

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 photomultiplier tubes.

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 angstroms) 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!). 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 2-9 for more details on the spectrometer design and components.

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 ($T \approx 5000^\circ \text{C}$), 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.

Part I - 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. 2-1, 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.

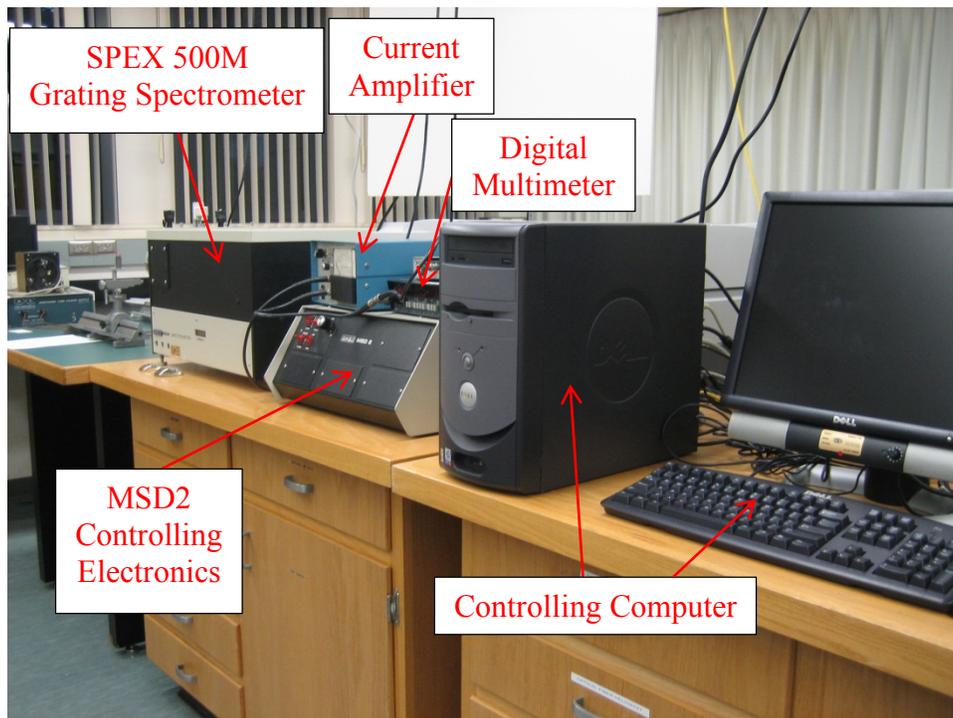


Fig. 2.1 The SPEX 500M grating spectrometer with controlling electronics and computer.

The optical system consists of an entrance slit, a collimating mirror, the grating, a focusing mirror, and an exit slit (see Fig. 2-3 in the Appendix on page 2-9). 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. 2-2) The light which passes 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 a printout at the computer called Waller. A more detailed description of the spectrometer system is given in the Appendix (see page 2-9).

