Experiment 2

Grating Spectrometer

References

- *Optics* by Eugene Hecht. Section 10.2.8 contains a good discussion of gratings and grating spectroscopy.

- *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles* by Robert Eisberg and Robert Resnick.

- *Experimental Physics* by R.A. Dunlap. Chapter 10 contains a concise description of photo-multiplier tubes.

2.1   Introduction

In this experiment you will become familiar with a research-quality grating spectrometer, the SPEX 500M, and use it to study the spectra of a variety of laboratory sources; e.g., Hg, Na, H, D, as well as the solar spectrum. There is considerable freedom to choose the measurements you will perform — just be sure to consult with your instructor regarding the light sources you are considering. The SPEX 500M is an impressive instrument with a resolution of 0.03 nm (0.3 Å) over a wavelength range 0–1500 nm, and it collects lots of light with an f-number of 4.0 (the *lower* the f-number, the better!).[1] The designation "500M" is shorthand notation for the 500 mm focal length of the spherical mirrors used in the instrument design. See the Appendix on page **??** for more details on the spectrometer design and components.

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[1] A note on units. The SPEX 500M displays wavelengths in the non-SI unit of angstroms (10^{-10} m). While a lovely dimension, particularly as regards atomic radii, it is hardly more serviceable than the standard SI unit of nanometers when it comes to visible wavelengths. As a former employee of the National Institute of Standards and Technology (NIST), Prof. Saeta is duty-bound to eschew such archaisms. Hence, he wrote the Igor Pro software to work in nanometers, not angstroms.

Most of the first laboratory meeting will be needed to familiarize yourself with the instrument and to perform a calibration procedure with a cool (roughly room temperature) low pressure mercury source. Collision broadening of spectral lines in this source is negligible, and the Doppler width of lines is less than the resolution of the instrument. The narrow spectral lines of this source and the well-documented wavelengths of the mercury spectral lines make this source ideal for calibration.

The second and third lab meetings will be spent performing measurements of spectra of a number of different light sources. For example, the Balmer series in the hydrogen spectrum played a critical role in the development of modern quantum physics. You can perform measurements of this spectral series to test the predictions of the Bohr and Schrödinger theories of the hydrogen atom. With our SPEX 500M grating spectrometer the Rydberg constant can be measured to five or six significant figures. In addition, you can cleanly resolve the isotope shift in the hydrogen spectrum by comparing the spectra of hydrogen and deuterium which are present in the same special "Balmer tube" source.

Instead of studying the hydrogen spectrum, you may wish to study the spectrum of the Sun. While the general shape of the spectrum is that of a blackbody ($T \approx 5000°$C), there are many absorption lines due to cooler gaseous elements in the Sun's atmosphere. You are challenged to identify the spectral lines of as many elements as you can; for example, helium was first discovered during studies of the Sun's spectrum. Of course, some of the most famous solar lines are due to hydrogen. You may also wish to observe the Doppler shift in the Sun's spectrum due to solar rotation. It's not an easy measurement, but it's an exhilarating challenge!

All students are urged to measure the sodium doublet splitting using the low-pressure sodium street lamp. This splitting is the most famous example of spin-orbit coupling in elements of relatively low atomic number. Everyone is also urged to measure the width of the collision-broadened green line emitted by a high-pressure mercury source. The sodium doublet and the pressure-broadened mercury line are also studied in the Fourier transform spectroscopy experiment, so your observations in these two experiments will provide an interesting comparison of the two spectroscopic techniques.

2.1.1   The SPEX 500M Scanning Grating Spectrometer

Two top views of the optics of the spectrometer are sketched in Fig. 2.1. The entrance slit is located in the focal plane of the collimating mirror, and the exit slit is located in the focal plane of the focusing mirror. Hence, light emanating from a point in the entrance slit is collimated (parallel rays) onto the grating, and parallel rays diffracted from the grating at the correct angle are focused to a point in the exit slit. In the top panel of Fig. 2.1, light is incident upon the grating at an angle α, and the zero-order diffraction maximum ($m = 0$) is specularly reflected at an angle α and focused onto the exit slit. In the bottom panel of Fig. 2.1, the grating is rotated by an angle β so that light is incident upon the grating at an angle $\varphi = \alpha + \beta$. The light focused onto the exit slit must now be diffracted away from the specular reflection by an angle $\theta = 2\beta$. Hence the
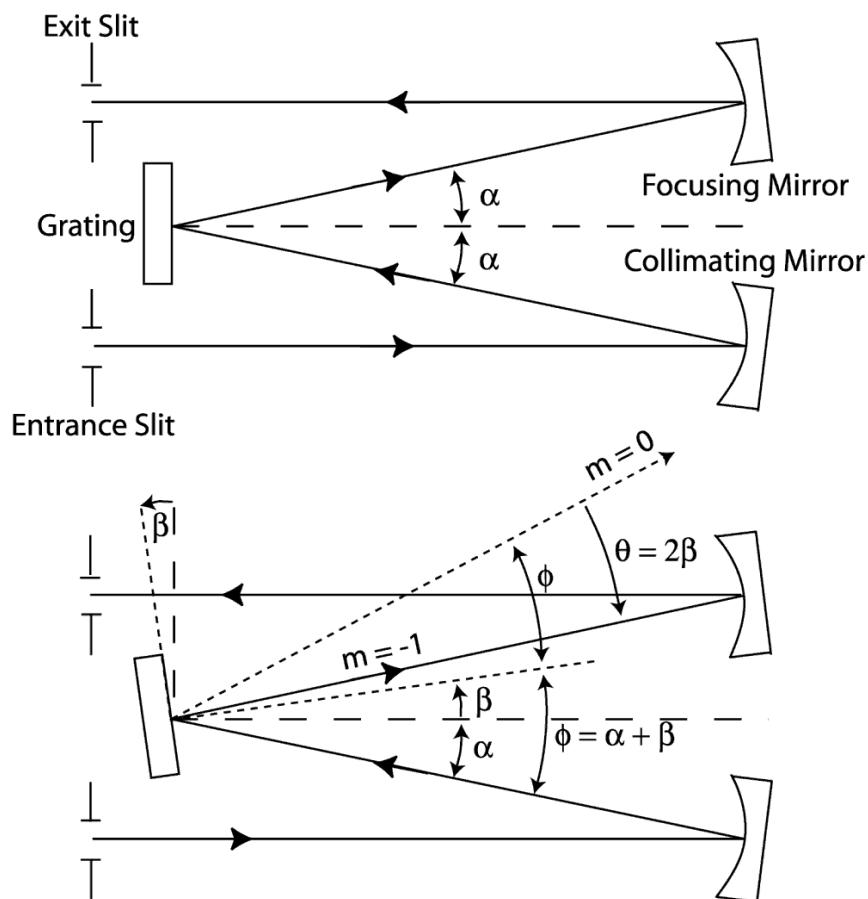
Figure 2.1: The design and operation of the SPEX 500M Spectrometer.

