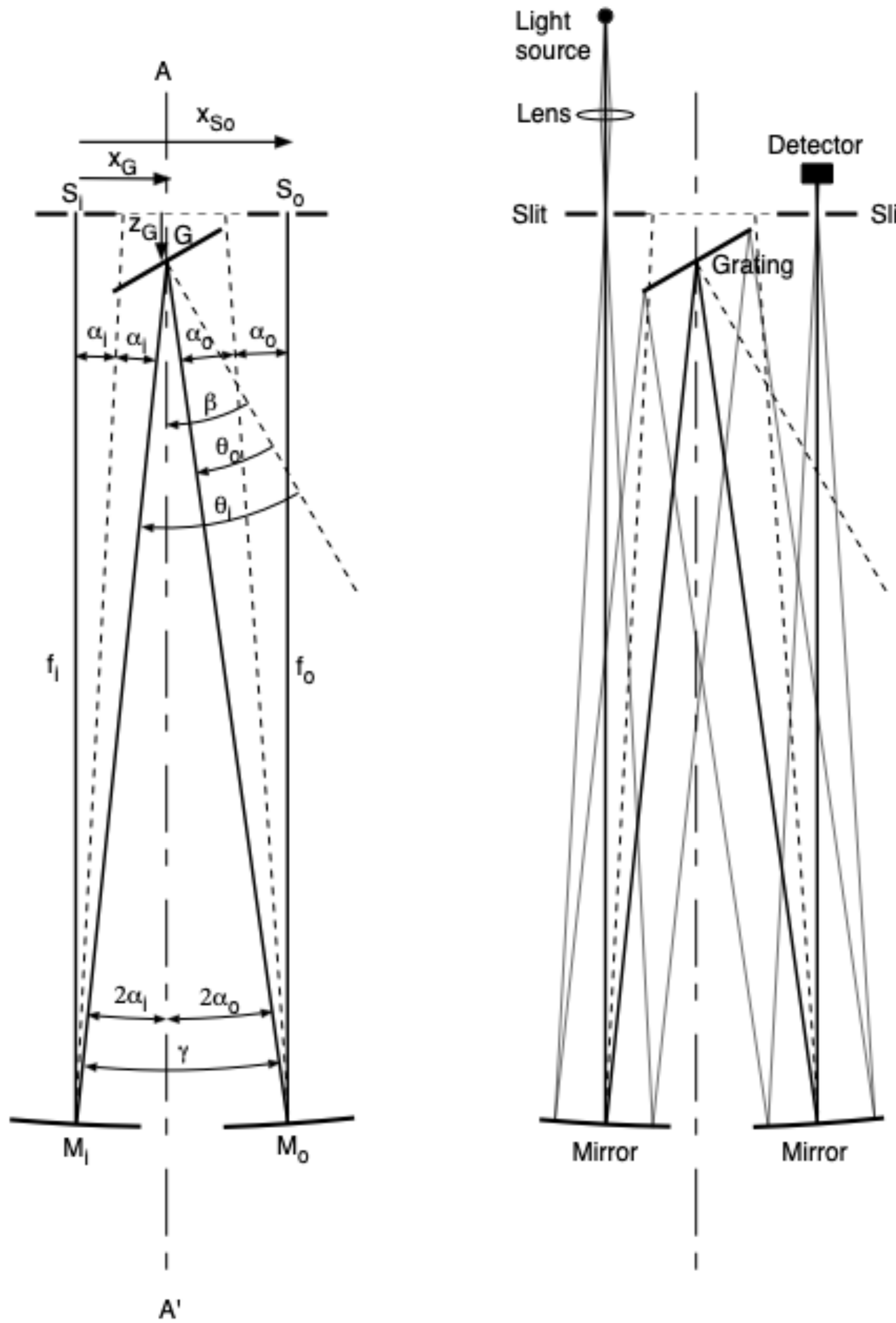


Figure 4a Monochromator geometry as defined by principal rays entering and exiting parallel to the instrument axis. Relationships between the indicated angles are derived and related below to the condition for constructive interference at the instrument exit. The grating angle β is swept by a stepper motor to scan through constructive interference for a range of wavelengths

Figure 4b A ray bundle originating from the light source is gathered by a lens and focused into the monochromator entrance slit. The principal ray that is parallel to the instrument axis is drawn as a heavier line. The entrance slit is also at the focal point of the first spherical mirror so the ray bundle is reflected into a collimated parallel-ray beam directed to the diffraction grating. Light scatters from the rulings of the grating: those rays that are parallel at the angle satisfying the constructive interference condition (see below) are gathered by the second spherical mirror and focussed into constructive interference at the exit slit. The light emerging from the exit slit is collected into a photomultiplier tube detector.

Modeling the ray paths

(Note: the notation for angles in this discussion is different from the notation used at the Horiba website.)

A ray of light goes from the center of entrance slit $\mathrm{S_i}$ to the center of spherical mirror $\mathrm{M_i}$. This defines the direction of the optical axis of the monochromator. The slit is located at a distance equal to the mirror's focal length $\mathrm{f_i}$ from the mirror center. The mirror is rotated so that its normal at mirror center makes an angle α_i with the axis. Thus the ray is reflected at an equal angle α_i to strike the center of diffraction grating G. The grating is rotated so that the direction of the instrument axis A-A' drawn through the center of the grating is at angle β from the normal to the grating. The ray coming into the grating makes an angle θ_i with respect to the grating normal. Here the ray and other rays parallel to it scattering from the ruled lines of the grating are assumed to be of a wavelength suited to constructive interference when refracted an angle θ_0 from the normal according to the criterion described in the next section. The outgoing ray from the center of the grating strikes the center of spherical mirror $\mathrm{M_o}$ at an angle α_o from the normal to the center of the mirror. The mirror is rotated so that this ray then is reflected at an equal angle α_o to the mirror's center normal so that the reflected ray goes through the center of exit slit $\mathrm{S_o}$ that is at distance equal to the focal distance $\mathrm{f_o}$ of mirror $\mathrm{M_o}$.

