Hydrogen-Deuterium Mass Ratio

1 Background

1.1 Balmer and Rydberg Formulas

By the middle of the 19th century it was well established that atoms emitted light at discrete wavelengths. This is in contrast to a heated solid which emits light over a continuous range of wavelengths. The difference between continuous and discrete spectra can be readily observed by viewing both incandescent and fluorescent lamps through a diffraction grating; hand held gratings are available for you to do this in the laboratory.

Around 1860 Kirchhoff and Bunsen discovered that each element has its own characteristic spectrum. The next several decades saw the accumulation of a wealth of spectroscopic data from many elements. What was lacking though, was a mathematical relation between the various spectral lines from a given element. The visible spectrum of hydrogen, being relatively simple compared to the spectra of other elements, was a particular focus of attempts to find an empirical relation between the wavelengths of its spectral lines. In 1885 Balmer discovered that the wavelengths λ_n of the then nine known lines in the hydrogen spectrum were described to better than one part in a thousand by the formula

$$\lambda_n = 3646 \times n^2/(n^2 - 4) \text{ Å (angstrom)}, \tag{1}$$

where $n = 3, 4, 5, \ldots$ for the various lines in this series, now known as the Balmer series. (1 angstrom $= 10^{-10}$ m.) The more commonly used unit of length on this scale is the nm (10^{-9} m), but since the monochromator readout is in angstroms, we will use the latter unit throughout this write-up.

In 1890 Rydberg recast the Balmer formula in more general form as

$$1/\lambda_n = R(1/2^2 - 1/n^2) \tag{2}$$

where again $n = 3, 4, 5, \ldots$ and R is known as the Rydberg constant. For reasons to be explained later, its value depends on the mass of the nucleus of the particular isotope of the atom under consideration. The value for hydrogen from current spectroscopic data is

$$R_{\mathrm{H}} = 109677.5810 \text{ cm}^{-1}[1],$$

and the current value for an infinitely heavy nucleus is

$$R_{\infty} = 109737.31568525(73) \text{ cm}^{-1}[2].$$

A generalization of the Rydberg formula to

$$1/\lambda = R_{\mathrm{H}}\left[\left(\frac{1}{n_1^2}\right) - \left(\frac{1}{n_2^2}\right)\right] \tag{3}$$

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suggested that other series may exist with n_1 taking on the values $1, 3, 4, 5, \ldots$, subject to the restriction that $n_2 > n_1$. This proved to indeed be the case. In 1906 Lyman measured the ultraviolet spectrum of hydrogen and found the series, now bearing his name, corresponding to $n_1 = 1$. In 1908 Paschen measured the infrared spectrum of hydrogen and discovered the series, now bearing his name, corresponding to $n_1 = 3$. Figure 1 shows some of the lines in these series. The vertical axis in this figure is linear in energy (given in units of electron-volts, or eV, at the right), so you can get some sense of the relative energies of the different series.

The remarkable success of the Rydberg formula in describing the spectrum of atomic hydrogen was in stark contrast to theoretical understanding of the atom in the early 1900's. Attempts to understand the emission of light at discrete wavelengths, or frequencies, using principles of classical mechanics and electrodynamics proved fruitless, as classical theory does not allow for an electron to circulate about a nucleus in a stable orbit. Rather, classical theory predicted that the negatively charged electron, circulating about the positive nucleus under the influence of a Coulomb potential, would emit radiation due to the centripetal acceleration associated with circular motion (recall that accelerating charges emit radiation). As the electron emitted radiation and lost energy, the orbit would shrink and eventually (in a predicted 10^{-12} seconds!) the electron would spiral into the nucleus, emitting a continuum of radiation in the process. The stability of atoms, and discrete atomic spectra clearly demonstrate that such a theory does not describe atomic behavior.

1.2   The Bohr Postulates

in 1913 the Danish physicist Niels Bohr, working at Ernest Rutherford's laboratory in Manchester, England, proposed a blend of classical and radically new ideas to describe atomic behavior. His three postulates were:

1. The electron moves in a circular orbit about the nucleus under the influence of the Coulomb potential, obeying the laws of classical mechanics;

2. In contrast to the infinite number of orbits allowed classically, the electron can occupy only orbits for which its orbital angular momentum is quantized in units of $\hbar$, i.e., $L =$ orbital angular momentum $= n\hbar$ where $n = 1, 2, 3, \ldots$. Electrons are stable in such orbits, i.e., they have a well defined energy and do not emit radiation even though they are undergoing centripetal acceleration. Bohr termed these orbits *stationary states*;

3. Radiation is emitted when an electron transitions from one stationary state to another. The energy of the radiation, $E = h\nu$, is equal to the difference in the energies of the initial and final stationary states.

