BUILD A SPECTROMETER!

INTRODUCTION

In the research lab it is common to design and build custom equipment to carry out the measurement. One of the course goals for the advanced lab is to prepare you for this through the guided labs and the final project. In this lab you will start with a basic design for and spectrometer, build it, calibrate it, and characterize its performance, and identify the aspects of the design that limit the performance most significantly.

In the second week of the lab you will redesign your week 1 setup to improve some the most significant sources of uncertainty. The redesign gives you an opportunity for creativity guided by quantitative scientific reasoning.

GOALS

1. You will be able to create a good model of your measurement device, which means having a good calibration fit to your data, and also a quantitative estimate of the various uncertainty sources and how they limit the resolution, precision, and accuracy of your spectrometer.
2. You will also be able to make well-reasoned decisions about how to improve the design of your spectrometer based on your model of the spectrometer.
3. You will be able to explain how diffraction gratings can be used to separate different colors of light using both physical ideas and mathematics.

LAB NOTEBOOK GUIDELINES

The lab notebook will play an important role in this course. You will use your notebook for keeping records of many things including

- Answering pre-lab questions from the lab guide.
- Answering in-lab questions.
- Recording data.
- Including plots of data.
- Analysis and results.
- Diagrams and pictures.
- Procedures of experiments that you design.

The lab notebook will be an important part of your grade because learning to keep a good lab notebook is an important part of your professional development. You may find it helpful to write up many of your notes on the computer, for example, within Mathematica or another program. This is fine. However, before your notebook is turned in, the notes, plots, and analysis should be transferred to the lab notebook by printing and taping the pages or keeping them in a three ring binder. There will also be formal lab reports and oral presentations, but these will be restricted to a limited portion of the experimental work you have conducted in the lab.

DIFFRACTION GRATING AND SPECTROMETERS

A spectrometer is a device that can measure the wavelengths of light emitted from a source. One basic requirement for a spectrometer is that it can spatially separate different wavelengths. There are two common options for separating different wavelengths of light: prisms and diffraction gratings. Prisms separate wavelengths because the glass has an index of refraction which depends on wavelength. The different colors get refracted at different angles. The diffraction grating causes different colors of light to be diffracted at different angles. Diffraction works using interference. The diffracted beams go off in directions where there is constructive interference between light scattering off the pattern on the grating.

KINDS OF DIFFRACTION GRATINGS

All diffraction gratings commonly used are reproduced from master gratings. The master gratings have a periodic pattern which causes the light to be diffracted. Two important distinguishing features among gratings are (1) Where does the diffracted light go? And (2) How is the master grating made?

The two options for where the light goes are reflection gratings and transmission gratings. Reflection gratings have a mirror surface so that the diffracted beams are reflected. Transmission gratings have some transparency so there are diffracted beams in the transmitted direction.

The two common options for producing a master grating are ruled gratings and holographic gratings. Ruled gratings are produced by etching grooves in a thin film of metal. Holographic grating masters are produced by exposing photoresist to an interference pattern produced by two beams of light. The molecular bonds in the thin layer of photoresist are altered by light allowing it to be preferentially dissolved where the light is the most intense.

If you want to know more about gratings you might find these resources helpful.

- A basic overview is available from the Thorlabs "grating selection guide" and "gratings tutorial" available as tabs on the product information for their diffraction gratings.
  http://www.thorlabs.com/NewGroupPage9.cfm?ObjectGroup_ID=25
- In depth guide on principles and manufacturing of gratings from Thermo RGL (Richardson Grating Laboratory).
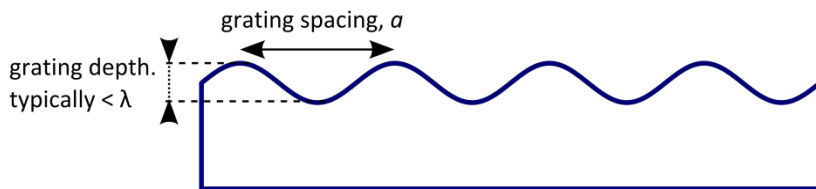 http://capem.buffalo.edu/lab-manuals/dgh.pdf

Figure 1: Zoomed in view of a the cross-section of a holographic grating.

