LOOKING AT LIGHT

Objectives

In the experiment Atomic Spectra, you determined wavelengths by measuring the angles of diffraction. It's important to know how spectra are acquired, but modern spectrometers can do all the angle measuring and data processing for you. This experiment will use a small computer-controlled spectrometer to rapidly acquire and study a variety of spectra.

Background

The Ocean Optics spectrometer (we have more than one model, but their operation is the same) is a hand-sized grating spectrometer that plugs into a computer through the USB port. Optical input is through a fiber-optic cable. The spectrum is dispersed across a 2048-channel (or 4096-channel) CCD array, and the entire spectrum is displayed on the computer screen in real time. The resolution (i.e., linewidth) depends on the model, but is 2 nm or less.

Procedure

This lab is a series of mini experiments. For each, you'll want to **print each of the spectra** to include in your report. Your observations and analysis should then refer to specific features in the spectra. For your report, report on each mini-experiment in its entirety (description/data/analysis) before going on to the next.

Launch the **SpectraSuite** software. The spectrometer should be acquiring a spectrum as soon as it starts. Point the optical fiber toward the overhead fluorescent lights to be sure.

1. Basic operation: Toward the top, in one of the toolbars, you'll see a Pause button. Clicking on this freezes the spectrum so that you can observe it or print it. The Start arrow resumes acquisition.



Clicking in the middle of the spectrum produces a cursor line.

Below the spectrum you'll see a data line showing the wavelength at the cursor, the wavelength or pixel number on the CCD array (0–2047), and the signal strength (0–70000).



2. **Integration time**: In the upper left is a box called "Integration Time" and, next to it, one called "Scans to Average." The integration time is how long the spectrometer spends acquiring each signal. Longer times give stronger signals, but an integration time too long will cause the signal from a strong source to saturate. Change the value to see what happens. Scans to Average, as you would expect, are the number of sequential spectra that are averaged together. A steady source shouldn't need any averaging, but averaging can improve the spectrum for sources that flicker or are not steady.



Above the spectrum graph itself is a toolbar with buttons that allow you to *scale/zoom/select* the different parts of the spectrum. You can also *print* the spectrum from there.

Freeze a spectrum, then display only the wavelength range 400–600 nm.

3. **Calibration:** Each spectrometer was calibrated at the factory, and this built-in calibration provides the wavelength shown at the bottom of the screen. It will be pretty close to the "true" wavelength, but – because the calibration can shift with time – it's not as accurate as the spectrometer is capable of achieving. Doing your own calibration is good practice at using the spectrometer and at using Matlab (or Python) to fit the data.

Install a helium discharge tube in the holder. Set the integration time to 10 ms and set the horizontal scale to display the region 300–800 nm. You'll see that the spectrum is rather jumpy. Although the light looks steady to your eye, it's actually flickering at a 60 Hz rate. You can improve the spectrum by setting Scans to Average to 10. Adjust the position of the fiber so that the tallest peak is just below the saturation value, then "freeze" the spectrum. You should be able to see 9 spectral lines, some of them rather weak.

Record the approximate *wavelength* at the center of the *strongest peak* ($\lambda \approx 588$ nm). Now from the menu Processing/X-Axis Units/ choose "pixels." To find the center, use the small up/down arrow buttons next to the pixel box to move the cursor back and forth across the peak while looking at the signal strength.

• If there's a clear maximum, with neighboring pixels on either side of the maximum of roughly the same strength, record an integer pixel value.

• If there are two pixels with roughly equal strength at the maximum, then record their midpoint (such as pixel xxx.5).

There's no need to be any more precise than one of these two options.

Start acquiring data again, but bring the fiber closer so that the peak at ≈ 707 nm is just below the saturation level, then freeze the spectrum. The 588 nm peak will now be saturated. Now, using the procedure above, record the pixel number and wavelength at the center of the 8 highest peaks (not including the 588 nm peak that you've already measured).

Note: The wavelength reported by the computer is simply what the computer thinks. It is *not* a measured wavelength. The pixels are your measurements, and from them - by calibrating - you're going to determine the measured wavelengths. So describe the wavelengths you see on the screen as simply "computer-reported wavelengths."