The first postulate is clearly based on classical theory; however the second and third postulates marked a radical departure from classical concepts. Applying these postulates to the hydrogen atom, Bohr's model predicted the total energy of an electron in a stationary state
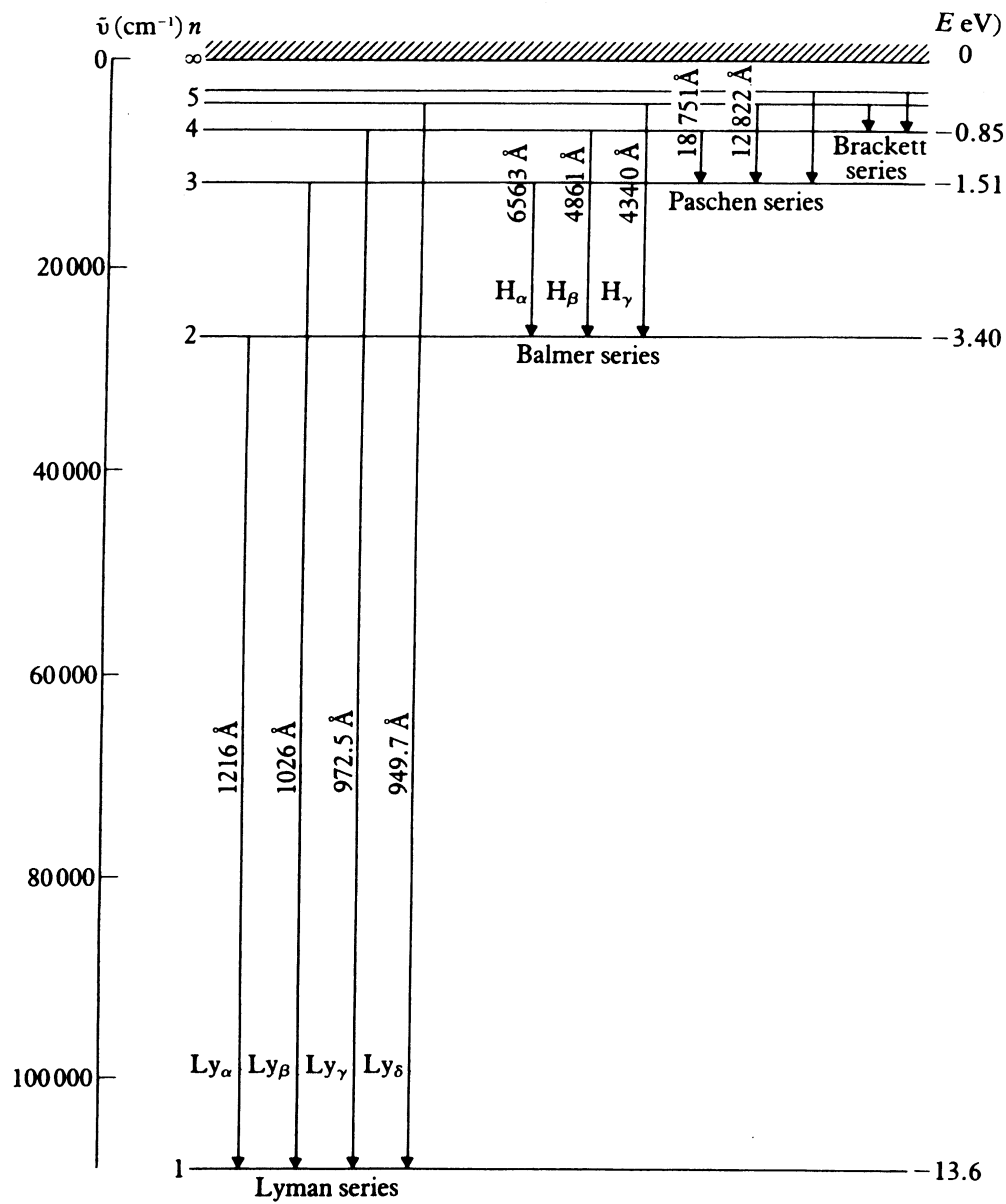
The spectrum of atomic hydrogen.

Figure 1: Energy level diagram of atomic hydrogen showing the transitions giving rise to the Lyman (UV), Balmer (visible) and Paschen (IR) spectra.

with orbital angular momentum $L = n\hbar$ to be

$$E_n = -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\frac{1}{n^2} \tag{4}$$

where m is the mass of electron, Z is the number of protons in the nucleus ($Z = 1$ for hydrogen) and e is the charge of the electron [3]. A transition from a state of higher energy to one of lower energy should result in the emission of radiation with energy

$$E_i - E_f = \frac{hc}{\lambda} = \frac{mZ^2e^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right] \tag{5}$$

where $n_i\hbar$ and $n_f\hbar$ are the electron orbital angular momenta of the initial and final states, respectively. Comparing this formula with the Rydberg formula we find that R_{H} should be

$$R_{\mathrm{H}} = \frac{me^4}{8\varepsilon_0^2 h^3 c}\ .$$

That Bohr's theory resulted in an expression for the Rydberg constant in terms of fundamental constants was a great triumph as it allowed for evaluation of the above expression and comparison to the value derived from spectroscopic data. Then current values for m, e, h and c indicated good agreement between R_{H} calculated from Bohr's theory and experimentally derived values.