$m = -1$ diffraction maximum of wavelength λ appears at the exit slit, according to the relation

$$d \sin\varphi - d \sin(\varphi - \theta) = m\lambda \tag{2.1}$$

In Eq. (2.1), d is the grating period, m is the diffraction order, and λ is the wavelength.

Equation (2.1) can be derived readily by examining Fig. 2.2. In the left panel, two rays are incident upon the grating at angle φ with respect to the grating normal, and strike points a distance d apart, where d is the grating spacing. The upper ray travels a distance $d \sin\varphi$ further, as indicated in the figure. In the right panel, the two associated secondary spherical wavelets (from diffraction theory) are emitting in the direction of the focusing mirror at an angle of $\varphi - \theta$ with respect to the grating normal. This time the upper ray travels a distance $d \sin(\varphi - \theta)$ shorter. Considering the total path length to and from the grating, the upper ray travels a longer distance, $d \sin\varphi - d \sin(\varphi - \theta)$. When this extra distance is equal to an integer number of wavelengths $m\lambda$, the
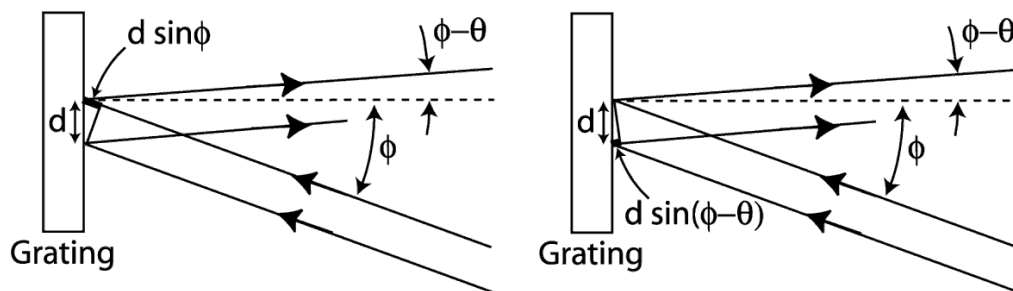
Figure 2.2: Derivation of the grating equation in reflection geometry.

diffraction maximum is focused onto the exit slit, in accordance with Eq. (2.1).

Using $\varphi = \alpha + \beta$ and $\theta = 2\beta$, Eq. (2.1) can be rewritten

$$d \sin(\alpha + \beta) - d \sin(\alpha + \beta - 2\beta) = m\lambda$$

which reduces to

$$2d \cos\alpha \sin\beta = m\lambda \tag{2.2}$$

Equation (2.2) relates the grating tilt angle β to the wavelength of the first order maximum that is focused onto the exit slit. Further information about the mechanics of the grating spectrometer, and a discussion of its resolution, are deferred to §2.5.

2.2   Calibration of the Spectrometer with the Mercury Source

The spectrometer system consists of an optical system, a scanning drive with mechanical readout (in angstroms), a photodetection system, and a controlling computer. (See the photo in Fig. 2.3, although the computer has been upgraded since the photo was taken.) We want to determine the precision of measurements performed using the complete system, so we must calibrate the entire system. Clearly, the resolution of the spectrometer system may be limited by components other than the grating, and we shall find that to be the case with our spectrometer.

The optical system consists of an entrance slit, a collimating mirror, the grating, a focusing mirror, and an exit slit (see Fig. 2.1). The scanning drive consists of a mini-step driver (MSD) which rotates the grating and can be operated either manually (local mode) or controlled by a computer (remote mode). Rotating the grating causes diffraction maxima of changing wavelengths to sweep by the exit slit. A mechanical readout indicates the wavelength (in angstroms) whose first-order maximum should be appearing at the exit slit. (See Fig. 2.4) The light that passes

Figure 2.3: The SPEX 500M grating spectrometer with controlling electronics and computer.

through the exit slit is detected by a photomultiplier tube, and the output current of the photomultiplier is measured by a microammeter. The microammeter displays the photocurrent reading on a front panel analog meter and provides an output voltage which is proportional to the photocurrent. The microammeter output voltage is fed into a multimeter for display and into an analog-to-digital converter board in the main chassis of the computer. The spectrum of a source can be recorded under computer control using a program written in Igor Pro and described in §2.6. A more detailed description of the spectrometer system is given in the Appendix (see page **??**).

