1. Reflection Gratings

The grating equation can be written for a reflection grating:

\[ d(\sin \theta_{\text{inc}} \pm \sin \theta_{\text{diff}}) = m\lambda \]  

(1)

where \( d \) is the grating constant, defined as \( d \equiv 1/N \), and \( N \equiv \) number of rulings per mm. The + holds when the diffracted beam is on the same side with the incident beam with respect to the normal to the grating’s surface. The – sign is when incident and diffracted beams are on opposite sides with respect to the normal. For simplicity, we are assuming that the incident beam is a plane wave, that is its angular spread is near zero.

Differentiating, we obtain, with \( \theta_{\text{inc}} \) constant:

\[ d(\pm \cos \theta_{\text{diff}})d\theta_{\text{diff}} = m d\lambda \]

This equation gives us the angular resolution \( d\theta_{\text{diff}} / d\lambda \) of the optical grating.

Now, we are ready to study the grating based monochromators.

Except of the case where intense laser beam is used, we have typically small optical signal directed to each angular direction due to the spectral analysis caused by the grating. Therefore, we are forced to use some concentrator (lens or mirror having a focal length \( f \)) in order to increase the signal to noise ratio. We need then to understand the effect of the chosen value of \( f \) on the spectrometer (monochromator) performance.

To simplify the above issue, we consider the quite simple case occurs when we have the so called Littrow arrangement, where we assume that \( \theta_{\text{inc}} = \theta_{\text{diff}} \).

It is left as an exercise to show that the linear resolution, \( d\lambda/dx \) is:

\[ d(2 \cos \theta_{\text{diff}}) f d\theta_{\text{diff}} = m d\lambda f \]  
or:

\[ d\lambda/dx = d(2 \cos \theta_{\text{diff}})/(m f) \]  and \( \delta x/\delta \lambda = m f / (d 2 \cos \theta_{\text{diff}}) = \]

\[ m f N / (2 \cos \theta_{\text{diff}}) \equiv R_d \]  

(1)

where: \( R_d \) is reciprocal linear dispersion.
Thus, for $\Delta x=1 \text{mm}$, we have $\Delta \lambda = 1 \times 1000 \text{ mm} \times 3600 \text{ grooves/mm}$

\[
/(2 \times 0.2) \text{ if } \cos \theta_{\text{diff}} = 0.2, N=3600 \text{ grooves/mm, and } f=1000 \text{mm, and } m=1.
\]

Thus, $\delta \lambda / \delta x = 0.4 \text{ mm} / (1000 \text{ mm} \times 3600) \approx 10^{-7} \times 10^6 \text{ nm/mm} = 0.1 \text{ Angstroms/mm}$

Now, if the linear resolution is about $25 \mu \text{m}$ (dictated by the segmentation of a linear CCD array), we expect a resolution of the order:

$$\Delta \lambda_{\text{lim}} \approx 0.1 \text{ Angstrom} \times 25 \mu \text{m} / 1000 \mu \text{m} \approx 2.5 \times 10^{-3} \text{ nm. \ (2)}$$

This could be one approach to the limiting resolution, but there may be another limit coming from the resolution of optical grating:

$$\lambda / \Delta \lambda_{\text{lim}} \approx \text{number of grooves} = 3600 \times 25 = 90000 \text{ for a typical grating.}$$

Thus, for $\lambda = 450 \text{ nm}$, we get $\Delta \lambda_{\text{lim}} \approx 0.6 \times 10^{-3} \text{ nm}.$

Thus, we see that this limiting resolution arising from Rayleigh’s criterion is not inconsistent to the relationship (2) which gives the expected accuracy of the spectroscopic system considered. However, there may be other factors which will cause worsening of the resolution predicted from (2), such as small signal to noise ratio due to the weakness of the spectral line, optical aberrations of the mirrors or lenses used, finite size of the slit used in the entrance of the monochromators etc.

The actual resolution may be obtained experimentally by measuring many times an almost ideal monochromatic line and then obtaining the statistical error.

**Another point of view on the accuracy of a grating Monochromator**

We go now to see the effect of various aspects which limit the accuracy of wavelength determination. These are enumerated as follows:

a) Natural linewidth, b) Imaging error due to the lenses or mirrors which are part of the monochromators system, c) slit size effects (in either input or output of the spectrometer)
The effect of finite size of spherical mirrors may be estimated by forming the ratio \( f/d \), where \( f \) the focal length and \( d \) the effective diameter of the mirror. This ratio is frequently called in optics “the f/number or f/# or f/No”. The larger the f/No, the smaller the contribution to the overall wavelength error. An optical instrument with large f/No has more accurate imaging capabilities than a small f/No instrument. That is why we frequently have long telescopes.