But doubters of Bohr's theory remained, with skepticism on the continent being particularly strong. His brother Harald wrote Bohr in the fall of 1913 from Göttingen, Germany, saying that the physicists there considered Bohr's model to be too "bold" and too "fantastic". Rutherford himself was skeptical, asking Bohr, "How does the electron decide what frequency it is going to vibrate (radiate) at when it passes from one stationary state to another? It seems to me that you would have to assume the electron knows beforehand where it is going to stop."

And skeptics were buttressed by new experimental results. Measurements of the spectral lines of singly ionized helium (one electron orbiting around a nucleus with two protons) showed that the ratio of the wavelengths of corresponding helium and hydrogen lines (same n_i and n_f) was not 1:4 as predicted by Bohr's formula, but rather 1:4.0016. (The ratio 1:4 results from increasing Z from one to two in the above expressions for the electron energy.) Bohr quickly revised his postulates, now requiring that the *total* angular momentum, the combined angular momentum of both the electron *and* the nucleus, be quantized in units of $\hbar$. The result of this requirement is that in the expression for the electron energy, the electron mass m must be replaced by the reduced mass μ,

$$\mu = mM/(M + m) \tag{6}$$

where M is the mass of the nucleus. (See the appendix for a derivation of this result.) The expression for the radiation energy of hydrogen-like ions (i.e., one electron orbiting Z protons) is now

$$E_i - E_f = \frac{hc}{\lambda} = \frac{\mu_X Z^2 e^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right] \tag{7}$$

where μ_X is the reduced mass of atom X. According to Bohr's revised theory, the wavelength ratios between corresponding hydrogen and helium lines should be $4\mu_{\text{He}}/\mu_{\text{H}}$. It turns out that

$$\frac{\mu_{\text{He}}}{\mu_{\text{H}}} = 1.0004 \ ,$$

(you may wish to verify this) resulting in complete agreement between theory and observation. When Einstein learned of this latest success of the Bohr theory, he responded: "This is an *enormous achievement*. The theory of Bohr must then be right."

The inclusion of the nuclear mass M into the equation for the spectral energies indicates that different isotopes of the same element should show different spectra, since these atoms would have different reduced mass. The existence of the isotope of hydrogen, deuterium, whose nucleus contains one neutron and one proton, was discovered by Harold Urey and his co-workers around 1930 using spectroscopic methods after they successfully produced samples of deuterium-enriched hydrogen by a distillation process [4]. Harold Urey was awarded the Nobel Prize in Chemistry in 1934, "for his discovery of heavy hydrogen."

2 The experiment

Experimental Goal: measure the hydrogen-deuterium nuclear mass ratio.

In this experiment you will measure the wavelengths of both the hydrogen and deuterium spectral lines for at least four transitions in the Balmer series. From a plot of measurements of the wavelength difference for a set of transitions, you will derive the ratio of the masses of the hydrogen and deuterium atoms.

The spectral lines are produced by a gas discharge lamp. In our setup, the lamp contains hydrogen enriched with deuterium so that both spectra are produced simultaneously. Enrichment of the hydrogen is necessary as the natural abundance of deuterium is about .015%.

From the Rydberg formula corrected for reduced mass, Eq. (7), we see that the wavelength of light emitted from a particular transition is inversely proportional to the reduced mass:

$$1/\lambda_X \propto \mu_X \ . \tag{8}$$

Because of this proportionality, we see that the nuclear masses of hydrogen and deuterium, M_{H} and M_{D}, are related to the different wavelengths of light produced by each isotope:

$$\frac{\Delta\lambda_{\text{HD}}}{\lambda_{\text{H}}} = \frac{\lambda_{\text{H}} - \lambda_{\text{D}}}{\lambda_{\text{H}}} = \frac{1/\mu_{\text{H}} - 1/\mu_{\text{D}}}{1/\mu_{\text{H}}} = \frac{1 - M_{\text{H}}/M_{\text{D}}}{1 + M_{\text{H}}/m} \ . \tag{9}$$

The mass M_{H} is, of course, just the mass of the proton M_p, and the ratio of the proton and electron masses is well known, $M_p/m = 1836.15$. Combining this with the results of your measurements, the ratio of the masses of the two nuclei, $M_{\text{H}}/M_{\text{D}}$ can easily be derived and compared to established values:

$$\frac{M_{\text{H}}}{M_{\text{D}}} = \frac{1.007276}{2.013553} = 0.500248 \ .$$

Extension Ideas

1. Try to measure the H$_\epsilon$ peak and compare to your other measurements. Investigate the λ dependence of your measured ratio, if any.

2. Use the setup to measure the emission spectrum of a light source of your choice (some bulb, a mobile phone LED, etc).

3   Apparatus and Procedure

Before describing the apparatus and measurement process, it is instructive to observe the difference between continuous and discrete light sources. Turn off the bright fluorescent tube lights in the experiment area and turn on the smaller overhead lights in the cylindrical shades. Take one of the slide-mounted diffraction gratings and look at the two overhead lights in the cylinders near the experiment and near the desk area. One of the bulbs is incandescent and the other fluorescent. The fluorescent bulb emits light at discrete wavelengths in the mercury spectrum, and the incandescent bulb emits light over a continuum of wavelengths. The colored images overlap, so make sure you identify which image goes with which bulb. Describe the images you see from each bulb, and justify your claim as to which one is the fluorescent bulb.