By proper construction, the final ray path can be aligned to be parallel to the incoming ray axis. In practice this is achieved by proper positioning of the center of the diffraction grating G at transverse and axial displacements $\mathrm{x_G}$ and $\mathrm{z_G}$ respectively relative to the center of entrance slit $\mathrm{S_i}$. In fact, we may think of the position of the grating center being defined as the intersection of laser beams shone into each slit $\mathrm{S_i}$ and $\mathrm{S_o}$ to the mirrors $\mathrm{M_i}$ and $\mathrm{M_o}$ which have been placed so their center normals angles of rotation $\mathrm{M_i}$ and $\mathrm{M_o}$ with respect to the respective incoming laser beam directions. The beams reflect from the mirrors and intersect at an angle $\gamma = 2\alpha_i + 2\alpha_0$ at the point where the center (and rotation axis) of the diffraction grating is placed. Note that α_i, α_0, and hence γ are constants for the instrument.

A key point whose importance will become evident below is that the instrument works by scanning the grating angle β. More precisely, we will see that the wavelength λ of light that is brought to a constructively interfering focus at the exit slit is advanced in value by uniform steps in the function $\sin\beta$.

From the drawing, we may deduce how the ray angles θ_i and θ_o are related to the angles α_i and α_o designed into the instrument and, importantly, to the scanned graing angle β:

$$\theta_i = \beta + 2\alpha_i.$$

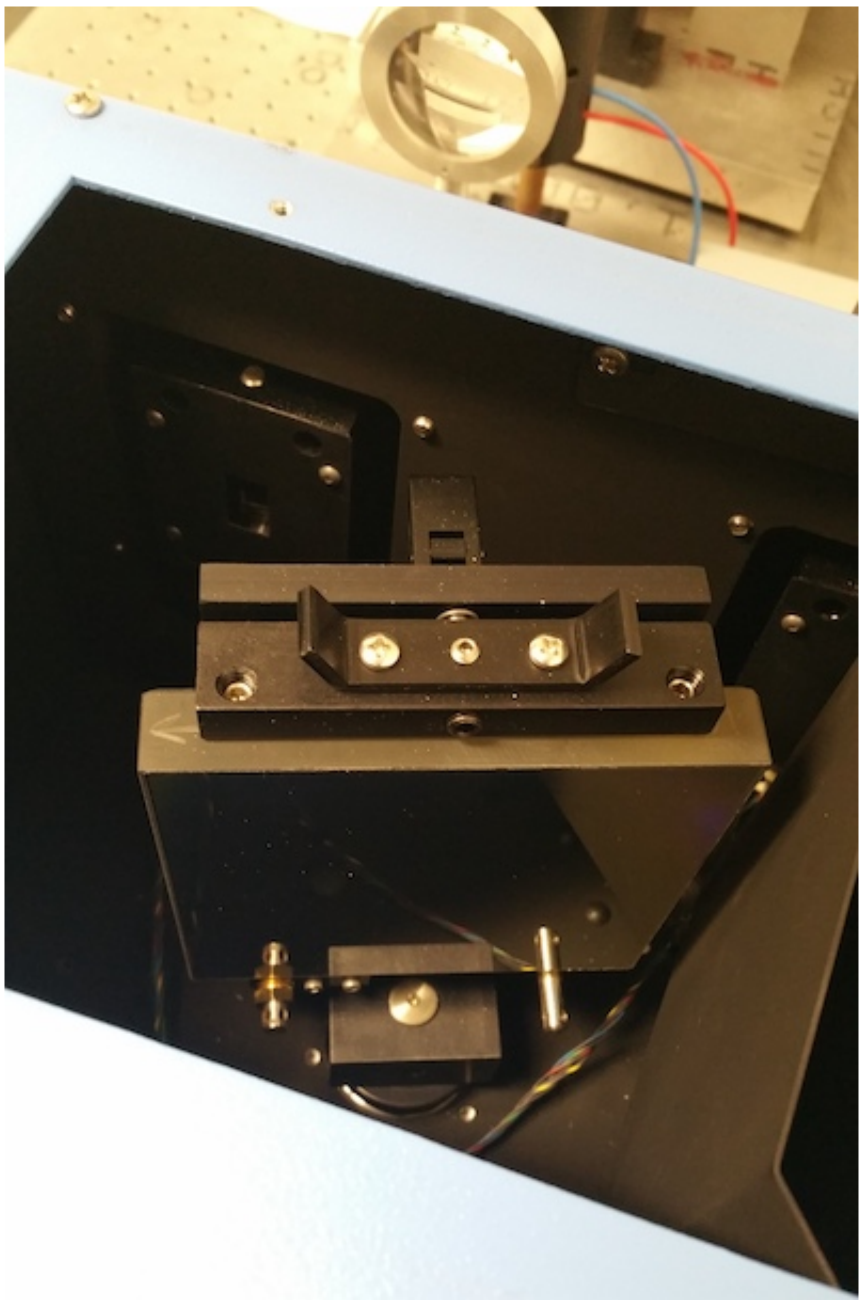
$$\theta_o = \beta - 2\alpha_o.$$

Notice that regardless of the rotation angle β of the grating, the net angle subtended by the incoming and outgoing (diffracted) rays is

$$\theta_i - \theta_o = 2\alpha_i + 2\alpha_o = \gamma,$$

which is constant.