These 9 wavelengths of the helium spectrum are well known. They are:

388.86 nm 447.14 nm	492.19 nm 501.57 nm	667.81 nm 706.52 nm

The computer-reported wavelengths should be close, but likely not exact. To improve the wavelengths, you want to fit the *known* wavelengths (above table) to a second-order polynomial

$$\lambda = a + b_1 p + b_2 p^2$$

where p is the pixel number. This is the calibration equation that can then turn any pixel number into the corresponding calibrated wavelength.

Using Matlab, enter the pixel numbers and the corresponding *known* wavelengths. Plot wavelength versus pixel number. It should look like a straight line, although it does have a slight curvature, which is why we'll use a second-order polynomial to fit the data. Any points not on the line were either incorrectly measured pixels or data entered incorrectly. Fix them.

Note: Be sure you're graphing λ (vertical) versus p (horizontal), not p versus λ . Also be sure you're using the known wavelengths, from the table above, not the computer-measured wavelengths.

To do the fit just adapt your fitting function to be a second order polynomial.

Finish getting your calibration equation while in lab. Then go on to the rest of the experiment. The remainder of the analysis for this section (3.) can be done later.

Now that you know the calibration equation, you can both use it and check its accuracy. Using the equation you determined from the fit and your measured pixel values at the various spectral peaks, compute the wavelengths. Now you have *measured* wavelengths.

You can determine the accuracy of your calibration by computing the *root mean square* deviation of your measured wavelengths from the known values. Calculate the *square of the* deviation for each of the 9 wavelengths, find the average of the squared deviations, then take the square root. **This is your best estimate of** $\delta\lambda$, the uncertainty in wavelength measurements that you make using your calibration equation. Report your value of $\delta\lambda$ in nm, and use this value to determine the appropriate number of significant figures to report in the remainder of this experiment.

4. **Resolution:** Lasers and LEDs. Shine a HeNe laser at a book or the side of the computer. Record the spectrum by looking at the *reflected* light. (CAUTION: It's not a good idea to shine a laser beam directly into the optical fiber.) Expand the horizontal scale to look at the region 600–650 nm. Find the wavelength of the center of the line (by measuring the pixel number and using your calibration equation) and compare it to the known value 632.82 nm. How well did you do? Is your measurement within two standard deviations ($2 \times$ your value of $\delta \lambda$) of the known value?

The laser linewidth is essentially zero (a monochromatic source), so an ideal spectrometer would show a signal at only one pixel. The fact that you see a bell-shaped curve spanning several pixels is due to the *instrumental linewidth*. We'll define the instrumental linewidth to be the full width at half maximum (FWHM) of a spectral peak from a narrow-linewidth source such as a laser.

Determine the instrumental linewidth of your spectrometer *in nm*. The instrumental linewidth is also called the *resolution* of the spectrometer. Two separate spectral lines can be resolved only if the distance between their centers is greater than the FWHM of each peak.

Compare the instrumental linewidth with your measurement uncertainty $\delta\lambda$. These are not the same thing. Which is smaller? Explain what the difference is between these two numbers.

It is interesting to compare the spectrum of the laser with that of an LED. There are several small LED flashlights of various colors in the lab. Set Averaging to 1 and, shining the light directly into the fiber, observe the spectrum of the LEDs. Record the spectra of the LEDs. Make any relevant measurements that allow you to give an accurate description of their spectra, including the FWHM. As you can see, the LED spectra are very broad compared to the laser. In fact, our spectrometer is incapable of making a direct measurement of the

spectral width of the laser and one has to resort to other techniques to get sufficient resolution.

5. **Hydrogen:** In the Atomic Spectra experiment, you spent an hour or more measuring three spectral lines in hydrogen. Install a hydrogen discharge tube and – in a few seconds – acquire its spectrum. You should see the three visible lines of the Balmer series **and** a few more lines extending into the ultraviolet. Measure the wavelengths of *as many* of the Balmer series lines as you can. Increasing the integration time will help you see the weaker lines.