3.1   Apparatus

A diagram of the apparatus is shown in Fig. 2. Light from a discharge tube containing both hydrogen and deuterium is focused by a lens onto the entrance aperture (slit) of the monochromator. (A monochromator is just a spectrometer that detects one wavelength at a time.) The dispersive element, i.e., the element which separates light according to its component wavelengths, inside the monochromator is a diffraction grating—a fancier version of the hand held grating you used to look at the overhead lights. The angle of the grating and mirrors inside the monochromator can be varied with the wavelength-adjust knob to select the wavelength of the light passing through the exit slit and on to the detector. The detector is a photomultiplier tube (PMT) located inside the housing attached to the exit slit port. The readout dial on the front of the monochromator indicates the wavelength of the detected light to the nearest angstrom.

The output of the PMT is a current, typically a fraction of a microampere at maximum detected light intensity in this experiment. The PDA-700 amplifier converts this current to a voltage which is recorded on a chart recorder or digital scope. To record the output light intensity over a wavelength interval, a stepper-motor + reduction-gear drive is attached to the wavelength adjust shaft. Here are some numbers to help you get a sense of the scan rate:

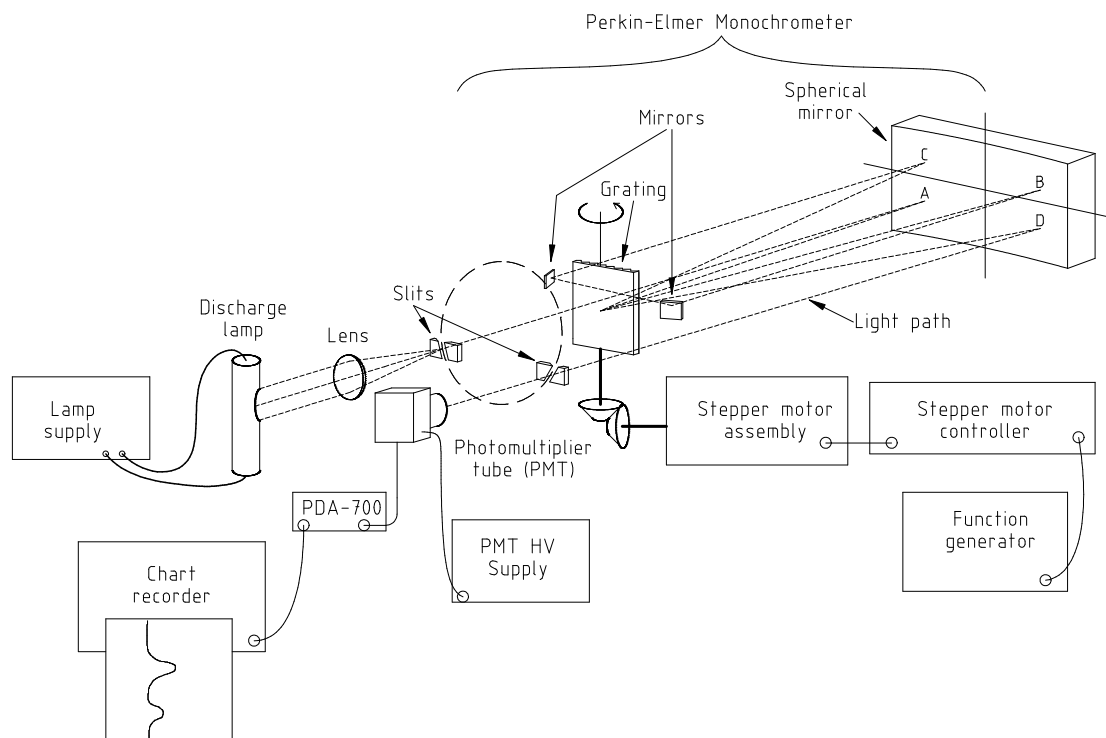|	
Stepper motor:	200 steps per revolution of output shaft
Reduction gear ratio:	1:36
wavelength adjust shaft:	20 Å per revolution.

Figure 2: Apparatus used to measure the spectral lines of the hydrogen-deuterium lamp.

You do want to record data slowly and smoothly, but you don't want it to take all day. The following exercise will help you develop a good first set of scanning parameters, you may adjust them from there at your discretion.

Exercise 1 *As an initial estimate of the experimental parameters, calculate the difference in wavelengths of the hydrogen and deuterium α lines, assuming that the mass ratio is 1:2. Then also calculate the difference in wavelength of the sodium D lines, listed in section 3.2. What would be the expected ratio of peak separations, $\Delta\lambda_{HD}/\Delta\lambda_{Na}$?*

Now assume you want to place the D lines about 40 seconds apart. What should the stepper-motor control frequency be? How many seconds separation would this rate give for the α lines?

Feel free to speed up or slow down the stepper motor rate and scan speed from these starting values as you see fit, but keep the rate below 100 Hz. (It is hard on the apparatus to use a high frequency.) However, once you are comfortable with your scanning rate, it is recommended to use the same set of values for all of your measurements.