The diffraction grating



> **Figure 5** The diffraction grating is viewed through a port in the top of the monochromator. Notice the grating's orientation relative to the entrance/exit face of the monochromator housing. The entrance slit is to the left behind the grating. The focusing lens is seen at the top of the photo.

More information about the grating may be found at

https://www.horiba.com/gbr/diffraction-gratings-ruled-holographic/#c8330 (https://www.horiba.com/gbr/diffraction-gratings-ruled-holographic/#c8330)

as well as

https://optics.org/products/P000020260 (https://optics.org/products/P000020260)

See also:

https://www.thorlabs.com/catalogpages/805.pdf (https://www.thorlabs.com/catalogpages/805.pdf)

The design parameters for the monochromator are the mirror focal lengths f_i and f_o, mirror rotation angles α_i and α_o, and spacing between input and output slits x_{So}. The manufacturer's literature suggests that there may be some advantages for reducing aberation by designing the system with an asymmetric confirguration where $f_o \neq f_o$ and $\alpha_i \neq \alpha_o$. However we will find it convenient to assume a symmetric design with common focal length f and mirror rotation angle α in some of the discussions below.

EXERCISE Grating Position

(a) Assuming that the input and output slits are both at axial position z = 0, show that the grating center must be located at:

$$z_G = \frac{f_i \sin 2\alpha_i + f_o \sin 2\alpha_o - x_{So}}{\sin 2\alpha_i + \sin 2\alpha_o}.$$

$$x_G = [(f_i - f_o) \sin 2\alpha_o + x_{So}] \frac{\sin 2\alpha_i}{\sin 2\alpha_i + \sin 2\alpha_o}.$$

(b) In the symmetric case $f_i = f_o = f$ and $\alpha_i = \alpha_o = \alpha$. Show that:

$$z_G = f - \frac{x_{So}}{2} \frac{1}{\sin 2\alpha}$$

and

$$x_G = \frac{x_{So}}{2}.$$

(c) Suppose that in the symmetric case, we have the mirror focal length $f = 0.75$ m and the distance between slits is $x_{So} = 0.15$ m. Suppose the grating center is located at $z_G = 0.12$ m. Show that the mirror tilt angle must be $\alpha = 3.419°$.

Modeling constructive interference from light scattering from the diffraction grating

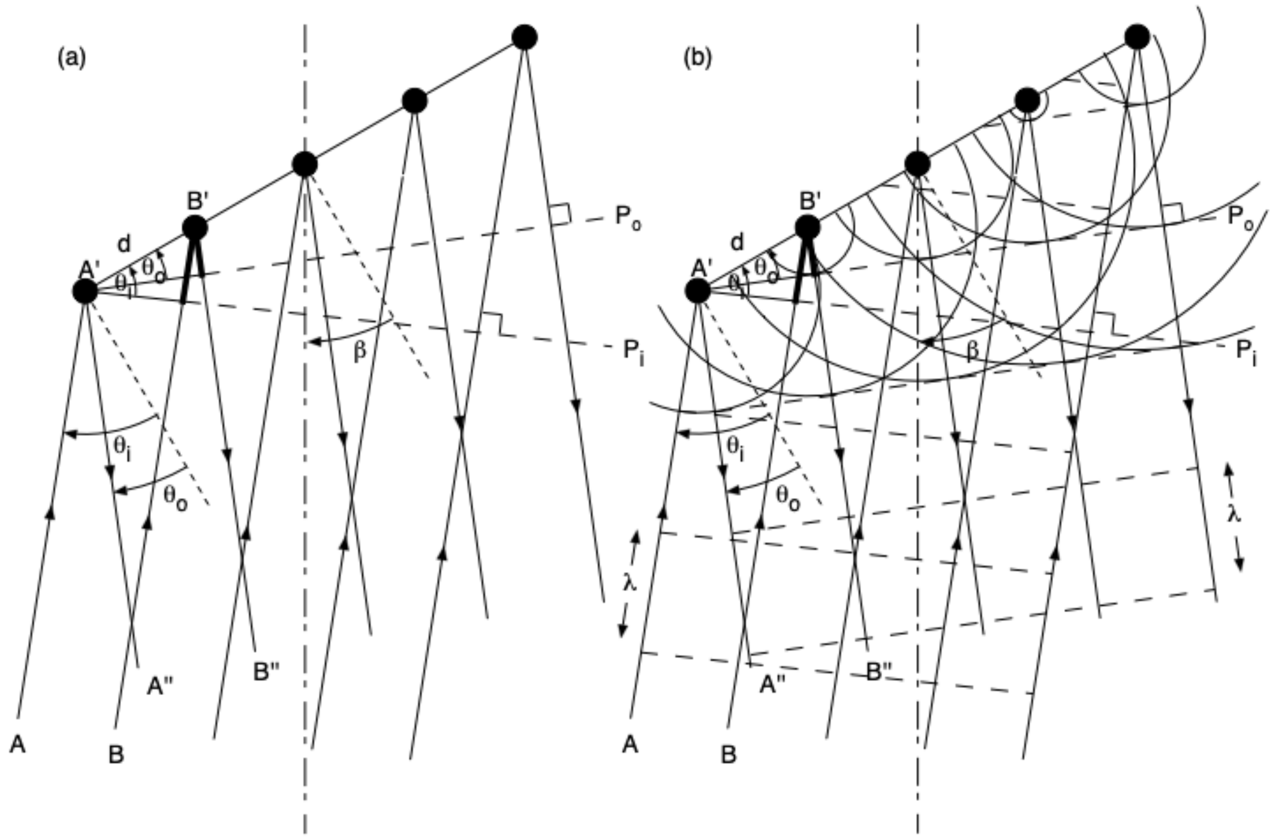


Figure 6 (a) Ray paths are shown for light incident upon and emerging from the grating. The path difference between the second pair of incident and exiting rays and the first pair is shown with heavy line segments. (b) Wavefronts and scattering waves are superimposed on the ray diagram.