Mount the low-pressure mercury source (housed in an aluminum cylindrical cap) on the entrance slit of the spectrometer. The glass envelope of this source is quartz and transmits the ultraviolet spectral lines of mercury, which prove useful for calibration. However, be careful not to turn the lamp on before it is mounted on the entrance slit of the spectrometer, because **the ultraviolet light can damage your eyes!** Set the widths of the entrance and exit slits to 6 μm. (One small division on the slit micrometers equals 2 μm.) A horizontal slide on the entrance slit has settings for slit heights of 2 cm, 1 cm, and 0.2 cm. There are also settings that superpose 1-mm-diameter circular apertures over the top, center, or bottom portions of the entrance slit. The "S" setting means "Shut". The height of the entrance slit should be set at 1 mm using the 1 mm aperture over the center of the slit. Power ON the high voltage on the photomultiplier tube (it is
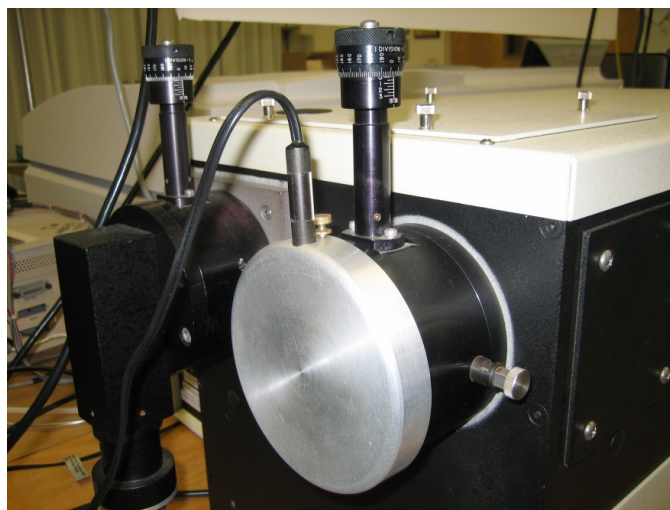
Figure 2.4: The entrance and exit slits of the SPEX 500M grating spectrometer.

set at -900 V). Use the 1-µA full-scale setting on the microammeter.

Instructions for scanning a spectral line under computer control have been placed with the computer. Perform a scan of the 546 nm line of Hg just to familiarize yourself with the spectrometer system.

Next scan the neighborhoods of the following eight spectral lines of Hg, which span the visible spectrum:

365.015 nm	546.074 nm
404.656 nm	576.959 nm
435.835 nm	625.132 nm (2nd order 312.566 nm)
507.304 nm (2nd order 253.652 nm)	730.030 nm (2nd order 365.015 nm)

In addition, you may want to check the calibration of the instrument across its entire range to 1500 nm by scanning the lines:

- 871.670 nm (2nd order 435.835 nm)

- 1092.148 nm (2nd order 546.074 nm)

- 1307.505 nm (3rd order 435.835 nm)

Measure the positions, full-widths-at-half-maximum (FWHM), and intensities of these lines. Make sure you understand the origin of the "lines" labeled as 2nd and 3rd order in the lists above. For instance, if you scan both the 365.015-nm line and the 730.030-nm line, how should you expect the two scans to compare to one another? After measuring the positions of the eight (or eleven) spectral lines, it is a good idea to spot check a few lines to see how repeatable your mea-

surements are.

Notice that the computer always begins a scan by moving several nanometers below the starting wavelength, then rapidly approaches the starting wavelength and finally performs the scan slowly in the direction of increasing wavelength. This manipulation removes the "backlash" of the mechanical drive. *Backlash is present in all mechanical drives, and you should always take it into account.*

You may notice that your measured positions of the Hg spectral lines (based on the mechanical readout) deviate slightly from the above literature values (found also in published tables placed with the spectrometer). These deviations represent the limits of the precision of the spectrometer drive, though most of the deviations consist of a simple additive constant and a slight correction to the slope of the wavelength drive. The linear calibration described below is aimed at removing *most* of these deviations, leaving only nonlinearities which indeed represent shortcomings of the wavelength drive.

Some general advice is in order regarding the use of the photomultiplier tube at the exit slit of the spectrometer.

> **Caution**
>
> The spectrometer photomultiplier tube is a Hamamatsu R928 that has an extended red multialkali photocathode that is sensitive to light of wavelength 185 nm to 900 nm. **The anode current (measured with the microammeter provided) has an absolute maximum rating of 100 μA.** Should you exceed 100 μA, there is a good chance you will damage the photomultiplier tube irreparably.