The resolution of a spectroscopic instrument is limited by the FWHM of Instrumental Profile:

More specifically,

\[
\text{FWHM} = \left( d\lambda^2_{\text{slits}} + d\lambda^2_{\text{resolution}} + d\lambda^2_{\text{line}} \right)^{1/2}
\]

Where

\( d\lambda^2_{\text{slits}} \rightarrow \text{bandpass determined by finite spectrometer slit widths and the linear dispersion of the grating.} \)

\( d\lambda^2_{\text{resolution}} \rightarrow \text{the limiting resolution of the spectrometer which incorporates system aberrations, diffraction effect of our system and the laser line width of our system*.} \)
and, 
\[ d\lambda^2 \] (line) \rightarrow \text{natural line width of the spectral line being probed.}

This FWHM is our limit of resolution for the spectrometer.

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* In case the spectrometric system studies some laser line

**How do you calculate the FWHM of the Instrumental Profile?**

- The instrumental profile FWHM is something you can measure experimentally.
- \[ d\lambda^2 \] (line): By only observing a laser line with the spectrometer we can eliminate the broadening of the FWHM due to the natural line width of a spectral line **.
- \[ d\lambda^2 \] (slits): The bandpass due to the slit width and the grating of the spectrometer can be calculated.
- \[ d\lambda^2 \] (resolution): The limiting resolution of the spectrometer is something that you solve for knowing the other variables of the FWHM equation.

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** see the following graph to understand the thermal broadening of a line and at the same time the peaks corresponding to longitudinal, laser modes within this line width:
How to Calculate Bandpass (BP)
We can apply, for this purpose, equation (1), above.

Then,

\[ BP = W \times R_d \]

Where \( W \) is the slit width of the entrance or exit slit
(which ever is larger)

Therefore, due to Equation (1),

\[ BP = W m f N / (2 \cos \theta_{\text{diff}}) \] \hspace{1cm} (2)

Thus, if we wish to achieve a specific band pass (BP), we can select the appropriate
value of entrance slit \( W \), given the other values of \( m, f, N, \) and \( \cos \theta_{\text{diff}} \).

**Further discussion about the slit size \( W \):**
We may stress that we have two slits, the entrance slit and the exit slit of a
monochromators. Normally, the two slits should be conjugate, that is the exit slit
should be the image of the entrance slit. However, this need not be always the case.
Thus, we propose that the value \( W \) inserted in formula (2) above, is the smallest of the
two slits in the case that they are conjugage. If they are not conjugate, the \( W \) value
should be the part of the smaller slit width imaged on the larger slit.

Figure 3.

![Graph showing FWHM of 600 and 1200 gratings Vs Entrance Slit Width](image)
We present in figure 3, a bibliographical case in which the bandwidth is computed with respect to the entrance slitwidth. In the case we study in our lab exercise, where the number of grooves per millimeter is 3600, we estimate that we may expect up to 3 times better bandpass than the one corresponding to the case 1200 groves per mm, all the other factors being equal. To achieve this better result could be achieved, with a CCD based monochromators we must be careful that each CCD pixel is equivalent to an effective output slit size. We, therefore, must always take into account the pixel size.

**Signal to Noise Ratio**

We must be aware, and worry!!, that frequently the CCD area is very small as typically, the CCD has a 20 µm x 100 µm area or even smaller. This means that the overall signal must be compared to the optical noise, which is independent from the optical signal to be measured. This is described by the so called “signal to noise ratio, or simply S/N”. This can add another uncertainty in the wavelength to be measured, and therefore we have the expression:

\[
\text{FWHM} = \left( d\lambda^2_{\text{slits}} + d\lambda^2_{\text{resolution}} + d\lambda^2_{\text{line}} + d\lambda^2_{\text{S/N}} \right)^{1/2}
\]

The latter expression is appropriate when we deal with weak line sources or line sources in the presence of appreciable optical background.

**Application of Monochromator Theory in design of 1 meter spectrograph**

Having discussed in some detail the monochromators design, we focus now in specific implementation to achieve a reasonable approach to the theoretical limit. We have available one concave aluminum mirror of reflectivity near 93%, focal length 914 mm, and diameter 152 mm. The situation is seen in Figure 2.
In the plane xz, the view can be described as seen in Figure:

Figure. A: input slit, B: Mirror, C: Spectrum image
Factors influencing grating efficiency

The efficiency depends on:

- $m$ (diffraction order)
- angles of incidence and diffraction
- $\lambda/d$
- polarization
  - P-Plane $\Rightarrow$ no anomalies
  - S-Plane $\Rightarrow$ anomalies

P-plane is TE polarized light
S-plane is TM polarized light
The above graph shows that the efficiency, that is, the percentage of intensity dispersed at a certain angle, depends on the wavelength.