Rays to and from the grating

Light expanding from the entrance slit of the monochrometer is collimated by the first mirror, resulting in plane waves that are incident onto the diffraction grating at a fixed angle θ_i to the normal of the grating. The grooves of the grating scatter the incident light into roughly cylindrical waves. When viewed at a distance from an angle θ_o to the normal to the grating and/or brought to a focus by a second mirror, the waves scattered from different grooves will superimpose. The result of the superposition from many grooves is to form a very sharp peak of constructive interference at a particular scattering angle θ_o that depends on the wavelength, the spacing between the grooves, the incident angle θ_i , and the scattered angle θ_o. The following is a simplified way to understand this that provides useful quantitative insight.

Ray path difference

Consider rays scattering from two adjacent grooves. Refering to Figure 6, the path difference between the A-A'-A" and B-B'-B" is

$$\Delta s = d \sin \theta_i + d \sin \theta_o,$$

where d is spacing between the grooves, θ_i is the angle of the incident light, and θ_o is the angle of scattered light when viewed from a particular direction.

Note that the groove spacing d is the recipricol of the grating line density n:

$$d = \frac{1}{n}.$$

For a grating with 1800 lines per mm, the groove spacing is $\frac{1}{1800} = 0.0005555 \text{ mm} = 555.5 \text{ nm}$.

Total scattering amplitude at the exit focus

When the rays are brought to a focus at the exit slit, the amplitudes of the individual scattering fields are summed. Note: for simplicity and since the rays are nearly parallel, we treat the light as a scalar field ψ. Because of the path difference Δs, each amplitude from the next groove is shifted in phase by an amount $\frac{2\pi\Delta s}{\lambda}$. The output amplitude summed by the focusing of the output mirror at the exit slit is:

$$\psi_o = \psi_i(\lambda)\psi_s(\Delta\theta, \lambda)\left(1 + e^{i\frac{2\pi\Delta s}{\lambda}} + e^{i2\frac{2\pi\Delta s}{\lambda}} + \ldots + e^{i(N-1)\frac{2\pi\Delta s}{\lambda}}\right)e^{i\phi}$$

Here $\psi_i(\lambda)$ is the amplitude of the incoming beam across the input reference plane denoted by P_i in Figure 6 above. $\psi_s(\Delta\theta, \lambda)$ is the amplitude of scattering into direction θ_o from each groove of the wavefront coming in with direction θ_i. It can depend on $\Delta\theta = \theta_i - \theta_o = 4\alpha$ (a constant for the apparatus), which is the angle subtended by the incoming and scattered rays. It can also depend, somewhat gradually, on wavelength. Finally, $e^{i\phi}$ represents a constant phase shift of all rays due to the equal path length from output reference plane P_o to the exit slit.

N is the total number of grooves in the grating. For grating density n lines/mm and grating width W,

$$N = nW.$$

For example, if $n = 1800$ lines/mm and $W = 110$ mm, then $N = 198000$, which is quite large!

EXERCISE Total scattering amplitude

Show that:

$$\psi_o = \psi_i(\lambda)\psi_s(\Delta\theta, \lambda)\frac{1 - e^{iN\frac{2\pi\Delta s}{\lambda}}}{1 - e^{i\frac{2\pi\Delta s}{\lambda}}}e^{i\phi}.$$

Hint: the series expression for Ψ is in the form of a geometric series $\text{constant} \times (1 + \xi + \xi^2 + \ldots + \xi^{N-1})$, which can be expressed in closed-form.

EXERCISE Total scattered intensity

Define the input intensity $I_i \equiv |\psi_i|^2$ and the output intensity $I_o \equiv |\psi_o|^2$.

Show that:

$$I_o = I_i|\psi_s(\Delta\theta, \lambda)|^2\left|\frac{\sin\left(\frac{N}{2}\frac{2\pi\Delta s}{\lambda}\right)}{\sin\left(\frac{1}{2}\frac{2\pi\Delta s}{\lambda}\right)}\right|^2.$$

Show that in the limit $\frac{\Delta s}{\lambda} = m$ (an integer) that the peak intensity is

$$I_{o_{\text{peak}}} = |\psi_s(\Delta\theta, \lambda)|^2 N^2.$$

Constructive interference condition

Large intensity maxima occur when the denominator of the above expression vanishes. This happens when

$$\frac{1}{2}\frac{2\pi\Delta s}{\lambda} = m\pi$$

for some integer m. This simplifies to:

$$\frac{\Delta s}{\lambda} = m,$$

which is rearranged to say that the path difference must be an integer number of wavelengths:

$$\Delta s = m\lambda.$$

In terms of angles, this then becomes a condition for constructive interference:

$$d(\sin\theta_i + \sin\theta_o) = m\lambda \text{ where } m = 0, 1, 2, \ldots$$

Re-expressing the constructive intereference condition in terms of

Re-expressing the constructive interference condition in terms of the grating angle β

