Physics 308 Laboratory
Experiment F: Grating Spectrometer

Motivation:

Diffraction grating spectrometers are the single most widely used spectroscopic instrument. They are incorporated into many devices used by analytical chemists. They are found in many solid state physics labs, most plasma physics labs, and nearly every atomic physics lab. They are widely used on major astronomical telescopes. The primary purpose of this lab is to gain both practical experience with a grating spectrometer and a thorough understanding of key grating spectrometer components.

References: Fundamentals of Physics, Halliday and Resnick, Ch. 41. Fundamentals Optics: Jenkins and White, Ch. 17.

Theory:

The theory of the diffraction grating spectrometer is built on the concept of a multiple slit Fraunhofer diffraction pattern. We studied multiple slit diffraction with two and three slits. The theory for a thousand or more slits \((N \geq 1000)\) is much the same. The principal maxima become very, very large and extremely narrow. We saw this start to happen when we compared the two and three slit pattern. The equation describing the multiple slit pattern is

\[
I_T = \frac{A_0^2 W^2}{r^2} \text{sinc}^2(\pi W \sin \theta/\lambda) \frac{\sin^2(\pi N D \sin \theta/\lambda)}{\sin^2(\pi D \sin \theta/\lambda)}. \tag{1}
\]

The first term is an overall scale factor and not important, the second term is an envelope function determined by the width \(W\) of a single slit. The third term which involves a ratio of sine functions is the most important. The principal maxima occur when the \(\sin^2\) in the denominator vanishes. Principal maxima occur for

\[
\pi D \sin \theta/\lambda = m\pi \tag{2}
\]

or

\[
D \sin \theta = m\lambda. \tag{3}
\]

This is the grating equation for illumination at normal incidence. The integer \(m\) is the order. It is important to see that for angles defined by Eqn. 3, Huygens wavelets from all slits interfere constructively.
D for principle maximum, path difference = \( m \lambda \).

For non-normal illumination we get a more general equation which is usually called “The Grating Equation”,

\[
D(\sin \alpha + \sin \beta) = m\lambda .
\] (4)

The figure below illustrates the essential idea of Eqn. 4: A principal maximum occurs whenever the path difference for light from adjacent slits is an integral number of wavelengths.
Suppose collimated light of two wavelengths is incident on the multiple slits (or diffraction grating). The incidence angle $\alpha$ is the same for both wavelengths, but the diffracted angle $\beta$ is different for different wavelengths. Thus we say the grating disperses the light. Equation 4 gives us the relation between $\beta$ and $\lambda$.

$$D \sin \alpha = m \lambda$$

Figure 3: Positions and intensities of the principal maxima from a grating, where light containing two wavelengths is incident at an angle $\alpha$ and diffracted at various angles $\beta$.

If the grating is illuminated with collimated light of many wavelengths, we might be concerned about different wavelengths interfering with each other. This does not happen. Light of each wavelength interferes only with itself to produce its own diffraction pattern. If five wavelengths are present in the incident light, then five superimposed diffraction patterns are produced. The $m = 0$ primary maxima are all exactly on top of each other or undispersed. All other primary maxima are dispersed, they occur at different angles for different wavelengths.

Modern instruments usually have reflection rather than transmission gratings shown above. We can imagine little mirrors located behind each slit and we simply fold the drawing at the plane of the slits. The little slits with mirrors are called grating grooves or grating lines. The grating grooves are generally too small to see without a microscope. Often grating are described as having some number (300, 600, 1200 or 1800) grooves/mm. The inverse of
the number is $D$ in mm.