Try to keep the photocurrent below 20 μA, using the microammeter front panel as a guide. You must narrow the widths of the slits, decrease the height of the entrance slit, or attentuate the source intensity to ensure that the photocurrent of each spectral line does not exceed this nominal 20-μA rating at any point in your scan across the spectrum. *Please be nice to our spectrometer PMT.*

Finally, use our linear least-squares method to fit a straight line to a plot of literature wavelengths versus measured wavelengths. Ideally the slope should be 1 and the y-intercept should be zero. The value of χ^2 should give some indication of the linearity of the spectrometer drive over the full visible spectrum spanned by our calibration lines. The linearity is even better over short wavelength intervals. Usually when an unknown spectral line is recorded, two bracketing calibration lines are also scanned, and the wavelength of the unknown spectral line is calculated by interpolation of the two literature wavelength values of the calibration lines.[2]

The χ^2 for your straight-line fit will be sensible only if you use sensible uncertainties for the measured positions of spectral lines. There are two contributions to the uncertainty of a mea-

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[2]In practice, it is common to use a low-order polynomial, rather than a line, to calibrate a grating spectrometer. A polynomial of order greater than one can correct for slight errors in the definition of the origin of wavelengths and misalignments of the sine bar.

sured spectral line position. First, the uncertainty with which you can locate the center of a line is best measured by a sample variance technique. Second, the resolution of the instrument is reflected in the width of the spectral line (when the source is the low pressure mercury lamp). **You will have to think carefully about which of these two contributions is more appropriate for the linear regression procedure.** If the sample variance technique yields a number which is much larger than the half width at half maximum (HWHM), then clearly the sample standard deviation should be used. If, however, the sample standard deviation is much smaller than the HWHM (which is in fact the case), it may be that structure in the line is obscured by the resolution of the instrument, and the HWHM may be a reasonable number to use as an uncertainty in the position of a spectral line. (You will probably find that the quarter-width-at-half-maximum (QWHM) is a good uncertainty to use.)

You should also take data to measure the resolution of the instrument as a function of the slit widths. The information in the Appendix (see pages **??** through 18) will allow you to compare your measured line widths of a Hg spectral line with the theoretically expected values given the dispersion of the grating and the widths of the slits. It is a good idea to roughly analyze this data as you proceed, so you can be sure to take data over a reasonable range of slit widths.

What you have learned about the instrument in your experimentation so far should be used to guide your data-taking and analysis for subsequent parts of this experiment.

2.3 Measurement of the Hydrogen Spectrum or the Solar Spectrum

2.3.1 The Balmer Series of Hydrogen

Position the hydrogen "Balmer tube" source so that the source is imaged by the lens onto the entrance slit of the spectrometer. (Even if you decide to study the solar spectrum, you may want to use the Balmer tube as a comparison source when searching for hydrogen lines in the solar spectrum.) Your instructor can suggest an arrangement that has proven satisfactory. If you decide to devise your own arrangement, be sure to direct the fan onto the lower portion of the tube; cooling the tube by convection prolongs the life of the tube considerably. You should measure the position, FWHM, and intensity of as many lines of the Balmer series as possible (at least eight). If you plot the reciprocal of the wavelength of a series line versus $1/n^2 - 1/m^2$, where n and m are the final and initial principal quantum numbers of the transition, you can use a linear fitting procedure to deduce a value *and an uncertainty* for the Rydberg constant of hydrogen. In comparing your measured value with literature values, be sure to compare apples with apples and oranges with oranges. Literature values are often quoted for R_∞, the Rydberg constant assuming an infinitely heavy nucleus. When you have finished the data analysis, take a moment to muse on how beautifully a straight line fits your data. The fundamental postulates of quantum mechanics have led to predictions which agree awfully well with measured values, whereas classical mechanics and electromagnetism predict that atomic electrons should spiral into the nucleus.

You can measure another interesting feature of the hydrogen spectrum by replacing the hydrogen Balmer tube with the deuterium Balmer tube. Be sure to allow the hydrogen tube to cool; the operating temperature of the tubes usually renders them too hot to touch. The deuterium tube actually has enough hydrogen to give roughly equal intensity lines for the two isotopes. Measure the spectral lines of deuterium and deduce a value *and an uncertainty* for the Rydberg constant.

2.3.2 The Solar Spectrum

You will need a little luck with the weather (and even more luck if you have an evening section), but after all, this is sunny southern California! Use the heliostat and fiber optic cable to bring a little sunshine into the spectrometer. Your instructor will help you position the heliostat outdoors near the rear door of the building; the fiber optic cable and power cord for the heliostat motor should be carefully laid out through an open window in the lab. Position the fiber optic cable so that it is protected from sharp kinking or compression, which will quickly degrade its performance. The body of the heliostat must be correctly oriented (angled plate facing north) for proper operation. When focusing sunlight onto the fiber optic, be careful not to melt the cable cladding. The end of the fiber optic cable inside the lab can be held at the entrance slit of the spectrometer with the optical rider provided.

Leave the heliostat unplugged at first and watch it (outdoors) for a minute or so to see the focused sunlight spot drifting due to the Earth's rotation. Now realign the heliostat and plug it in; if you have oriented it correctly, the drift you observed before should be nearly eliminated by the tracking which is now taking place. Do not expect to see or hear rapid motion from the motor when the device is tracking properly!

The Sun's spectrum is, in general, a jumble of absorption lines superposed on a continuous blackbody spectrum. You will have to do a little reading on the solar spectrum and decide which prominent features you are going to try to observe. It may prove helpful to alternate or even superpose the spectra of the Sun and an appropriate laboratory source. You will have to think through your approach to these measurements and come to the laboratory prepared. Don't lose sight of the fact that elements in the Sun which are heavier than helium came from the same place that those elements in your body came from: exploding stars, or at least stars that are long dead!