From trigonometric identities,

$$\sin\theta_i + \sin\theta_o = 2\cos\frac{\theta_i - \theta_o}{2}\sin\frac{\theta_i + \theta_o}{2}.$$

Using the relations

$$\theta_i - \theta_o = 2(\alpha_i + \alpha_o)$$

and

$$\theta_i + \theta_o = 2\beta + 2(\alpha_i - \alpha_o),$$

we have

$$\Delta s = d\cos(\alpha_i + \alpha_o)\sin[\beta + (\alpha_i - \alpha_o)].$$

Then condition for diffraction maxima $\Delta s = m\lambda$ becomes

$$2d\cos(\alpha_i + \alpha_o)\sin[\beta + (\alpha_i - \alpha_o)] = m\lambda.$$

Symmetric case

For the symmetric case $\alpha_i = \alpha_0 = \alpha$,

$$\Delta s = 2d\cos 2\alpha\sin\beta.$$

The condition for diffraction maxima is given by

$$2d\cos 2\alpha\sin\beta = m\lambda.$$

To obtain a maximum, we must rotate the grating an angle β such that

$$\sin\beta = \frac{m\lambda}{2d\cos 2\alpha}.$$

Finally we re-arrange the above constructive interference condition and use the fact that $d = \frac{1}{n}$ to show that wavelength of light passed through to the exit slit of the monochromator is related to the grating angle β by:

$$\lambda = \frac{1}{m}\frac{2}{n}\cos 2\alpha\sin\beta.$$

EXERCISE Grating angle for passage of the 546.1nm mercury line through the exit slit

Show that for the mercury line $\lambda = 546.1$ nm, a grating density $n = 1/d = 1800$ lines/mm, and a mirror tilt angle $\alpha = 3.419°$, the grating must be rotated so that its normal is at an angle $\beta = 29.67°$ from the instrument axis to obtain maximum transmission for order m=1.

Calibration

(Assume a symmetric optical configuration in the following discussion.)

Suppose we find that at a specified wavelength λ_{cal} such as the mercury line 546.1 nm, the instrument has positioned its grating at an angle β_{cal} to obtain a peak in the output intensity at order m. So we have

$$\lambda_{\text{cal}} = \frac{1}{m}\frac{2}{n}\cos 2\alpha \sin \beta_{\text{cal}}.$$

Thus

$$\frac{1}{m}\frac{2}{n}\cos 2\alpha = \frac{\lambda_{\text{cal}}}{\sin \beta_{\text{cal}}}.$$

The path difference

$$\Delta s = \frac{2}{n}\cos 2\alpha \sin \beta = m\frac{\lambda_{\text{cal}}}{\sin \beta_{\text{cal}}}\sin \beta.$$

Then we can re-write the intensity function

$$I_o(\beta, \lambda) = I_i(\lambda)|\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(\frac{N}{2}\frac{2\pi\Delta s}{\lambda}\right)}{\sin\left(\frac{1}{2}\frac{2\pi\Delta s}{\lambda}\right)} \right|^2 = I_i(\lambda)|\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(Nm\pi\frac{\sin\beta}{\sin\beta_{\text{cal}}}\frac{\lambda_{\text{cal}}}{\lambda}\right)}{\sin\left(m\pi\frac{\sin\beta}{\sin\beta_{\text{cal}}}\frac{\lambda_{\text{cal}}}{\lambda}\right)} \right|^2.$$

Importantly, we see that the output intensity is a function of both the grating angle β and incoming wavelength λ:

Light will be maximally transmitted (with a very sharp maximum) whenever there is intensity in the incoming spectrum ($I_i(\lambda) \neq 0$) and $\lambda = \tilde{\lambda}$ where $\tilde{\lambda}$ satisfies

$$\frac{\sin\beta}{\sin\beta_{\text{cal}}}\frac{\lambda_{\text{cal}}}{\tilde{\lambda}} = 1.$$

In other words, in plotting the output intensity as $\sin\beta$ is scanned, we can label our horizontal axis with $\tilde{\lambda}$ instead of $\sin\beta$ where:

$$\tilde{\lambda} = \frac{\lambda_{\text{cal}}}{\sin\beta_{\text{cal}}}\sin\beta.$$

We employ this as a change of variable to write:

$$I_o(\tilde{\lambda}, \lambda) = I_i(\lambda)|\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(Nm\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(m\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2.$$

NOTE: it will be useful to recall that we can also express $\tilde{\lambda}$ in terms of the instrument parameters:

$$\tilde{\lambda} = \frac{1}{m}\frac{2}{n}\cos 2\alpha \sin \beta.$$

Instrument function and the actual measured spectrum

Supppose we have a spread-out spectrum of input intensity I_i where, for a incremental range of wavelength $d\lambda$,

$$dI_i = S_i(\lambda)d\lambda,$$

where S_i is the *spectral density function* of the input light. The total intensity of the input light is then

$$I_i = \int_0^\infty S_i(\lambda)d\lambda.$$

The output intensity can be assumed to be the incoherent sum (integral) of the transmitted intensities:

$$I_{\text{o\_total}}(\tilde{\lambda}) = \int_0^\infty S_i(\lambda)|\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(N\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2 d\lambda.$$

We define the *instrument function* $F_{\text{inst}}(\lambda, \tilde{\lambda})$ of the spectrometer to be

$$F_{\text{inst}}(\lambda, \tilde{\lambda}) \equiv |\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(Nm\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(m\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2.$$

$$I_{\text{o\_total}}(\tilde{\lambda}) = \int_0^\infty S_i(\lambda)F_{\text{inst}}(\lambda, \tilde{\lambda})d\lambda.$$

Ideally, we'd like the output intensity from the scanned monochomator to be a close replica of the input:

$$I_{\text{o\_total}}(\tilde{\lambda}) = \text{constant } \times S_i(\tilde{\lambda}).$$

This would occur if

$$F_{\text{inst}}(\lambda, \tilde{\lambda}) = \text{constant } \times \delta(\lambda - \tilde{\lambda}).$$

where $\delta(\lambda - \tilde{\lambda})$ is the Dirac delta function.