A diffraction grating by itself is not a grating spectrometer. A grating spectrometer has optical components to collimate the light incident of the grating and to refocus the dispersed light in the exit plane. The collimation is accomplished with a small entrance aperture, usually a slit parallel to the grating grooves, and a lens or concave mirror one focal length away. The collimated light is, of course, never perfectly collimated. If the entrance slit has a width “$a$”, then the collimated light includes at least a range of angles $a/F$. If we improve the collimation by reducing “$a$” then we eventually run into the diffraction limit. The light transmitted by the lens will include at least a range of angles $\lambda/A$ where $A$ is the width of the lens. Modern grating spectrometers use collimating mirrors tipped slightly off axis instead of lenses. Lenses are not used primarily because they have slightly different focal lengths for different wavelengths. Achromatic lenses are corrected for this problem but the correction is never perfect.
After the grating has dispersed the light into a range of angles we need a lens or mirror to refocus the light at the exit plane. A mirror is preferable here too, usually of the same focal length as the collimating lens. The popular Ebert Fastie design, shown below, used the same mirror for collimating and refocusing. The refocusing operation forms an image of the entrance slit in the exit plane when monochromatic light is used. If five different wavelengths are present, then five different separated images of the entrance slit are formed in the exit plane. A spectrometer which has a single exit aperture, usually a slit which matches the entrance slit, is often called monochromator. It is essentially a very sophisticated filter which transmits one wavelength to a detector or other apparatus. A spectrometer which has either a detector array or a photographic plate in the exit plane is often called a spectrograph. It can detect many wavelengths simultaneously.

A key figure of merit for a grating spectrometer is the limit of resolution, $\Delta \lambda$, which is the minimum separation of two resolved spectral lines. The figure of merit is sometimes quoted as a dimensionless resolving power,

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

These figures are determined from the angular dispersion of the instrument $\frac{d\beta}{d\lambda}$. The angular dispersion is derived by linearly differentiating Eqn. 4

$$ \frac{d\beta}{d\lambda} = \frac{m}{D \cos \beta}. $$

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Sometimes a linear dispersion in the exit plane is quoted. It is just \( F \frac{d\beta}{d\lambda} \), where \( F \) is the focal length of the refocusing mirror. If we assume the light incident on the grating is adequately collimated and that the exit slit width is “a”, then the limit of resolution is

\[
\Delta \lambda = a / \left( F \frac{d\beta}{d\lambda} \right). \tag{7}
\]

Wavelengths dispersed within an angle \( a/F \) are not resolved, because \( a/F \) is the angular acceptance of the exit slit. The resolving power is

\[
R = \lambda F \frac{d\beta}{d\lambda} / a. \tag{8}
\]

The laboratory monochromator in this experiment has entrance and exit slits of fixed width. Many research instruments have adjustable slits. More light can be sent through the instrument by increasing the slit widths “a”, but the resolving power decreases as \( 1/a \). One can trade off throughput for resolving power with adjustable slits. There is a limit, though, if you close the slits down sufficiently you run into the diffraction limit and the resolving power fails to increase further.

The most advantageous choice of relative entrance and exit slit widths is to make the widths equal in a spectrometer with equal focal lengths for the collimating mirror and refocusing mirror.

A key question which needs to be addressed is the question of the relative strength of the different diffraction orders. Our multiple slit diffraction pattern provides the answer in the form of the \( \text{sinc}^2(\pi W \sin \theta / \lambda) \) envelope function. If the grating has little mirrors each of width \( W \) which are parallel to the grating surface then the zeroth order \((m = 0)\) will always dominate. Unfortunately the zeroth order provides no dispersion and thus is useless in a grating monochromator. The solution is to tip the little mirrors by some angle \( \xi \) as shown below.

![Diagram showing normal to the grating surface, normal to the groove facet (i.e., tilted mirror), and the tilt angle ξ.]

This improvement throws a “blaze” of light into a particular order. Such a grating is a “blazed” diffraction grating. For the normal incidence illumination \((\alpha = 0)\) the order near
\( \beta = 2\xi \) is greatly favored. For a Littrow or near Littrow \((\alpha \approx \beta)\) arrangement the order near \(\alpha \approx \beta \approx \xi\) is favored. The light reflected off each little mirror is not reflected into a single angle, but rather into a range of angles because each little mirror is so very narrow it produces a wide single slit diffraction pattern.

**Experimental procedure and analysis:**

The photomultiplier will be used to detect the light passing through the exit slit. It requires a few hundred **negative** volts from the power supply. The white cables are the high voltage cables. **Do not exceed 600 volts.** The current from the anode of the photomultiplier tube (PMT) is detected with a Keithley 610 electrometer. The brightest line (to the PMT) is the blue one. Adjust the power supply voltage so that the anode current is less than \(10^{-6}\) amps at the peak of this line. The red/black banana jack output on the back of the electrometer is used to drive a strip chart recorder or the Pasco interface. (The Pasco interfaces can follow the 120 Hz flicker of the discharge lamps and high frequency noise from the electrometer. To minimize these effects you should pass the output of the electrometer through the low-pass filter box.) Adjust the PMT high voltage to make small changes in the amplitude. Electrons are collected at the anode of the PMT, so set the meter switch to “−”. The output is 0 to +3 V for negative input, independent of the meter switch setting.