MATHEMATICAL AND PHYSICAL UNDERSTANDING OF DIFFRACTION

The "grating equation" gives the relationship between the incident angle of the beam θ_i and angle of the n-th order diffracted beam $\theta_{r,n}$ for a particular wavelength of light λ, and grating spacing a. The grating spacing a is explained in Figure 1. The grating equation is given in Eq. (1):

$$a\left(\sin \theta_{r,n} - \sin \theta_i\right) = n\lambda \qquad \text{(1)}$$

| Pre-lab Question 1	Figure 2 shows two pictures of diffraction. a. Mathematically show that the diagram on the right, which uses wave vectors, predicts same "grating equation" given in Eq. (1). b. Explain the wave vector diagram in terms of constructive interference. In particular, why does the y-component of the wave vector change in integer increments of $\delta k_y = 2\pi/a$?
Pre-lab Question 2	In the basic spectrometer you will build later in the lab, a lens is used to image the light source, but a diffraction grating is placed prior to the image being formed. a. Draw a diagram of how a point source of light images as it diffracts off the grating. Where do the different colors of images go? b. Do the images focus the same distance away?
Question 3	How does the grating equation simplify when we only look for diffracted beams which return along the incident angle (i.e., $\theta_{r,n} = -\theta_i$)?
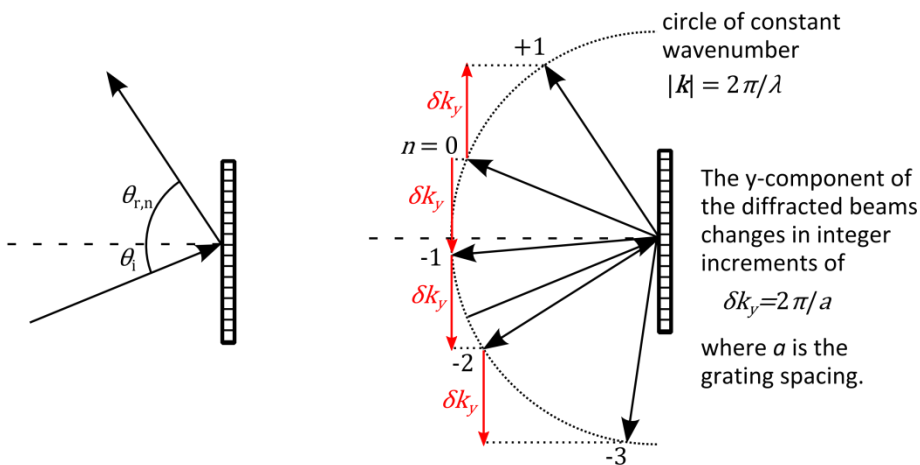
Figure 2: Two views of diffraction of a single wavelength of light from a grating. The left diagram shows the diffraction in terms of the incident angle θ_i and diffracted angles. The right diagram shows the same phenomena but considering the change in the wavevector, $\vec{k}$, rather than angle.

HYDROGEN SPECTRUM FOR CALIBRATION

In this lab, you will use the emission spectrum of hydrogen to calibrate your spectrometer. Hydrogen has a theoretically predictable spectrum given by the Rydberg equation.

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

(2)

where $R_H = 1.0973731 \times 10^7 \text{ m}^{-1}$.

The calibrated spectrometer will then be used to measure the wavelengths of mercury, which has no easily predictable formula for the spectral wavelengths.

Question 4	Using the Rydberg equation for the spectrum of hydrogen, predict the visible lines between 400 and 700 nm.

SIMPLE SPECTROMETER DESIGN

This section of the lab will ask you to construct a simple spectrometer design. Often times when designing an apparatus, it is best to start with an existing basic design, test it, understanding its limitations, and then redesign it to make improvements. In this lab you will perform the following four steps:

- Build a basic diffraction spectrometer.
- Characterize its performance (accuracy, precision, resolution).
- Calibrate it using the hydrogen spectrum.
- Measure the mercury spectrum.

The questions throughout the rest of this week are designed to guide you through this process in more detail.

Pre-lab Question 5	**Geometric imaging limit to spectrometer resolution.**
	 One limit to the resolution of the spectrometer is set by the width of the image of the lamp tube (see Figure 3). If two spectral lines are very close to the same wavelength, the two images in their respective colors will overlap. This question asks you to predict the resolution limit using simple geometric optics and error propagation.
	    a. For the spectrometer shown in Figure 3, derive a formula for the angular width of the diffracted image of the tube.
	    b. Using error propagation and the simplified grating equation derived in Eq. 3 to relate θ_i and $\theta_{r,n}$, how does uncertainty in the angular width propagate into uncertainty in wavelength?