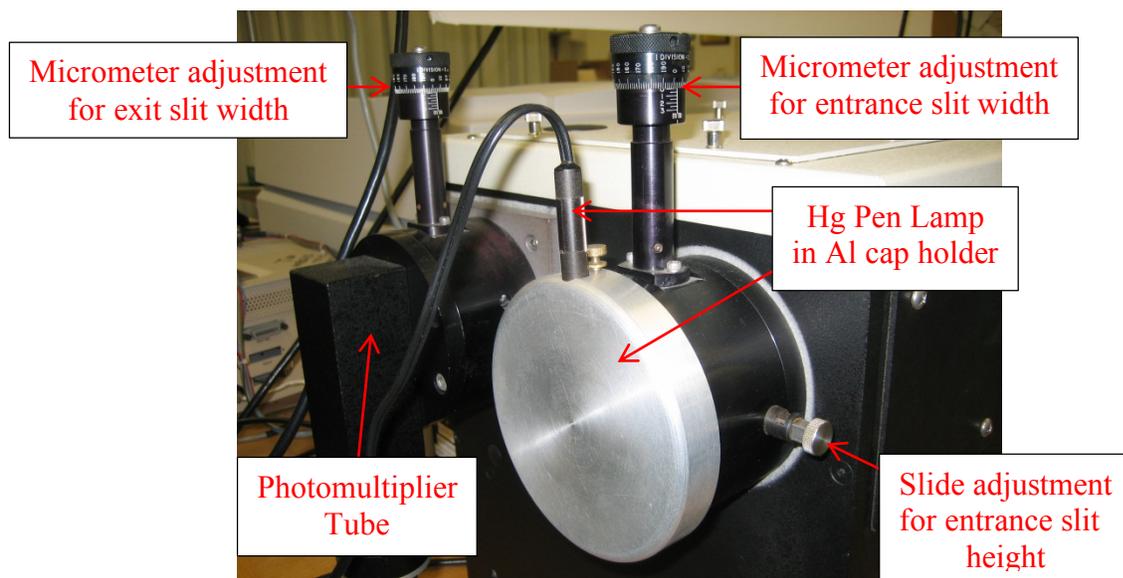


Fig. 2-2 The entrance and exit slits of the SPEX 500M grating spectrometer.

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 that 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 $6\ \mu\text{m}$. (One small division on the slit micrometers equals $2\ \mu\text{m}$.) 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 set at -900 volts). Use the 1 microamp 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 (2 nd order 312.566 nm)
507.304 nm (2 nd order 253.652 nm)	730.030 nm (2 nd order 365.015 nm)

In addition, you may want to check the calibration of the instrument across its entire range of 0 to 1500 nm by scanning the lines:

871.670 nm (2 nd order 435.835 nm)
1092.148 nm (2 nd order 546.074 nm)
1307.505 nm (3 rd 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 measurements are.

Notice that the computer always begins a scan by moving 10 nm (100 angstroms) 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 non-linearities 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.

IMPORTANT MESSAGE CONCERNING THE SPECTROMETER PHOTOMULTIPLIER TUBE

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 MICROAMPERES. Should you exceed 100 μA , there is a good chance you will damage the phototube 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 attenuate the source intensity to insure 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.

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 measured 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 2-9 through 2-12) 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.

Part II - Measurement of the Hydrogen Spectrum or the Solar Spectrum

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. 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. Also, the high precision of your measurements will require you to convert the measured wavelengths in air to wavelengths in vacuum before plotting and fitting your data. 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.

The Solar Spectrum

You will need a little luck with the weather, 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 now 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!

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

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 meter 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 Eisberg and Resnick.

The Mercury Linewidth

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 meter 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 fit with a Lorentzian. Also, do you notice a hint of self-absorption in the spectral profile?

Appendix to Experiment 2

The SPEX 500M Scanning Grating Spectrometer

Two top views of the optics of the spectrometer are sketched in Fig. 2-3. 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. 2-3, 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. 2-3, the grating is rotated by an angle β so that light is incident upon the grating at an angle $\phi = \alpha + \beta$. The light focused onto the exit slit must now be diffracted away from the specular reflection by an angle $\theta = 2\beta$. Hence the $m = -1$ diffraction maximum of wavelength λ appears at the exit slit, according to the relation