The monochromator does not detect light at just a single wavelength but rather detects light over a small spread of wavelengths centered about the wavelength indicated on the readout dial. Here we face the common trade-off between signal strength and resolution. The width of the entrance and exit slits is variable, and is set (for both slits simultaneously) by the slit width control. Increasing the slit width allows more light to come through, but degrades the resolution of the monochromator. For the purposes of this experiment, a slit width of about

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50 microns allows for a good signal level and more than adequate resolution; the slit readout should show "0 0 50".

3.2   Calibration standards

As mentioned above, the readout dial indicates the absolute wavelength to the nearest angstrom. We are working with wavelength *differences* on the order of 1 Å, and will want to measure the $\lambda_H - \lambda_D$ interval to fractions of an ångstrom, which is not possible using the wavelength readout.

To calibrate the monochromator output, the wavelength difference between the two lines of the yellow sodium doublet, the 3^2S–3^2P transition, is used as a standard. The wavelengths of these two lines, called "the sodium D-lines," are

$$
\begin{array}{ll}
D_1: & 5895.92 \text{ Å} \\
D_2: & 5889.95 \text{ Å}
\end{array}
$$

The calibration procedure will be described in detail below.

For reference in the next section and for use in data analysis, we also state the wavelengths of the four strongest Balmer lines:

$$
\begin{array}{ll}
H_\alpha: & 6562.852 \text{ Å} \\
H_\beta: & 4861.33 \text{ Å} \\
H_\gamma: & 4340.47 \text{ Å} \\
H_\delta: & 4101.74 \text{ Å}
\end{array}
$$

It is possible, with some effort, to measure higher energy lines in this series as well.

Exercise 2 *Calculate the wavelengths of the next three higher-energy lines in the Balmer series from Eq. (3).*

3.3   Procedure

Turn on the power supply for the sodium discharge lamp. Press the white button on the power supply if the lamp does not start. It will take a little while for the lamp to reach full intensity, but you can begin aligning the optics and looking for a signal before it is fully warmed up.

The wavelength interval of the sodium lines is used to calibrate the recording apparatus, and the peak separation is much greater for the sodium doublet than for the hydrogen-deuterium splitting, so it is best to run the sodium scans first to establish the scan settings.

Turn on the power to the SRS Model PS 325 high voltage power supply and the PDA-700 amplifier. The PDA-700 should be on the ".xxxx" microamp range. This corresponds to a maximum current of 2.000 μA.

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If the stepper motor drive coupling is still attached to the wavelength adjust shaft, remove it. A hex-socket (Allen) wrench is available for attaching and removing the coupling from the wavelength-adjust shaft. Turn the know smoothly to set the wavelength to approximately 5890 Å. (Please be gentle: small parts inside the monochromator are easily damaged by rough treatment.)

Remove the plastic dust cover from the lens. Check that the distance from the sodium lamp to the lens is about 240 mm and that the distance from the lens to the entrance slit is also about 240 mm (this corresponds to a carriage position of 725 mm on the optical track). The focal length of the lens is 120 mm, so these distances will result in the formation of an image of the lamp with magnification 1 at the entrance slit. Adjust the lamp position to optimize the focus of the image on the entrance slit.

Exercise 3 *Prove the above claim about the image of the lamp by making a ray diagram.*

Check that the high voltage setting displays "1000" volts. This is the number that should be displayed at the center of the high voltage power supply. Turn on the high voltage with the switch at the lower left of the front panel. The output voltage should read -1000 volts (polarity is negative) within a volt or two. Slowly scan *by hand* through the D_2 line at 5890 Å while watching the PDA-700 reading; you should see an increase in the PMT output current as you scan through the line. Keep turning the knob and scan through the second D-line, D_1 at about 5896 Å to verify that you are seeing both peaks. Scan back through the lines and set the wavelength on D_2 to give maximum output current, typically about 0.1 microamp for a slit width of 50 microns. (Note: the exact value is unimportant, and your value may be very different depending on how warmed up your lamp is and how well aligned your setup is.) Then fine-tune the focus by moving the lamp carriage along the track, looking for maximum output. If you are having trouble getting any output, consult with the TA, Professor or Lab Manager.

Once you are getting a signal from the sodium lamp, log into the computer near the setup. It is connected to a National Instruments (NI) data acquisition system. The NI box will be used with a LabVIEW application that acts as a chart recorder. Start the **Chart Recorder** application from its icon on the desktop.

After the Chart Recorder application starts, click on the tabs at the top left to set the scan parameters. The following settings should produce a nicely visible trace (if the setting is not specified, the default value is acceptable):

Channel 1 Check Enable Ch 1. Also check Invert signal; the current from the detector (and thus voltage from the current amplifier) is negative, so this option makes the peaks point up rather than down.

Sample Clock The sample clock controls how often a measurement is recorded by the interface box. We will use a little signal averaging to reduce noise. Check Pre-bin samples and set Bins/Read-cycle to 10.

Go back to the Scan Controls tab, click TAKE SCAN, and see what you get as you manually turn the knob through the two sodium lines.