Analysis: For the three longest wavelengths, compare your measured values to the accepted values listed in Atomic Spectra. Then use *all* of your experimental wavelengths to show that the wavelengths in the Balmer series (n = 3, 4, 5,...) obey the equation

$$1/\lambda = C (1/m^2 - 1/n^2)$$

To do so, use Matlab to calculate $1/\lambda$ for each n, graph $1/\lambda$ versus $1/n^2$, then add a *linear* trend line. From the slope and the intercept of the trend line (think about how much precision is appropriate for the coefficients):

- Determine C. Be sure to report it with proper units.
- Determine m. How close does it come to the theoretical value of 2?
- Determine the *series limit* wavelength of the Balmer series.
- 6. **Mercury:** Observe the mercury spectrum from a discharge tube. You should see the yellow doublet (expand it to be sure), the green, and the bright violet lines that you measured in the Atomic Spectra experiment. Focus on the doublet and see how well the spectrometer resolves the two lines. How does this compare to the resolution measurement you made in part 4?
- 7. **White light:** The spectra you have observed so far have displayed the raw output of the Ocean Optics detector. That's fine for many applications, but it doesn't allow you to compare the intensity at one wavelength to the intensity at a different wavelength. The reasons are threefold. First, the efficiency of the detector array is wavelength dependent. Second, and even more important, the efficiency of the diffraction grating is wavelength dependent. That is, the grating diffracts a larger fraction of the light energy at some wavelengths than it does at other wavelengths. Third, the optical fiber itself attenuates different wavelengths of light by different amounts.

To do *irradiance measurements*, which compare the intensities at different wavelengths, we must first calibrate the spectrometer with a *continuous* source of radiation of known intensity (or at least known relative intensities). An obvious source that meets this need is a blackbody radiator. The radiation from a black body – as given by the Planck distribution law – depends only on the temperature and not on how the object is made.

True black bodies are hard to construct, but a glowing tungsten filament is a reasonably close approximation to a black body. You have a light bulb with a bare filament. The only piece of information you need is the filament's temperature, which you can measure with a device called an *optical pyrometer* in which you match the color of the filament, as seen through a filter, to the color of a reference filament. The pyrometer is at the side of the room. Bring your light bulb to it and your instructor will show you how to use the device. Use it to measure the filament temperature. Note that the pyrometer measures in Celsius, so make sure you convert your temperature to Kelvin.

When you return to your bench drive the light bulb using the Variac, setting it at 120 V and 100%

On the toolbar above the spectra are a dark bulb and a bright bulb. These save reference spectra. Set your integration time to 10 ms, Scans to Average to 10, start acquiring a spectrum of the glowing filament, and adjust the intensity to be about half to a third of full scale. When you have this, click the bright bulb on the toolbar. Then cover the end of the optical fiber so that no light gets in and click the dark bulb on the toolbar.



To the right of the toolbar, where an S is now clicked, click on the <u>I</u> (for *irradiance*). Under the Processing menu, select Set Color Temperature and enter the temperature (in Kelvin!) that you measured for your filament.

Now observe the filament spectrum again. It should look quite different from the "raw data" spectrum you first saw. At these temperatures, the blackbody spectrum has its peak intensity at $\approx 3~\mu m$ in the infrared. You can't see the peak. Instead, you're seeing the rapid decrease of intensity on the short-wavelength side of the peak.

Note: *Once in irradiance mode, you cannot change any settings.* Don't change the integration time or the number of averages. If you need to change these, due to a very weak source, you'll need to go back to "Scope Mode," (the **S** on the toolbar) and reacquire the bright-bulb and dark-bulb spectra. However, since you've already entered the filament temperature, these only take a few seconds if you need to do so.

Another note: Be careful not to saturate the detector. This is hard to tell since you're not seeing the raw signal. The indication that the detector is saturated is a spectrum that "goes funny," such as kinks in a spectrum that should be smooth or peaks with flat tops.

You can determine the temperature of a black body by measuring the intensities at 600 nm and 800 nm and calculating the ratio I_{800}/I_{600} . The short-wavelength approximation to the Planck blackbody curve is

$$I_{\lambda} = C\lambda^{-5}e^{-hc/\lambda kT} = C\lambda^{-5}e^{-14,400,000/\lambda T}$$

where λ is in nm and T in K. C is a constant whose value we do not need because we're going to take a ratio.