Next, you will be asked to build the basic spectrometer shown in Figure 3, and to choose some of the parameters to optimize the performance of the spectrometer.
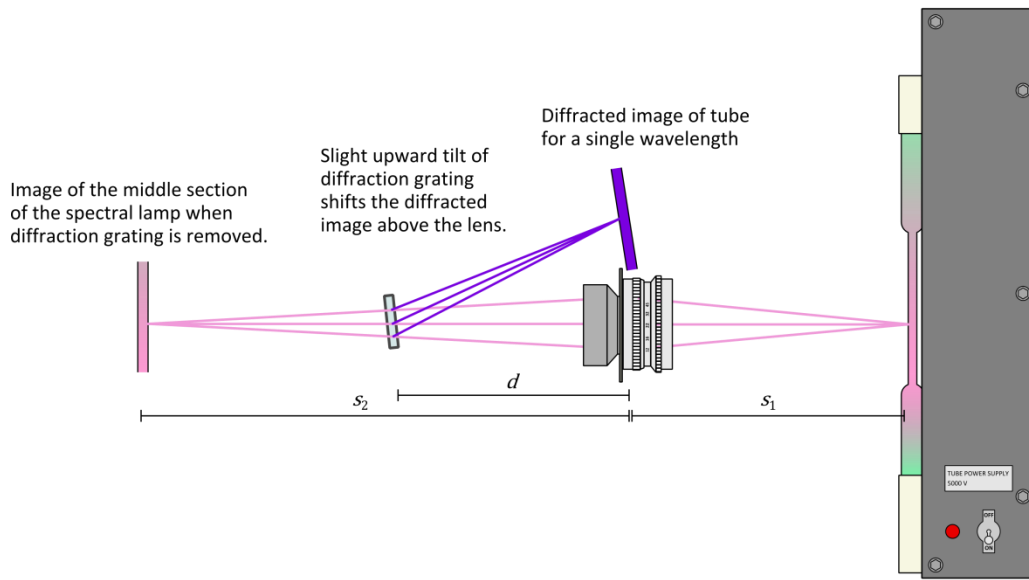

Question 6	**Build the spectrometer shown in Figure 3.** As you assemble the device consider the following questions. You might find it helpful to first assemble the spectrometer and then consider how you would answer the questions once you have a setup to play with.
	
	    a. How will you align the laser with the spectral lamp light so that you know the angle of incidence is same for both beams?
	    b. At what height should you set your optics? Why?
	    c. How far should the lens be placed from the lamp to optimize the light collection and resolution? Are the any obviously bad choices? Is there an optimal choice?
	    d. How far from the lens should the diffraction grating be placed to optimize light collection and resolution? Are there any bad choices? Is there an optimal choice?
	    e. Where do you want to put your detector/viewing slit?

Question 7	**What detector should be used?**
	Try to measure spectral lines with both your photodiode and lamp.
	    a. Both your eye and the photodiode are light sensors. Considering the kinds of information they can record, how are they similar and different?
	    b. Which detector lets you observe more spectral lines?
	    c. Is there a difference between where you would put the photodiode vs your eye?

Question 8	**Random and systematic error in the lever arm measurement of the angle.**
	    a. What are the sources of random uncertainty? Quantitatively estimate the random uncertainty sources, and their combined error in a single measurement of the tilt of the diffraction grating.
	    b. Are there any sources of systematic uncertainty? If so, describe them, and estimate the size of the systematic error source, and the error it produces in the angle.
	    c. What are the most significant sources of error?

Question 9	**Comparison of the uncertainty sources.**
	Quantitatively compare the three sources of uncertainty in the measurement of diffraction angle.
	Are any of these the dominant source of measurement imprecision?
	Is there uncertainty predominantly random or systematic?
	    a. Lever arm measurement of angle of diffraction grating.
	    b. Geometric imaging limit to spectrometer resolution (angular width of imaged tube).
	    c. "Diffraction limit" i.e., Fraunhofer diffraction from the finite size of the grating causing the image to spread out
	        • $\frac{\Delta\lambda}{\lambda} = \frac{a}{n\,W_g}$, where a is the grating spacing, and W_g is the width of the diffraction grating.
	    d. Size of the light detector (eye/slit/photodetector).
	    e. Any other sources?

Question 10	**Estimation of the total random uncertainty in angle.**
	    a. Do a repeated measurement of a particular spectral line to estimate the total random uncertainty in the angle measurement.
	    b. How does this compare to your different sources of estimated error?
	    c. Does the random uncertainty in the angle measurement depend on angle?