In fact, over spectral ranges of interest

$$|\psi_s(\Delta\theta, \lambda)|^2 \approx \text{constant}$$

and

$$\left| \frac{\sin\left(Nm\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(m\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2 \approx \frac{N\tilde{\lambda}}{m}\delta(\lambda - \tilde{\lambda}).$$

This is based on the estimate that the instrument function peak area ≈ 1/2 x peak height x peak base ≈ $\frac{1}{2} \times N^2 \times 2\frac{\tilde{\lambda}}{Nm} = \frac{N\tilde{\lambda}}{m}$, where the peak base is estimated as twice the resolution estimate $\Delta\lambda$ discussed below in the section "Resolution and Resolving Power". This area estimate is tested in the code below by comparing it to a numerical integration of the peak area.

Since the actual instrument function is not infinitely sharp like a delta-function, it acts to slightly smear out the spectrum. This is a form of *convolution*. There are approaches to try to *de-convolve* the effect of instrument function (plus effects of slit width – see section on "Dispersion" below) but we will not explore these here.

Computing the instrument function

The following computes values of

$$F_{\text{inst}}(\lambda, \tilde{\lambda}) \equiv |\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(Nm\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(m\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2$$

for a 1000-element array of arguments λ on either side of the specific value

$$\tilde{\lambda} = \lambda_{\text{cal}} = 546.0735 \text{ nm}$$

assuming for simplicity that

$$|\psi_s(\Delta\theta, \lambda)|^2 = 1.$$

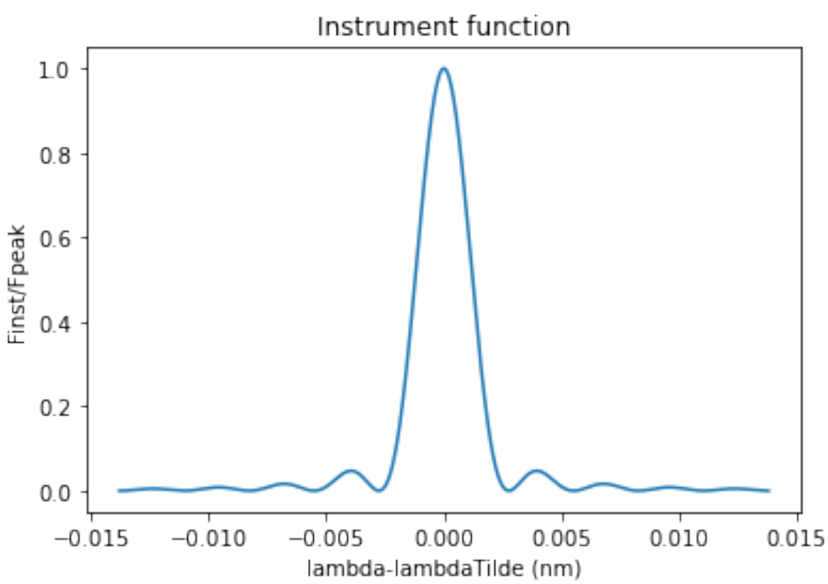
In [1]:

```
%matplotlib inline
'''
This code computes of diffraction grating profile versus the sin of 
R Tagg 26 Nov 2021
'''
```

```python
import math
import numpy as np
import matplotlib.pyplot as plt

lambdaCal = 546.0735 # mercury line

# Light source characteristics
lambdaTilde = lambdaCal # look at the case where the input light is

#Diffraction grating parameters
alphaDegrees = 3.419 # rotation angle in degrees of input and output
n = 1800 # grating lines per mm
W = 110 # mm horizontal size of grating
m = 1 # first order diffraction

alpha = alphaDegrees/180*math.pi
N = n*W

psi_s_squared = 1 # simple constant unity depedence of scattering am

sinBetaTilde = 0.5*m*n*lambdaTilde*1e-6/math.cos(2*alpha) # must lam
Fpeak = psi_s_squared*N**2
halfWidth = lambdaTilde/(N*m)

print('m = ',m)
print('lambdaTilde = {0:.4f} nm'.format(lambdaTilde))
print('sinBetaTilde = {0:.4f}'.format(sinBetaTilde))
print('betaTilde = {0:.2f} degrees'.format(math.asin(sinBetaTilde)*1
print('Peak value of instrument function Fpeak = {0:.3e}'.format(Fpe
print('Half width to first zero = {0:.5f} nm'.format(halfWidth))

Nstep = 1000
lambdaTildeRange = 5*halfWidth
lambdaTildeStep = 2*lambdaTildeRange/Nstep
lambdaArray = np.linspace(lambdaTilde-lambdaTildeRange,lambdaTilde+l
#lambdaArray = np.linspace(lambdaTilde-0.02,lambdaTilde+0.02,1001)
#lambdaArray = np.linspace(lambdaTilde-0.02/m,lambdaTilde+0.02/m,100

arg = m*np.pi*lambdaTilde/lambdaArray
numerator = np.sin(N*arg)
denominator = np.sin(arg)
# Avoid a zero-divided-by-zero singularity at the peak
numerator[500]=math.sqrt(Fpeak)
denominator[500]=1.

# Now compute the instrument function
Finst = psi_s_squared*np.square(np.divide(numerator,denominator))

# Numerically integrate the area under the peak by summing values of
# between the zeros to the left and right of the peak
NhalfWidthL = int(Nstep/2-halfWidth/lambdaTildeStep)
NhalfWidthR = int(Nstep/2+halfWidth/lambdaTildeStep)
```

```
peakArea = np.sum(Finst[NhalfWidthL:NhalfWidthR])*lambdaTildeStep
print('NhalfWidth L R = ',NhalfWidthL,NhalfWidthR,'Nstep = ',Nstep)
print('Peak area      = {0:.3e}'.format(peakArea))
print('Est peak area = {0:.3e}'.format(N*lambdaTilde/m))

plt.plot(lambdaArray-lambdaTilde,Finst/Fpeak)
plt.xlabel('lambda-lambdaTilde (nm)')
plt.ylabel('Finst/Fpeak')
plt.title('Instrument function')

plt.show()
```

```
m =  1
lambdaTilde = 546.0735 nm
sinBetaTilde = 0.4950
betaTilde = 29.67 degrees
Peak value of instrument function Fpeak = 3.920e+10
Half width to first zero = 0.00276 nm
NhalfWidth L R =  400 600 Nstep =  1000
Peak area      = 9.762e+07
Est peak area = 1.081e+08
```