When you can see a signal with the manual scan, then connect the stepper motor as follows:

1. Make sure that the switch box between the function generator and the stepper motor controller is *off*, and turn on the power to the digital function generator.

2. Set the function generator frequency to 60 Hz by using the keypad on the front panel: push FREQ/PER, then 6, 0, then the units key Hz Vpp. By using the STEP SIZE button and the Up/Down buttons to select the 10's column (it will flash), you can then change the frequency quickly in steps of 10 Hz with the Up/Down buttons.

3. Turn on the switch box briefly to verify that the motor shaft turns. You may safely run the function generator up to 150 Hz for small adjustments, but for data taking, the frequency should be set at a value below 100 Hz.

4. Set the wavelength 2–3 angstroms less than the D_2 wavelength. Connect the stepper motor drive coupling to the shaft: **Note the location of the "FLAT" on the shaft. Turn the knob so that the FLAT is at the same angle as the set screw on the coupling. Then push the coupling onto the shaft and *tighten the set screw by hand* against the FLAT. Use the Allen wrench to make the screw snug against the shaft. *DO NOT OVER-TIGHTEN THIS SCREW!!* Just tight enough to keep it from getting loose is enough—over-tightening only wrecks the apparatus.**

Select the *increasing* wavelength direction on the stepper motor controller, and turn on the power to the controller.

Start the stepper motor by flipping the switch on the box between the generator and the stepper-motor controller on, then immediately click TAKE SCAN on the Chart Recorder. Watch to see the sodium peaks recorded.

After you have scanned through the lines, stop the scan and turn off the pulse train with the switch box. *Do not turn off the stepper motor controller power.* The sodium peaks should be well-shaped and pointed at the tops. If they are rounded or flattened at the tops, you have too much gain on the PDA-700 current amplifier. Reduce the Range switch on the amp, and try another scan.

IMPORTANT: **Once you decide on a stepper-motor frequency and chart speed, you must stick with it for all of the measurements, otherwise your calibration will be ruined. Also, scan in the same direction of "increasing wavelength" for all runs.**

You can filter noise with the Low Pass Filter settings. Do not be to aggressive with these filters! You do not want to distort the underlying signal, just remove the "fuzz" that may be obscuring the important response to the varying light intensity. See the effect of the different filter options on your scan. A good starting choice is the "Smoothing" filter with a setting of 5 points.

Save the scan in local memory to look at it later by clicking RETAIN SCAN. If you give the scan a name (in Scan Name), e.g., "Na cal", it will save this name with the scan. Otherwise it will use the default. Subsequent RETAIN SCANs will save more scans with the assigned name and a number.

A scan you want to save permanently should be saved to disk by clicking SAVE TO FILE. It is recommended to use the file extension .wfm, which indicates that it is a LabVIEW "waveform" file (a binary format). You can also load old scan files into the application to study and manipulate them.

While you are taking your good calibration scan, turn on the H-D discharge lamp and the cooling fan (separate power supply). The discharge tube runs very hot, and cooling it with the fan will help extend the lifetime of this expensive ($500) tube.

After the sodium scan is finished, turn the sodium lamp off, and carefully loosen the carriage screw and lift the carriage and lamp off the track. Place it on the track behind the H-D lamp, and then slide the carriage for the H-D lamp into the same position as the sodium lamp was.

The image of the H-D lamp is much narrower than that of the sodium lamp, so alignment is critical here. Check that the image of the lamp falls on the curved entrance slit to the monochromator (may be necessary to dim lights to see this). To see the slit better, you may want to open it up to 100 microns or more. Note that the lamp needs to be slightly tilted to maximize the coverage of the slit with the image of the lamp, as the slits are off-center of a circle at the focal plane of the monochromator (see Fig. 2) If the image does not fall on the slit, it may be necessary to move the lens back and forth across the light path with the small brass adjust screw marked with yellow tape at the base of the lens holder. If the beam is far out of alignment, it may be necessary to move the entire base on which the lamp and lens are mounted. If this seems to be necessary, please ask for help from the TA, Professor or Lab Manager. After checking the image alignment, reduce the slit width back to approximately 50 microns.

Remove the stepper motor drive. Dial in the approximate wavelength value for the H_α line (see table in the calibration standards section). As you did before, scan slowly through the H_α and D_α lines by hand.

The sodium lamp is considerably more intense than the H-D lamp so it will be necessary to increase the sensitivity ("range") of the PDA-700. As before, use the Wavelength knob on the monochrometer to park the wavelength at one of the H-D peaks and fine-tune the lens position by alternately moving it transversely with the yellow screw and also fine-tune the focus by moving the lamp carriage along the track until you obtain maximum output. If you are having trouble getting any output, ask for help!

Do not change the function generator frequency! If you do, you will have to repeat the Na calibration. Run a scan through both the H_α and D_α lines. Adjust the "range" of the PDA-700 if needed.