If you decide to measure the solar rotation, it will be critical to show that the position of a solar spectral line depends on which portion of the Sun's disk is being imaged onto the optical fiber. As the Sun rotates, light emitted from one side of the Sun's equator will be blue-shifted because that portion of the Sun is moving toward the Earth, while light emitted from the other side of the equator will be red-shifted as a result of motion away from the Earth. If you power off the heliostat and simply allow the Sun's disk to pass over the optical fiber while you take spectra as quickly as possible, you should see a small but systematic shift in the position of a solar spectral line. It will be a *small* shift because the Doppler shift is considerably less than the resolution of the spectrometer, 0.03 nm! Be sure to perform all the calculations before you come to lab!

2.4   Measurements of the Sodium Doublet Separation and the Width of the Collision-Broadened Mercury Green Line

2.4.1   The Sodium Doublet

The low-pressure sodium source (the bulb is sold commercially as a street lamp) is sufficiently bright that it can simply be placed 20 cm to 1 m from the entrance slit of the spectrometer (it need not be imaged onto the slit). Like the street lamps, the source requires several minutes to reach full intensity. Measure the positions, FWHM, and intensities of the two lines. From this data you can deduce a value *and an uncertainty* for the spin-orbit coupling energy in this alkali "one-electron" atom. Compare your measured value with literature values. You should review the treatment of spin-orbit coupling given by Townsend in Chapter 11 and/or by Eisberg and Resnick.

2.4.2   The Mercury Line Width

The high-pressure mercury source also requires several minutes to reach full intensity, but is then sufficiently intense that it may simply be positioned 20 cm to 1 m from the entrance slit of the spectrometer. Measure the FWHM of the green line and obtain a detailed plot of the shape of the spectral line. The bulb operates at approximately nine atmospheres and 5000°C. The slight tail on the long wavelength side is characteristic of a collision- (or pressure-) broadened line. Our treatment in lecture of collision broadening does not account for the tail but does predict a Lorentzian lineshape. It would be interesting to see how well the measured lineshape can be fitted with a Lorentzian. Also, do you notice a hint of self-absorption in the spectral profile?

2.5   Appendix: the Sine Bar and Resolution

Figure 2.5 illustrates how a linear relation can be obtained between an easily controllable parameter and the wavelength at the output of the spectrometer. The grating is mounted on a rotatable table, and the end of a lever of total length L slides on the end surface of a translatable rod. The key point is that as the rod is translated and the distance x is varied, the end of the lever may slide on the end of the rod (slide left-right in Fig. 2.5). The relation between the tilt angle β of the grating and the distance x is clearly $\sin\beta = x/L$. The arrangement depicted in Fig. 2.5 is commonly referred to as a "sine bar" by mechanical engineers. Substituting this relation into Eq. (2.2) we get

$$\lambda = \frac{2d\cos\alpha}{mL}x \tag{2.3}$$

which is indeed a linear relation between λ and x. A stepping motor turns a threaded rod and hence varies x in a linear way. As a result, the number of revolutions executed by the motor is
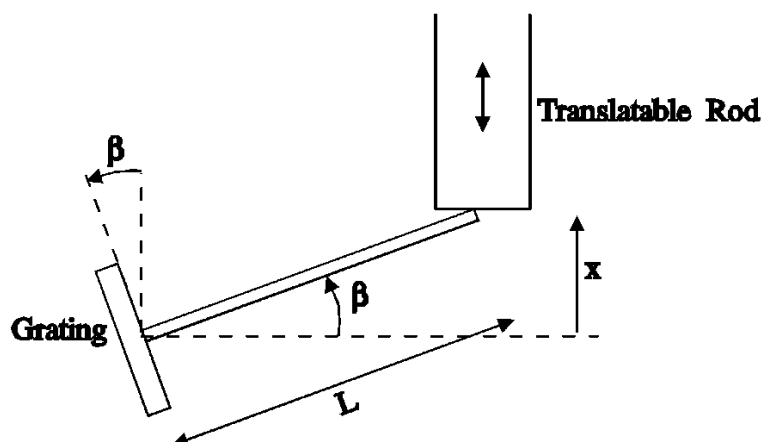
Figure 2.5: The sine bar.

linearly related to the wavelength at the output. A mechanical counter keeps track of the turns of the motor.

The dispersion of the spectrometer $D \equiv d\lambda/d\theta$ is the incremental change in the wavelength appearing at the exit slit for a given change in the angle θ of diffraction. The dispersion can be calculated by differentiating Eq. (2.1) with respect to θ while holding the angle of incidence φ constant:

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\theta} = \frac{d\cos(\varphi - \theta)}{m} \tag{2.4}$$

The dispersion is often expressed as the change in wavelength in nanometers per millimeter of travel in the direction of the exit slit width. If y measures the distance along the slit width direction, the relation between y and θ is $y = f\,\theta$, where f is the focal length of the focusing mirror ($f = 500$ mm). Substituting the differential form $dy = f\,d\theta$ into Eq. (24), we get

$$\frac{\mathrm{d}\lambda}{\mathrm{d}y} = \frac{d\cos(\varphi - \theta)}{mf} \tag{2.5}$$

The grating employed in the SPEX 500M has 1200 grooves/mm, so the grating spacing is 1/1200 mm or 833 nm. If we set $\cos(\varphi - \theta) \approx 1$, then the dispersion in first order ($m = 1$) is according to Eq. (2.5)

$$\frac{\mathrm{d}\lambda}{\mathrm{d}y} = \frac{833\,\mathrm{nm}}{500\,\mathrm{mm}} \approx 1.67\frac{\mathrm{nm}}{\mathrm{mm}} \tag{2.6}$$

The upper limit on the resolution of the spectrometer can now be calculated by multiplying the dispersion by the slit width. For a slit width of 10 µm, this calculation yields (1.67 nm/mm) (10µm) = 0.0167 nm ≈ 0.17 Å. This result is conventionally multiplied by 2 to account for the way the entrance slit is imaged onto the exit slit, giving a resolution of approximately 0.03 nm or 0.3 Å.