**Exercise:**
Consider the grating with the following parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Focal length (mm)</td>
<td>998.8</td>
</tr>
<tr>
<td>no. grooves/mm</td>
<td>2400</td>
</tr>
<tr>
<td>blaze λ</td>
<td>580 nm</td>
</tr>
<tr>
<td>blaze angle</td>
<td>44.2°</td>
</tr>
<tr>
<td>ruled dimensions (Hx W)</td>
<td>30mm x 80mm</td>
</tr>
</tbody>
</table>

**(α)** Determine the resolution of this grating. *(β)* A monochromators is constructed using this grating, with input and output slit of 50µm. Determine at the exit of the monochromators the plate factor, that is, the \( \frac{\Delta \lambda}{\delta x} \), where \( \delta x \) is the width of slit. *(γ)* Determine the wavelength resolution of the monochromators for the above slit sizes. Examine, the case with slit sizes 20 µm, and 10 µm

**Solution:**

**(α)** It is \( \lambda / \Delta \lambda = N \). Grooves x m = 192,000. Thus, for \( \lambda = 580 \text{ nm} \), we have \( \Delta \lambda = 3 \times 10^{-3} \text{ nm} \)

**(β)**

**Plate factor:**

\[
\frac{d\lambda}{dx} = \frac{d( 2 \cos \theta_{\text{diff}})}{( mf)} = \frac{2 \cos \theta_{\text{diff}}}{(N \text{ mf})} \approx 2 / (2400 \text{mm}^{-1} \times 1000 \text{mm}) = 2 \text{ nm/} (2400 \times 1000 \times 10^{-6} \text{ mm}) = 0.83 \text{ nm/mm}
\]

**(γ)** The best we can expect, for the accuracy, is \( \Delta \lambda_{\text{slit}} = (0.83 \text{ nm/mm}) \times 50 \mu \text{m} = \)
=0.04 nm. For the case of 10 µm, we obtain, Δλ≈0.008 nm. Be careful, however, for the diffraction effects in the slits, as we have that the slit size is 20 times less than the wavelength.

2. Transmission gratings
In this case, we have the simplified expression,

d sin θₘᵢ=ₘₗᵢ

where i is the index of the wavelength under consideration, assuming that the light beam is perpendicular to the grating surface. In reality, we have a deviation from the fully perpendicular case, and therefore, the exact expression is:

± d sinθᵢᵣ+ d sin θᵢᵢ=ₘₗᵢ

with θᵢᵣ very near zero, and thus sinθᵢᵣ ≈ θᵢᵣ. For symmetrical orders, we have:

d θᵢᵣ − (-d θᵢᵣ) + d sin θᵢᵢ - d sin θᵢᵣ ≈ 2 m λᵢ

or

θᵢᵣ + sin θᵢᵢ = m λᵢ/d  (1)

etc.

and

θᵢᵣ= m λᵢ/d - |sin θᵢᵢ|

This gives us an estimate of θᵢᵣ. By changing in very small steps the orientation of the grating, we may reduce very much the absolute value of θᵢᵣ until it is zero within errors. In this case, the angles θᵢᵢ and θᵢᵣ should be equal, and in this way, we may get rid of one important systematic error. This systematic error may lead to wavelength errors of the order of 5-20 nm!! If we don't pay enough attention to assure a perpendicular to the grating beam.

On the other hand, by using a calibrated spectral line λ_calib, we may use equation (1) to determine the value of θᵢᵣ, which we may use to determine unknown spectral lines with respect to the line λ_calib. Thus, we may use as calibration line the one at 586 nm of the Hg spectrum, and therefore determine the value of wavelength of the line at 588 nm with respect the calibration line. If we work with the 4th order, then the experimental deviation from the expected 2 nm difference is normally around 1 nm, which indicates the expected statistical error in determining the peak corresponding to the 588 nm yellow line. Remember, that this error does not include the systematic error discussed above, which is due to the non perpendicular beam and perhaps to other reasons.

Vibrational spectroscopy. Atom spectroscopy:
Grating theory files:
   1. GratingTheory-joa4_5_026

ROWLAND.pdf

4. Optical grating fabrication:
   4.2 GratingFabricationInterferenceLaserBeams
5. NIST:
   http://physics.ship.edu/~mrc/pfs/308/atomic_spectroscopy/Pubs/AtSpec/index.html
      AstrophysicsSweden-spectroscopy2006.pdf

   SpectroscopyNotesStructureB1
   SpectroscopyNotesStructureB2.pdf
   AstrophysicsSweden-spectroscopy2006.pdf