As a check that we have correctly gone through the setup above, calculate the theoretical I_{800}/I_{600} ratio using the temperature of your filament, as measured using the pyrometer, and compare it to the I_{800}/I_{600} ratio measured from your spectrum. These should be the same; a reasonably close agreement (within 20%) is sufficient. A disagreement larger than 20% indicates a poorly measured temperature (the most likely cause), incorrect intensity measurements, or that you didn't follow carefully all the steps described above. Try again.

Now we can see the effect of changing the temperature of the source. Use the Variac provided to change the voltage driving the light bulb's current. Set the Variac to 50% and you will see that the bulb is much dimmer. Acquire a spectrum again – but do not adjust the settings on the spectrometer - and use the ratio of the irradiances at 800 nm and 600 nm to determine the temperature. You can check the temperature using the pyrometer and the two measurements should be in reasonable agreement.

Appendix: The Mercury Spectrum and Atomic structure

Analysis: The bright green, bright violet, and dim violet lines are transitions from the 7^3S_1 state in mercury to the three 6^3P_J states with total angular momentum quantum numbers J=0,1, and 2. (You should review atomic physics notation in the Appendix of Atomic Spectra and look at the mercury energy-level diagram at the end of that experiment.) The three P states, all with quantum numbers L=1 and S=1, are split apart by the **spin-orbit interaction**.

Electrons have a magnetic moment $\vec{\mu}$, due to their spin, with $\vec{\mu} \propto \vec{S}$. In an electron's rest frame, the positive nucleus orbits about it and – like a current going around a loop – produces a magnetic field $\vec{B} \propto \vec{L}$, where \vec{L} is the orbital angular momentum. A magnetic moment in a magnetic field (i.e., a compass needle) has potential energy $E \propto \vec{\mu} \cdot \vec{B}$. We needn't worry about the proportionality constant but can use what we've noted about $\vec{\mu}$ and \vec{B} to write

$$E_{\text{s-o}} = A \vec{S} \cdot \vec{L}$$

where A is a proportionality constant.

This is called the **spin-orbit interaction energy**. It is a magnetic energy due to the interaction of the electron's magnetic moment with the magnetic field generated by the moving charges. The size of the spin-orbit energy depends on the orientation (i.e., angle) between \vec{S} and \vec{L} . Although the three 6^3P_J states have the same total spin S and same total orbital angular momentum L, they have different angles between these two vectors and thus have different spin-orbit energies. This accounts for the energy differences between these three states that you can see in the mercury energy-level diagram.

To see how this interaction affects atomic energy levels, use the fact that the total angular momentum is $\vec{J} = \vec{L} + \vec{S}$ to write

$$J^{2} = \vec{J} \cdot \vec{J} = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S}) = L^{2} + S^{2} + 2\vec{S} \cdot \vec{L}$$
$$\vec{S} \cdot \vec{L} = \frac{1}{2}(J^{2} - L^{2} - S^{2})$$

From quantum mechanics, we know that the allowed values of J^2 are $J(J+1)^{-2}$, with a similar rule for L^2 and S^2 . Thus the spin-orbit interaction energy is

$$E_{\text{s-o}} = \frac{A\hbar^2}{2} (J(J+1) - L(L+1) - S(S+1))$$

where L, S, and J are the quantum numbers of the state. The three 6^3P_J states of mercury have the same values of L and S but different values of J, hence they each have a different energy.

Look at the energy-level diagram in Atomic Spectra. The energy difference between 6^3P_2 and 6^3P_1 (i.e., the "splitting" due to the spin-orbit interaction) is $E_{J=2} - E_{J=1}$. Similarly, the splitting between the J=1 and J=0 states is $E_{J=1} - E_{J=0}$.

Use the theoretical expression for E_{s-0} from above to find a <u>theoretical</u> value for the ratio of the energy splittings

splitting ratio =
$$\frac{E_{J=2} - E_{J=1}}{E_{J=1} - E_{J=0}}$$

Note: The energy levels listed in Experiment 2 are *experimental values*. They are not theory and have nothing to do with determining a theoretical splitting ratio.

Then use your measured wavelengths to determine an *experimental* value for the splitting ratio. How well does it compare to the theoretical value? A discrepancy between the two is an indication that our analysis of the spin-orbit interaction has been too simple – as, indeed, is known to be the case for the heavier elements in the periodic table.