At a wavelength of 550 nm, a resolution of 0.03 nm gives a resolving power of

$$R \equiv \frac{\lambda}{\Delta\lambda} = \frac{550\,\text{nm}}{0.03\,\text{nm}} \approx 18,000 \tag{2.7}$$

This value is quite a bit less than the theoretical resolving power of the grating $R \equiv Nm$ where N is the number of lines in the grating. Since the grating has 1200 grooves/mm and has a ruled width of 110 mm, N is equal to 1200 times 110 or 132,000! The grating is large so that more light can be focused at the exit slit, rendering the spectrometer a "faster" instrument. Resolution and speed of a spectrometer are two quite different (sometimes opposing) design considerations. While our instrument has only modest resolution, its speed or f-number (4.0) is excellent.

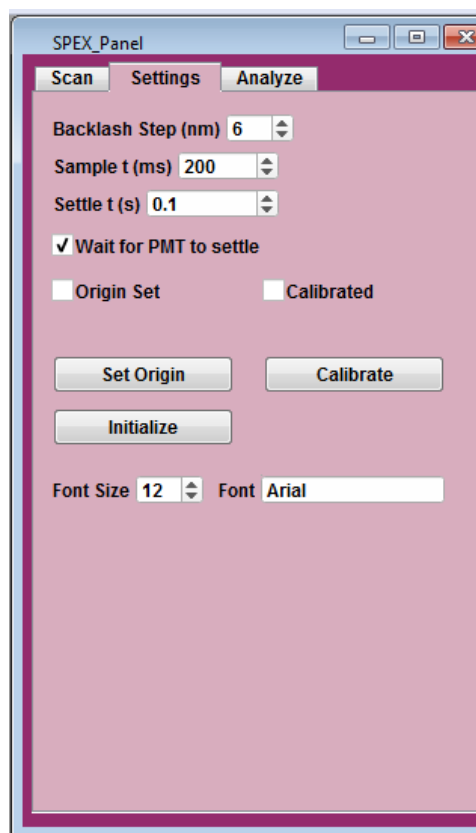## 2.6   Using Igor to Control the SPEX 500M Grating Spectrometer

These instructions describe the software that provides computer control of the SPEX 500M grating spectrometer. In this experiment, Igor interfaces a PC (a Dell Dimension 4600 computer named "Waller") running Windows 7 to the MSD2 electronics that drives the stepper motor that rotates the grating in the SPEX 500M spectrometer. These instructions will guide you through a scan of a mercury line (546.074 nm), and help you produce a printed plot of the spectral line on the HP Color LaserJet Enterprise M553 printer (named "Scandal", IP=134.173.33.114).

2.6.1   Recommended Startup Procedure

1. On the SPEX 500M grating spectrometer, set the widths of the entrance and exit slits to 6 µm, and set the height of the entrance slit to 1 mm using the middle 1 mm-diameter aperture.

2. Power ON the mercury calibration lamp and the photomultiplier tube high voltage (−900 V).

3. Power ON the MSD2 driver (power switch at right rear, local/remote switch on REMOTE).

4. Power ON the multimeter and the microammeter (full scale at 1 µA, multiplier at ×1).

5. Finally, power ON the computer main chassis and monitor.

6. As Windows 7 boots up, log in with the following account and password:

account name	**spex**
password	**grating**

7. Launch the program "Igor64.exe" using the shortcut on the desktop. If prompted, click $\boxed{\text{Yes}}$ to install a newer version of HMC.ipf, and then click $\boxed{\text{No}}$ to the question, "Do you want to save changes to experiment 'untitled'?"

8. Once Igor has loaded, go to the **Expt** menu option and click **SPEX** on the pulldown menu. A window named "SPEX_Panel" should open in Igor, as illustrated above. Within that window, the **Settings** tab should be frontmost.

9. Click $\boxed{\text{Initialize}}$. The command line window should then write several line of output ending with "Communications with the SPEX established properly." (See top of next page.)

```
Untitled
0  •SPEXScan()
1     path: "C:Users:SPEX:Documents:WaveMetrics:Igor Pro 7 User Files:prefs:"
2     Defaults are being saved in the directory : C:Users:SPEX:Documents:WaveMetrics:Igor Pro 7 User Files:prefs
3     Communications with the SPEX established properly.
4
```

(If this does not occur, turn off the SPEX MSD2 controller, wait 10 seconds, turn it back on, and initialize again.)

10. Now click $\boxed{\textbf{Set Origin}}$ under the **Settings** tab. You will be prompted to enter the current wavelength **in nanometers**. Do so, reading the spectrometer window display, *noting that the number on the instrument's display is reported in angstroms, not nanometers.*
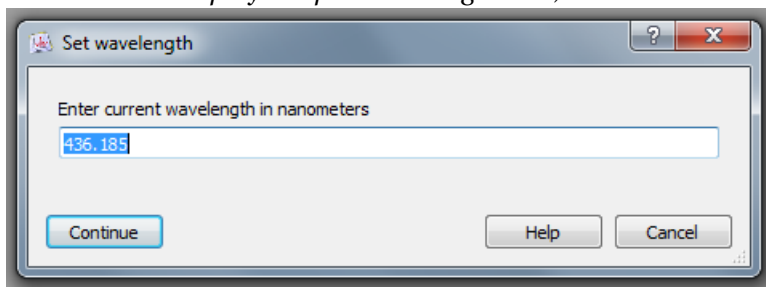

Click $\boxed{\textbf{Continue}}$. Note that the $\boxtimes$ Origin Set box has been automatically ticked in the SPEX **Settings** panel.