Resolution and resolving power

According to the Rayleigh criterion, two sharp lines at wavelengths λ and λ' in the input spectral density $S(\lambda)$ will just barely be resolved if the second line falls at the first minimum (actually first zero) of the instrument response function centered on the first line.

In other words, to establish the instrumental resolution for the grating, we must find what value of $\lambda' = \lambda + \Delta\lambda$ produces the first zero next to the m'th order peak at $\lambda = \tilde{\lambda}$ of

$$F_{\text{inst}}(\lambda, \tilde{\lambda}) \equiv |\psi_s(\Delta\theta, \lambda)|^2 \left| \frac{\sin\left(Nm\pi\frac{\tilde{\lambda}}{\lambda}\right)}{\sin\left(m\pi\frac{\tilde{\lambda}}{\lambda}\right)} \right|^2$$

This will occur when

$$\sin\left(Nm\pi\frac{\tilde{\lambda}}{\tilde{\lambda}+\Delta\lambda}\right) = 0$$

Assuming $\Delta\lambda$ is small relative to $\tilde{\lambda}$ (easily justified when looking at the plot of the response function shown above),

$$\begin{aligned}
\sin\left(Nm\pi\frac{\tilde{\lambda}}{\tilde{\lambda}+\Delta\lambda}\right) &\approx \sin\left[Nm\pi\frac{\tilde{\lambda}}{\tilde{\lambda}}\left(1+\frac{\Delta\lambda}{\tilde{\lambda}}\right)\right] \\
&= \sin(Nm\pi + Nm\pi\frac{\Delta\lambda}{\tilde{\lambda}}) \\
&= \sin(Nm\pi)\cos\left(Nm\pi\frac{\Delta\lambda}{\tilde{\lambda}}\right) + \cos(Nm\pi)\sin\left(Nm\pi\frac{\Delta\lambda}{\tilde{\lambda}}\right). \\
&= (-1)^{Nm}\sin\left(Nm\pi\frac{\Delta\lambda}{\tilde{\lambda}}\right).
\end{aligned}$$

Remembering that we assumed $\lambda = \tilde{\lambda}$, this will have its first zero when

$$Nm\pi\frac{\Delta\lambda}{\lambda} = \pi.$$

Re-arranging,

$$\Delta\lambda = \frac{1}{Nm}\lambda.$$

This may be taken as the half-width of the instrument function and determines the limiting *resolution* of the spectrometer.

The *resolving power* is defined to be

$$R \equiv \frac{\lambda}{\Delta\lambda} = Nm.$$

Example

For first order $m = 1$, $n = 1800$ lines/mm, grating width W = 110 mm, and $\lambda = 546.1$ nm, we have

$$N = nW = 198000 \text{ lines},$$

$$R = 1 \times 198000 = 198000, \text{ and}$$

$$\Delta\lambda_{\text{grating}} = 0.00276 \text{ nm}$$

This compares very well to the location of the first zero in the plot of the instrument function shown above.