Question 11	**Take calibration data using Hydrogen lamp.**
	The statistical error analysis methods will show their full power in this section. Creating a "good" fit of the calibration data requires that you have a good quantitative understanding of all the important sources of uncertainty and that you have a good mathematical model of your spectrometer.
	    a. What are the fit parameters?
	    b. What are the independent variables?
	    c. What are dependent variables you are comparing for your fit?
	    d. What are the estimated uncertainties in the calibration data?
	    e. Do a least-squares fit of the data and determine the best fit parameters and their errors. (For example, by using `NonlinearModelFit` in Mathematica)
	    f. Plot the residuals. Are they randomly scattered or is systematic variation observed?
	    g. Quantitatively determine the goodness of fit using χ^2. If your fit is not good, go back and reassess earlier parts of the lab to see if you underestimated uncertainties, incorrectly took the data, etc. Repeat until you get a good fit.

Question 12	**Performance specs for the basic spectrometer.**
	    a. Explain the difference between resolution, precision, and accuracy of a measurement.
	    b. What is the resolution in nm?
	    c. What is the precision in nm?
	    d. What is the accuracy in nm?

Question 13	**Test out your spectrometer on the Mercury spectrum.**
	Mercury is a more complicated atom than hydrogen and its spectrum cannot be accurately predicted.
	
	    a. Measure the wavelengths of the visible spectrum of mercury.
	    b. Can you resolve the yellow lines at 576.9 and 579.1?
	    c. Quantitatively compare your measurements to the wavelength. Are the measurements within the performance specifications you determined in the previous question?

Table 1: Mercury spectral lines from NBS/NIST

Color	Wavelength (nm)	Intensity (spark) (arb. units)
IR	1128.7	
IR	1014.0	
Yellow	579.054	1000
Yellow	576.959	200
Green	546.074	2000
Blue-Green	491.604	50
Blue	435.835	500
Violet	407.781	150
Violet	404.656	300
UV	366.328	400
UV	365.483	200
UV	365.015	500

Side View

Diffracted image of tube for a single wavelength

Slight upward tilt of diffraction grating shifts the diffracted image above the lens.

Image of the middle section of the spectral lamp when diffraction grating is removed.

s_2

d

s_1

TUBE POWER SUPPLY
5000 V

Top View

HeNe

This mirror is needed to fit the the setup on the breadboard.

Rotatable Diffraction Grating

210 mm f/5.6 Camera Lens

Images observed through slit above the lens.

Longer wavelengths diffracted at larger angles

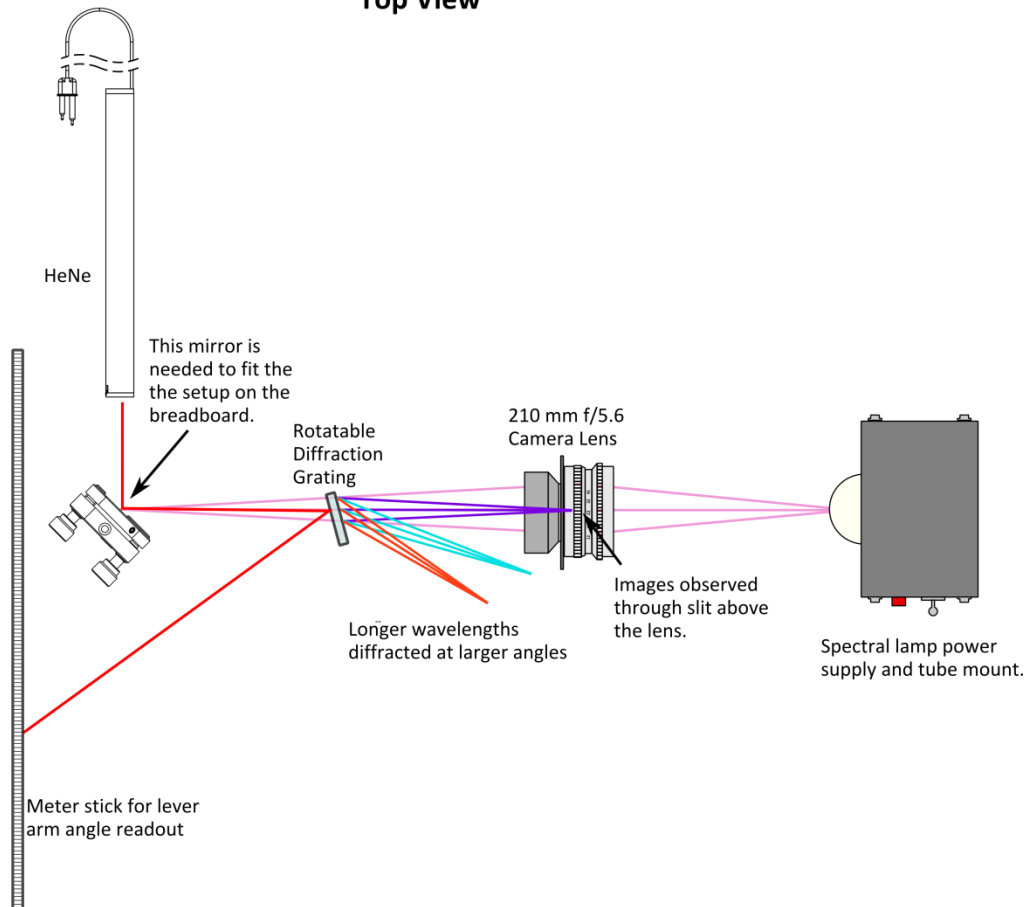Spectral lamp power supply and tube mount.