2.6.2 Taking Spectra

Go to the **Scan** tab and enter in the **wavelength (nm)** box a value smaller than that which you would like to scan. Press **enter** or click on the rose background outside the box; the spectrometer will move to the input wavelength. Verify on the front of the spectrometer that it has moved to the correct wavelength. Enter the range of your scan in the appropriate box using the "**start : stop : step**" syntax, as indicated above the box entry. You may enter a single range, as shown in the example here, or you may enter a range on each of several lines in the box. Note that the mercury lines are preloaded for you in the **Go to Hg** and **Scan Hg** menus. The green line at 546.074 nm is a good choice for a first scan, and a good step size to start with is 0.01 nm.

Enter a value for **Passes**, which corresponds to the number of passes over the specified wavelength range(s) you wish to make. A data point is taken at each specified wavelength on each pass. The point is obtained by sampling the signal voltage many times and averaging. The duration of averaging is set by the **Sample Time** variable on the **Settings** tab. If you choose one pass, Igor displays error bars using the standard error of the incoming data during the sampling time at each wavelength.
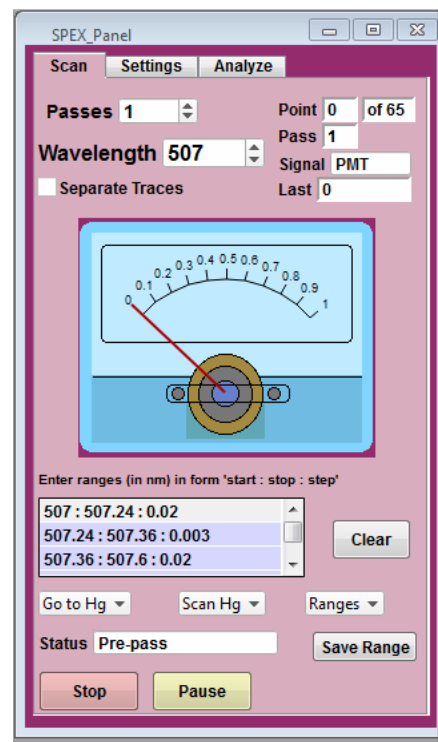
If you choose more than one loop, Igor uses the standard error of the repeated trials (passes) at each wavelength. Click $\boxed{\text{Start}}$. A new plot window with your data will automatically open. It is named for the time at which you begin the acquisition.

If you use more than 1 pass, you may check the ⊠ Separate Traces box if you wish to see a separate trace for each pass through the wavelength range. At the end of each pass, a new curve is added to the lower half of the plot window, as illustrated in Fig. 2.6. In this example, there are actually five separate traces in the lower panel, but because of the excellent signal-to-noise ratio, they are virtually indistinguishable. The discrete points in the top panel of Fig. 2.6 have the normal averages and their standard errors, computed as described above, and updated after each measurement.
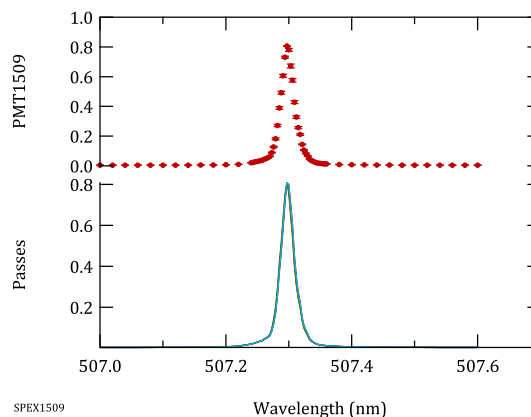

Figure 2.6: An example scan with separate traces for each pass.

2.6.3   Where are the Data?

Each spectrum is stored in its own data folder named after the date and time of the scan. At the start of each spectrum (run), an entry with the parameters of the scan is made in the Scan Diary, which is a standard Igor Notebook window. You can add your own notations to this window to help you keep track of any changes you may have made to the setup—such as amplifier gain, alignment, light source, etc.—and can even paste in copies of the graphs as a catalog. Each spectral entry shows the data folder holding the scan and then a line showing the number of passes requested in parentheses, followed by the wavelength range(s). An example Scan Diary window is shown in Fig. 2.7