The result of the scan should be a trace showing a pair of peaks of unequal height (fractions of H and D in tube are not equal), with each peak having a symmetric or nearly symmetric shape. If you are not satisfied with the results of the scan, you can repeat it: switch to

"decreasing λ" on the controller, dial the frequency up to 100–140 Hz, run the wavelength back down through the lines, and then repeat the above procedure. *Don't forget to reset the frequency on the generator to the correct value.*

Caution: when you reverse the scan direction, you need to allow the "backlash" in the gears to be taken up before recording your lines. If you fail to do this, you may see significant distortions in your trace: a peak will have a large flat part in the middle of it.

Don't forget to RETAIN and then SAVE TO FILE your best scans.

After successfully recording the H_α and D_α lines, remove the stepper motor drive coupling from the shaft. Adjust the wavelength to near the H_β line and repeat the checkout and scan process as above. (You do not need to readjust the lamp and lens position.) The signal strength of the H_β and D_β lines is different from that of the α lines. This is due to both a difference in light intensity at these wavelengths, and in sensitivity of the photomultiplier tube. (Study the sensitivity chart for the tube in the book which describes the apparatus; does it make sense?) It may be necessary to switch the PDA-700 to a different range to achieve a suitable displacement on the recorder.

After successfully recording the β lines, proceed to record the γ and δ lines. As the line strength decreases, you may need to adjust the PDA-700 gain to obtain peaks of reasonable height. You could also try to get the ε lines; these will be noisy.

You should have at least 5 scans total: the sodium lines and and at least four pairs of H-D lines.

After finishing collecting all of your data, turn off the H-D lamp, and five minutes later turn off the cooling fan. Turn off all other electronics (except the computer), put the plastic cover over the lens, and remove the pen and put the cap back on it.

Before closing the Chart Recorder application, make sure to

- Save the raw data for each scan with SAVE TO FILE and use the file extension `.wfm`.

- Filter, adjust the range, and export each data set so that it can be analyzed with another computer program (e.g., Python). See how to do these operations in the descriptions below.

- Make and export a plot of each scan to put into your notebook.

Make a copy of the data for each partner. Each person should carry out the data analysis separately.

Using the chart recorder plot controls

To adjust, analyze, or export chart recorder data, open the waveform file with the Chart Recorder application (or select it from the "retained scans" list, if it is still available). Then use the features under **Plot Controls and Adjustments** to manipulate the trace and

prepare it for exporting or printing. Here are the options.

Filters

There are three types of data "smoothing" or "low-pass" filters you may apply. Each only affects the displayed data, and may be added or removed at will.

LP Butterworth is a digital implementation of a "Butterworth" low-pass filter. It treats the data set as if it were a signal fed into an analog multi-stage LRC filter. The corner frequency of the filter is set by the "Time constant". Longer time constants have a stronger effect. One side-effect of using this filter is that it always forces the trace to start at zero (similar to the initial response of an uncharged RC filter). If your data starts near zero, this distortion may be minimal.

Smoothing Filter uses a simple data smoothing algorithm called "Savitzky-Golay." Briefly, the method replaces each data point with a weighted average of that data point and a selecton of neighboring data points. The more points you include (set by "Smoothing filter bins") the more strongly the data set is smoothed out.

Median Filter is a nonlinear filter that is similar to the Smoothing filter in that it averages over neighboring data points, but in this form the data points are replaced by the *median* value rather than a weighted average. This type of filter tends to preserve sudden overall changes in the trace level. One side effect is that as the number of "Median filter bins" is increased, the trace will take on a blocky or stair-step appearance.

However you use the filters, the proper amount of filtering should not noticeably affect the overall shape of the trace. Use filtering sparingly!

Number of points

This control allows you to replace the trace's original data with a set of interpolated points. For slow scans, the data sets may get very large, with many more points than one needs. This may be annoying when you want to import a data set into another application, such as a spreadsheet or Python notebook.

You can see the effect of changing the number of points by selecting this option and observing the trace. The default number is 1000 points, but you may select any number, even more points than the data set contains.

You should adjust the number of points *after* you have applied any filters. (See what happens if you do it in the other order.)

To make a set for export, use this feature before selecting Export Plot.

Crop Visible

This control allows you to Zoom into a portion of the trace, or extract a portion for export. There are two steps to use this control:

SELECT X REGION Click this button and two vertical blue cursors will appear. Use the mouse to move them so that they surround the region of interest you wish. Then click

the button again to extract the cursor locations. These will show up in the Low and High displays.

Enable This checkbox does the work. When selected, the data will be cropped to the selected range. Deselecting the checkbox brings the original range back into view.

One use for this feature is to get a better resolution on the positioning of the Measure cursor (see below). When you Zoom into the data, the smallest division recorded by the cursor decreases.

Export Plot

This is the output control for data sets to be plotted or to create a file usable by other applications.

EXPORT PLOT DATA builds a spreadsheet file (of type "CSV", or "comma-separated values") with columns for each of x-values and y-values. The values exported are subject to the results of the three previous adjustments (filtering, point interpolation, and cropping). You get the traces you see on the screen as a data file.

PRINT PLOT Opens a dialog box that shows only the plot window and a text box. You may add notes to the text box to describe what you see. Then you can send the results to the default web browser for the computer. From the browser you may cut and paste into your notebook, or print to PDF, or whatever you like.