The diffraction grating surface and the collimating mirror surface in the grating spectrometer are damaged by fingerprints. **Handle the grating carefully by the edges, and NEVER attempt to clean it.**

The Mercury (Hg) lamps produce significant UV radiation. Do not stare into the lamps. Prescription glasses or sun glasses will prevent eye exposure to UV. If you do not have glasses and if the UV causes you discomfort, please request protective glasses from the instructor.

1. Make an accurate scale drawing of the optical layout of the laboratory grating spectrometer. Assume the entrance slit is the slit furthest from the drive mechanism.

2. Use definition of the angles \(\alpha, \beta, \alpha_0\) and \(\delta\) that are given in the Ebert Fastie layout figure. Show that the grating equation \(D(\sin \alpha + \sin \beta) = m\lambda\) is consistent with

\[
2D \cos \alpha_0 \sin \delta = m\lambda
\]

3. Make an accurate scale drawing of the sine bar mechanism which shows the grating pivot point, pivot arm (or sine bar), and the pivot drive mechanism or micrometer. Derive an expression which shows that for the 600 groove/mm grating the micrometer reading in thousandths of an inch is the wavelength in nanometers. (Hint: Use the above expression at an appropriate angle.)
4. Put the Hg lamp in front of the entrance slit. Inspect the diffraction patterns to the left and right. Find the micrometer settings which put the yellow, green and blue lines at the exit slit. Rotate the grating to observe the effects of blazing.

5. Use the photomultiplier and the 5000 Å blaze grating to measure the relative intensity of the Hg green line with the grating put in right-side-up and up-side-down. Discuss the reason for the relative intensities.

6. Make a greatly magnified sketch of your expectation of the grating surface. Show the incident and diffracted rays relative to the grooves when the grating is right-side-up. What is the blaze angle ξ?

7. Scan the Hg spectrum from about 600 nm to 300 nm and identify the emission lines. You can use the “60 DN” setting on the motor drive. Momentarily change the current scale one notch more sensitive as you cross zero on the micrometer barrel about every other turn to make fiducial marks on your plot. Write the places you did this in your notebook and use them to calibrate the X scale.

8. Using Hg as the known spectrum, measure λ₁, λ₂ and (λ₁ − λ₂) of the D₁ and D₂ lines of Sodium, Na. This measurement should be carried out during a single scan of the spectrometer by exchanging lamps at the appropriate times. You will need to establish the full scale deflections and locations of the appropriate Hg reference lines.

9. Use the same procedure to measure the Rydberg constant.

Final Question: Derive an expression for the diffraction limited resolving power of a grating monochromator.
Supplement: A fiber optic array spectrometer

The scanning spectrometer just studied is ideal for studies in which high resolution, fast time dependence and/or high sensitivity are desired. Of great use are array spectrometers in which the exit slit is removed and a position sensitive detector is mounted in its place. Often the diffraction grating is rigidly fixed. Examples of the common Czerny-Turner arrangement are shown below. Important limitations are the increase in stray light reaching the detector and overlap of multiple diffraction orders. For later it is possible to put in place a filter that has a series of optical filters in order to attenuate unwanted orders. This last section is a qualitative look at a modern array spectrometer, the Ocean Optics USB4000 which comes “factory calibrated” and has a 3864 pixel 16 bit detector spanning from 180 to 890 nm. Integration time are as short as 10 \mu s as compared to the sub nanosecond response of the photomultiplier tube.

Procedure:

1. Plug the USB cable from the USB4000 into the PC
2. Click on the Ocean Optics Spectra Suite icon to start the data acquisition software
3. Carefully point the fiber optic at the sodium lamp and mercury lamps and acquire a sample spectrum.
   Question: How good is the factory calibration? Compare and contrast the spectral resolution with that of the scanning spectrometer.
4. Examine the output of the incandescent lamp.
5. Run the windows “Paint” program and examine the white, red, blue and green test patterns. Record one spectrum and comment on what you see.