Meter stick for lever arm angle readout

Figure 3: Diagram of the basic spectrometer built in week 1.

At the end of week 1 you should have a full understanding of the specifications of your spectrometer, and understand the various sources of uncertainty which limit its resolution, precision and accuracy.

GOAL 1: REDESIGN YOUR SPECTROMETER TO RESOLVE THE YELLOW MERCURY LINES

The yellow Mercury lines occur at 576.9 nm and 579.1 nm.

Question 14	**Considering all the sources of uncertainty identified in the previous week:** a. Are there any sources of random uncertainty which limit our ability to resolve and measure the two lines? If so, by how much does the random error need to be reduced? b. Should any of the systematic uncertainty sources limit the resolution? If so, by how much do they need to be reduced? c. In particular, do you need to improve the geometric imaging limit to the spectrometer's resolution? If so, by how much.

There are two options for reducing the geometric imaging width to resolve the yellow mercury lines. Both involve reducing the width of the light source. The two options are:

1. Put a narrow slit right in front of the mercury lamp
2. Or, create a "condenser stage" which involves first imaging the lamp and then putting narrow slit over the image.

The first option is simplest because it can be added to the existing setup with minimal other modifications.

Question 15	**Add an adjustable width slit in front of the spectral lamp to reduce the size of the source.** a. Predict: How narrow should the slit be to just resolve the two spectral lines? b. Position the adjustable width slit near the tube. How close should it be? Does the distance between the tube and slit affect the resolution? Does the distance between the tube and slit affect the brightness of the image? c. Once you have the adjustable width slit set up, do a quick test of the resolution change with d. Afterward, measure the slit width necessary to just resolve the spectral lines using the measuring microscope.

MODIFY DESIGN, CALIBRATE, RETAKE MERCURY DATA

The previous questions dealt specifically with resolving the two yellow mercury lines. The next set of questions pertain to other sources of uncertainty.

Question 16	**Other sources of uncertainty** a. Based on your Week 1 analysis of the various systematic and random uncertainty sources, what changes to the design would be most profitable for improving the precision and accuracy of the spectrometer? b. Modify the spectrometer design to address the uncertainty sources identified in part (a). c. Calibrate your redesigned spectrometer using hydrogen, including an analysis of the goodness of the calibration fit.

Question 17	**New performance specifications**
	   a. Determine the performance specifications (accuracy, precision, resolution) for your spectrometer.
	   b. Compare the performance specifications for the modified design to the original design from week 1.

Question 18	**Measure mercury spectrum**
	   a. Measure the wavelengths of the visible spectrum of mercury.
	   b. Did you resolve the yellow lines at 576.9 and 579.1?
	   c. Quantitatively compare your measurements to the wavelength. Are the measurements within the performance specifications you determined in the previous question?
	   d. Compare the week 1 measurements to the week 2 measurements.

THE FORMAL REPORT

For both the basic and redesigned setup you should report the following:

1. The spectrometer design
2. The calibration and goodness of fit
3. A quantitative analysis of the uncertainty sources (both random and systematic).
4. Performance specifications (resolution, precision, and accuracy).
5. The mercury data.

In all of those categories you should compare the two setups. You should also explain how and why you modified the basic setup based on the analysis of the sources of uncertainty.

PROJECT IDEAS

1. Use the photodetector as the light detector, and process the signal with a chopper and lock-in amplifier to increase the sensitivity to low light levels. Possibly, in addition, use LabVIEW to automate the spectrometer, and take spectral data for a variety of spectral lamps.

REFERENCES

1. A basic overview is available from the Thorlabs "grating selection guide" and "gratings tutorial" available as tabs on the product information for their diffraction gratings.
http://www.thorlabs.com/NewGroupPage9.cfm?ObjectGroup_ID=25
2. In depth guide on principles and manufacturing of gratings from Thermo RGL (Richardson Grating Laboratory).
http://capem.buffalo.edu/lab-manuals/dgh.pdf