After obtaining images of possibly cleaned-up data traces, you may use the Measurement Cursor to extract the locations of various features from the data and create spreadsheets for each.

Use of the Measurement Cursor is straightforward. Click the CENTER CURSOR button at the lower right of the Chart Recorder to bring the red cross-hairs into the center of the plot screen. Drag the cursor to the location of the feature you want to record.

Click CAPTURE CURSOR in the box at the lower left of the Chart Recorder. The coordinates of the cursor will appear in the little spreadsheet.

After the cursor is captured, you may edit/modify the Scan Name/Label cell, for example, to record the voltmeter value corresponding to a particular calibration point. (Note: do not edit this cell until the coordinates have been captured. See what happens if you violate this rule!)

After you have collected the points you need, click EXPORT TABLE to export the table to Microsoft Excel. Unless Excel has already been started, this may take a minute—have patience. Excel will open, and from here, you may edit the file and then save it.

3.4   Data reduction and analysis

Load the exported data file into your favorite computer program (e.g., Python). Then you have a couple options:

1. Make a curve fit to each peak, and use the fit parameter for center of the peak. This works best with symmetric peaks, because most peak functions are symmetric about their center, such as a Gaussian or Lorentzian.

2. Calculate a "centroid" which is a weighted average of the counts per channel. The centroid would be given by the formula

$$X_{\text{centroid}} = \frac{\sum x_i n_i}{\sum n_i} \,, \tag{10}$$

where the index i runs over the channels included in the peak. Note: a "channel" is a time value in scope file.

After you have found the peak positions, and determined the statistical uncertainty in each, use your Na D lines to make a calibration conversion: change the horizontal separation from inches or time into ångstroms of wavelength difference.

Then make a plot. Equation (9) suggests that $\Delta\lambda_{\text{HD}}/\lambda_{\text{H}}$ should be constant. How can you plot your data in a way that gives that constant from a line fit?

Some things to think about and discuss:

- How consistently do the data follow the predicted relationship? Are there obvious outliers?

- How should you deal with the fact that your calibration (the Na Lines) is also a measurement with uncertainty?

- What would happen if the calibration lines had a mistake (say, by being too far apart)?

Appendix – Reduced mass

Consider a classical system of two particles of mass M and m interacting via central forces (i.e., Coulomb or gravity). Let the position vector between the two particles be $\vec{r}$. When no external forces act on the system, the center of mass $\vec{R}$ will be at rest with respect to some inertial reference frame S. The center of mass is defined as

$$\vec{R} = \frac{M\vec{X} + m\vec{x}}{M + m} \,, \tag{11}$$

where $\vec{X}$ and $\vec{x}$ locate the particles of mass M and m with respect to the origin of S, and $\vec{x} = \vec{X} + \vec{r}$. Since the center of mass is at rest with respect to S, a physically equivalent reference frame S' has its origin at the center of mass itself; in S', the center of mass of the system

$$\vec{R}' = \frac{M\vec{X}' + m\vec{x}'}{M + m} = 0 \,. \tag{12}$$

Hence $M\vec{\boldsymbol{X}}' = -m\vec{\boldsymbol{x}}'$. It is still true that $\vec{\boldsymbol{r}} = \vec{\boldsymbol{x}}' - \vec{\boldsymbol{X}}'$, since $\vec{\boldsymbol{x}}$ and $\vec{\boldsymbol{X}}$ are related to $\vec{\boldsymbol{x}}'$ and $\vec{\boldsymbol{X}}'$ by a simple translation. These two equations can be solved to yield

$$\vec{\boldsymbol{X}}' = -\frac{m}{m+M}\vec{\boldsymbol{r}}\,, \tag{13}$$

$$\vec{\boldsymbol{x}}' = \frac{M}{m+M}\vec{\boldsymbol{r}}\,. \tag{14}$$

In S' the energy of the two particle system is given by

$$E = \frac{1}{2}m\dot{x}'^2 + \frac{1}{2}M\dot{X}'^2 + V(r)\,, \tag{15}$$

where the "dot" notation indicates a derivative with respect to time and $V(r)$ is the potential energy between the two particles. Upon taking derivatives of Eqs. (13) and (14) and substituting the result into the energy equation one obtains

$$E = \frac{1}{2}\left(\frac{mM}{m+M}\right)\dot{r}^2 + V(r)\,. \tag{16}$$

Clearly, the expression in parenthesis in the above equation is the reduced mass μ. An advantage of expressing the energy in terms of μ is that one transforms the problem of two particles of masses m and M into a problem of one particle of mass μ. A similar calculation shows that one can write the angular momentum about the center of mass in a similar way:

$$\vec{\boldsymbol{L}}' = \left(\vec{\boldsymbol{x}}' \times m\,\dot{\vec{x}}'\right) + \left(\vec{\boldsymbol{X}}' \times M\,\dot{\vec{X}}'\right) = \vec{\boldsymbol{r}} \times \mu\dot{\vec{r}}\,. \tag{17}$$

In the Bohr model and in the subsequent Schrödinger theory, these classical results translate directly into their quantum equivalents.

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