You can see all the data waves using the **Data Browser**, which you can find in the Data menu. The figure at the right shows the Data Browser corresponding to the series of traces shown in Fig. 2.6. Notice that at the bottom left corner of the figure is the label SPEX1509, which tells you that the run was initiated at 15:09 (3:09 p.m.).
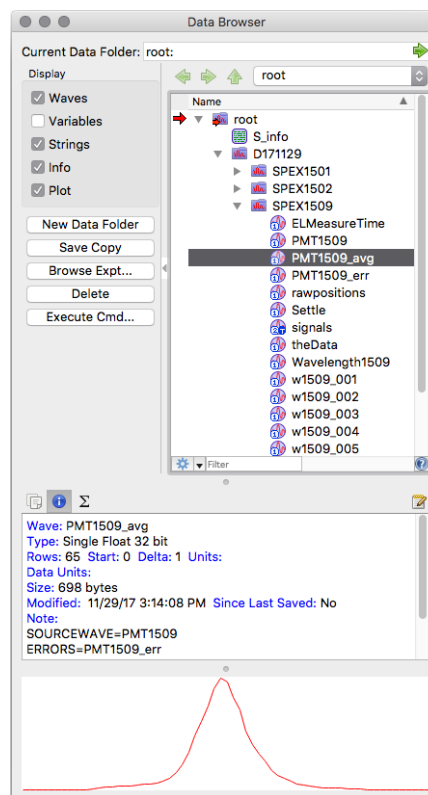
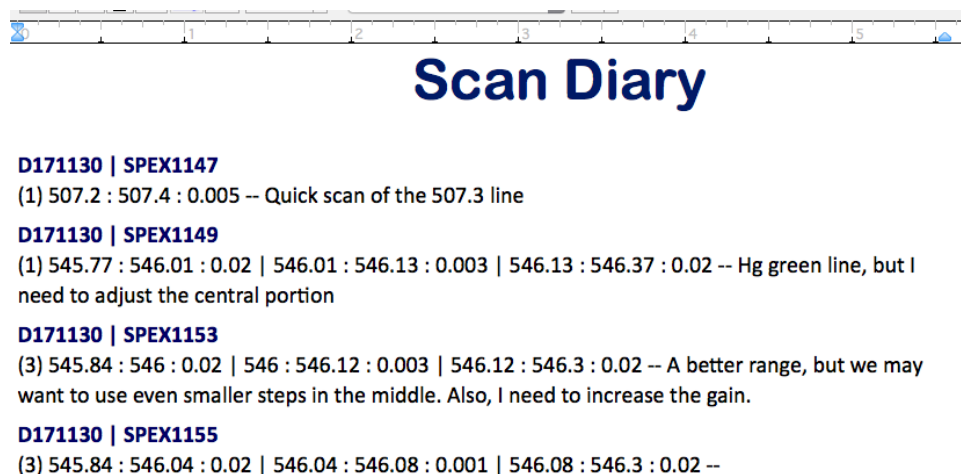The PMT1509_avg wave (illustrated at the bottom of the Data Browser, since it is highlighted)

Figure 2.7: The Scan Diary window.

shows the average computed for the 5 passes (loops). The individual passes are labeled w0953_001 through w0953_005. The wave note contains further information about the data source: the SOURCEWAVE is PMT1509 and the ERRORS are in PMT1509_err. This means that to produce a "proper" plot of these data, you would display PMT1509_avg vs Wavelength1509 and add error bars from PMT1509_err.

The result is shown in Fig. 2.8, after changing the y axis to logarithmic display and shrinking the markers so the error bars can be seen. You can print a copy on the color printer Scandal using **File | Print Graphics. . . .**

2.6.4   Remaking a Plot

If you have closed a spectrum plot and wish to regenerate it (or just find it, if it is buried on your display), select **SPEX Plot** from the **Expt** menu and choose the appropriate spectrum from the popup menu.

2.6.5   Working on Another Computer

The Igor SPEX software allows you to store all your scans in a single Igor Experiment file, organized by the date of the scan and the time it was begun. Make sure to save often. When you want to work with your data on another computer, copy the Experiment file to the other computer. You may see error messages that Igor cannot find some waves and/or procedure files. Just click to ignore those warnings. You should be able to access all of your data via the Data Browser.

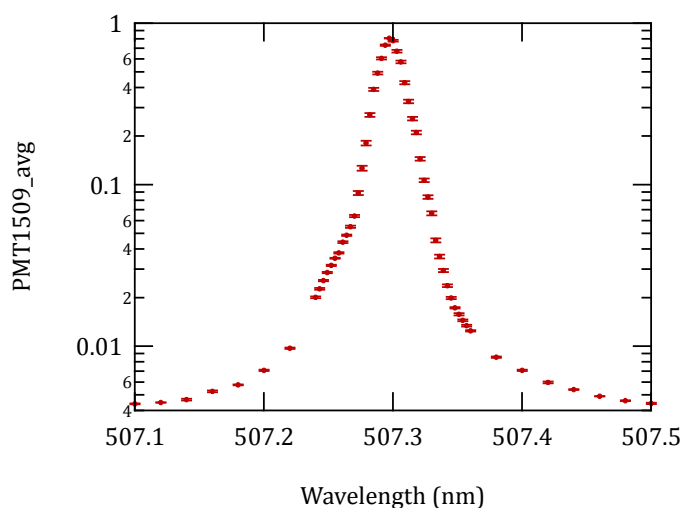If you would like the convenience of the **SPEX Plot** command, you can download the appropriate

Figure 2.8: Sample Hg line, the $\lambda = 253.652$ nm line at second order.

procedure file from the department server within Igor by typing the command

```
Install("SPEXPlot", targetFolder="User Procedures")
```

This will install the code in the **User Procedures** folder, which houses optional procedures that you may wish to use from time to time. You can make sure it is available in any particular experiment file by entering

```
#include "SPEXPlot"
```

in the Procedure Window (Cmd/Ctrl-M).

2.6.6   Calibration Lines

For easy reference, here are the mercury calibration lines.

365.015 nm		625.132 nm	(2nd order 312.566 nm)
404.656 nm		730.030 nm	(2nd order 365.015 nm)
435.835 nm		871.670 nm	(2nd order 435.835 nm)
507.304 nm	(2nd order 253.652 nm)	1092.148 nm	(2nd order 546.074 nm)
546.074 nm		1307.505 nm	(3rd order 435.835 nm)
576.959 nm			