Dispersion

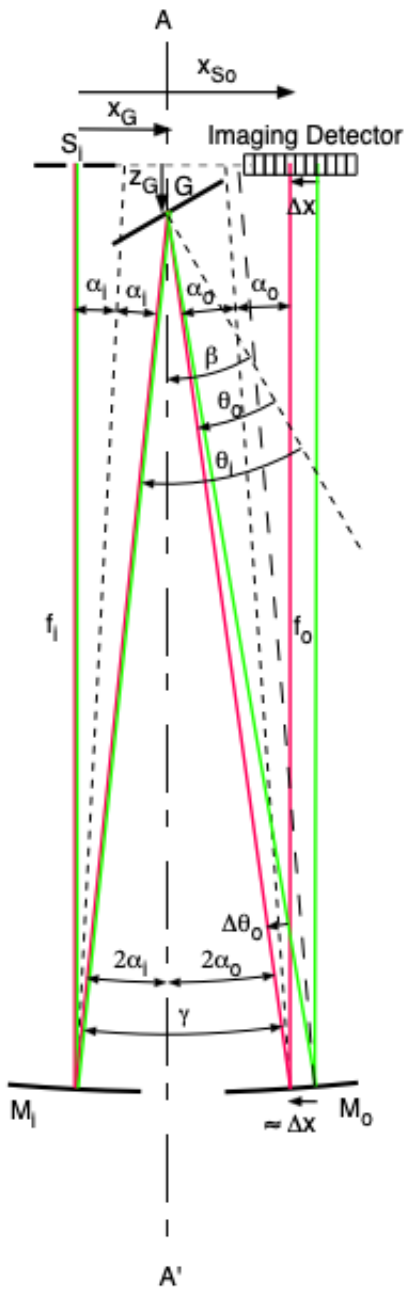


Figure 7 Tracing the paths of rays of different wavelengths (exagerated as red and green) shows the geometry of linear displacement of the position of constructive interference across the exit aperture.

THIS SECTION NEEDS CHECKING, INCLUDING POSSIBLE CONFIRMATION IN

REFERENCES.(The dispersion formulas and quoted values in the Horiba documentation are comparable but simpler in formation.)

An alternate design of the monochomator system is to place an imaging detector at the exit aperture. As seen in the Figure 7, different spectral lines will constructively interfere at different positions across the imaging detector.

Imagine a mixture of two wavelengths λ and $\lambda - \Delta\lambda$ emerging from the source, shown above as red and green lines. They have the same incident angles θ_i but will be diffracted into different output angles θ_o and $\theta_0 - \Delta\theta_o$.

Returning to the original condition for constructive interference, rearranged slightly and using $d = \frac{1}{n}$:

$$(\sin\theta_i + \sin\theta_o) = mn\lambda,$$

How does the above expression change with a variation in λ and consequent variation θ_o? (Remember that θ_i is the same for all wavelengths.) Taking the first-order variation (using derivatives) of both sides of the above equation, we can write

$$\cos\theta_o\Delta\theta_0 = mn\Delta\lambda.$$

The displacement Δx of the lines at the imaging detector is very nearly equal to the displacement of the lines where they strike the output mirror, because the exit principal rays all fall very close to being parallel to each other and to the instrument axis.

By examining the geometry in Figure 7, we find to a good approximation:

$$\Delta x = -\frac{f_o - z_G}{\cos 2\alpha_o}\Delta\theta_o$$

The negative sign indicates that increasing wavelength (green to red in the diagram) leads to shift to the left, which is negative in the selected coordinate system.

From above relation of variation of θ_o with variation of λ:

$$\Delta x = -mn\frac{f_o - z_G}{\cos 2\alpha_o \cos\theta_0}\Delta\lambda.$$

Earlier, we derived a relation for the grating position z_G such that (for the symmetric case where $\alpha_i = \alpha_o = \alpha$,

$$z_G = f - \frac{x_{So}}{2}\frac{1}{\sin 2\alpha}$$

where x_{So} is the separation between the entrance slit and the center of the exit aperture. Thus

$$\Delta x = -mn\frac{x_{So}}{2}\frac{1}{\sin 2\alpha \cos 2\alpha \cos\theta_0}\Delta\lambda.$$

Finally, using trigonometric identities and the fact that $\theta_0 = \beta - 2\alpha$,

$$\Delta x = -mn\frac{x_{So}}{\sin 4\alpha \cos(\beta - 2\alpha)}\Delta\lambda.$$

The ratio $\frac{\Delta\lambda}{|\Delta x|}$ of wavelength change to spatial shift is called the *dispersion*. We see that

$$\frac{\Delta\lambda}{|\Delta x|} = \frac{\sin 4\alpha \cos(\beta - 2\alpha)}{mnx_{So}}.$$

For first order m=1, grating density n = 1800 lines/mm, separation x_{So} $= 0.15$ m, α = 3.419°,and $\beta = 29.67°$, we get

$$\frac{\Delta\lambda}{|\Delta x|} = .000000807 \text{ mm/mm} = 0.807 \text{ nm/mm}.$$

Instead of an imaging detector, consider what wavelength range is passed through a slit of a given width. A minimum slit width w of 3 μm = 0.003 mm would then pass a band of wavelengths

$$\Delta\lambda_{\text{slit}} = 0.807 \text{ nm/mm} \times 0.003 \text{ mm} \;= 0.00242 \text{ nm},$$

which is of a magnitude similar to the resolution limit imposed by the grating.

Free Spectral Range (Bandwidth)

Now we want to know what wavelength shift has a peak at order m that overlaps with the peak of the original wavelength at next order m+1.

Suppose the condition for a maximum is satisfied at wavelength λ for order $m + 1$:

$$\Delta s = (m + 1)\lambda.$$

We want to know what wavelength shift $\Delta\lambda_{\mathrm{FSR}}$ satisfies the condition for maximum at previous order m

$$\Delta s = m(\lambda + \Delta\lambda_{\mathrm{FSR}}).$$

Equating right-hand sides

$$(m + 1)\lambda = m(\lambda + \Delta\lambda_{\mathrm{FSR}}).$$

Solving for the shift:

$$\Delta\lambda_{\mathrm{FSR}} = \frac{\lambda}{m}.$$

So for $m = 1$,

$$\Delta\lambda_{\mathrm{FSR}} = \lambda.$$

In other words, a peak at order 1 for wavelength 2λ will overlap with a peak at order 2 for wavelength λ.

References

https://www.horiba.com/gbr/diffraction-gratings-ruled-holographic/#c8330 (https://www.horiba.com/gbr/diffraction-gratings-ruled-holographic/#c8330)