$$d \sin \phi - d \sin(\phi - \theta) = m \lambda \quad (2-1)$$

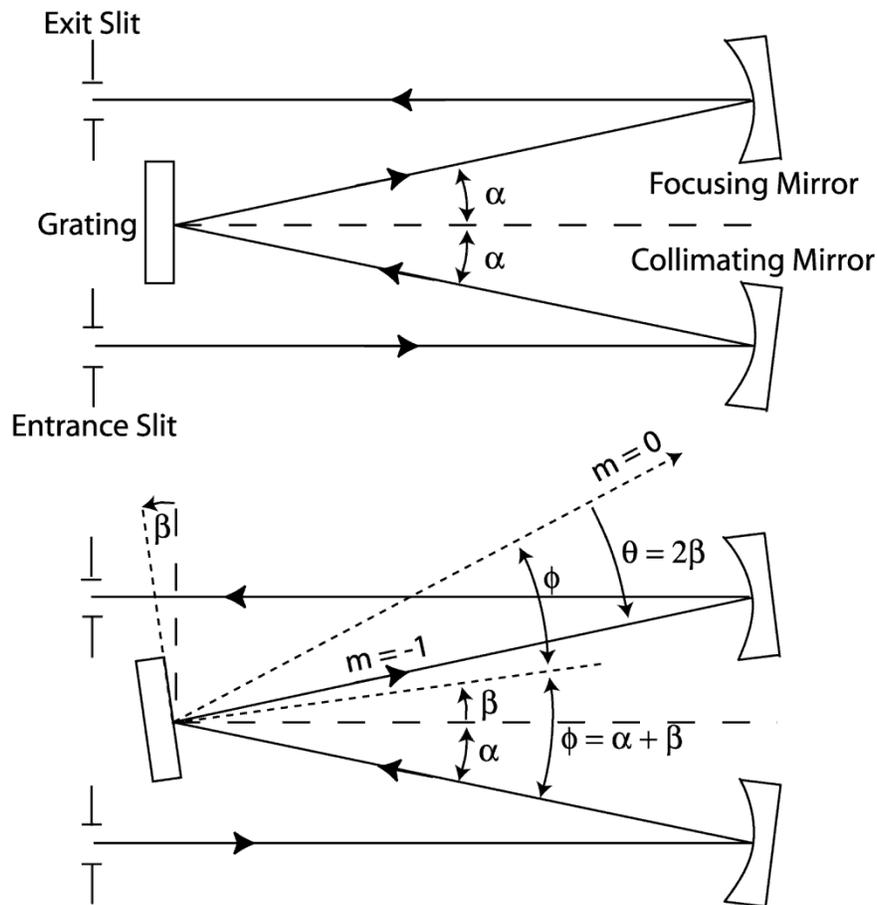


Fig. 2-3 The design and operation of the SPEX 500M Spectrometer.

In Eq. (2-1), d is the grating spacing, m is the diffraction order, and λ is the wavelength.

Eq. (2-1) can be derived readily by examining Fig. 2-4. 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 $d \sin \phi$ 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 $\phi - \theta$ with respect to the grating normal. This time the upper ray travels a distance $d \sin(\phi - \theta)$ shorter. Considering the total path length to and from the grating, the upper ray travels a longer distance, $d \sin \phi - d \sin(\phi - \theta)$. When this extra

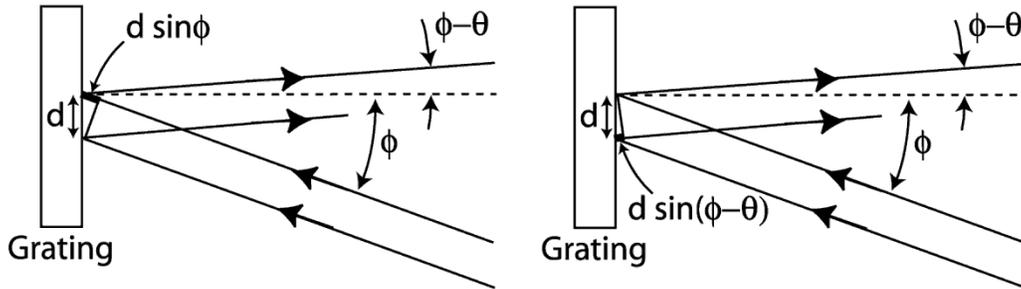


Fig. 2-4. Derivation of the grating equation in reflection geometry.

distance is equal to an integer number of wavelengths $m\lambda$, the diffraction maximum is focused onto the exit slit in accordance with Eqn. (2-1).

Using $\phi = \alpha + \beta$ and $\theta = 2\beta$, Eqn. (2-1) can be rewritten

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

which reduces to

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

Eqn. (2-2) relates the grating tilt angle β to the wavelength of the first order maximum that is focused onto the exit slit.

Fig. 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 Eqn. (2-2) we get

$$\lambda = \frac{2d \cos \alpha}{mL} x \quad (2-3)$$

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

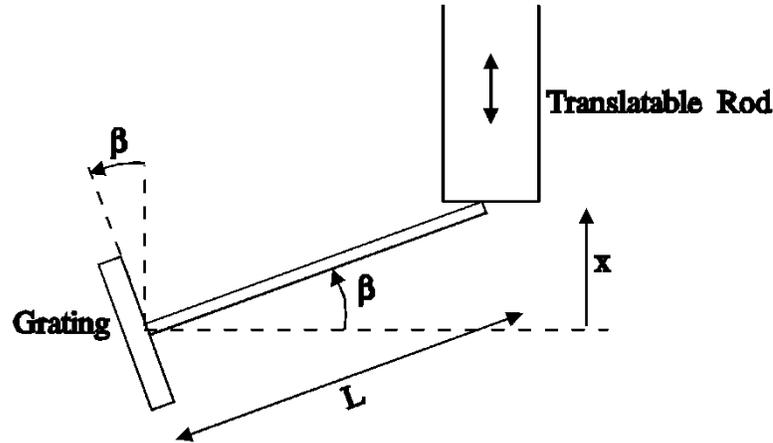


Fig. 2-5. The sine bar.

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 Eqn. (2-1) with respect to θ while holding the angle of incidence ϕ constant:

$$\frac{d\lambda}{d\theta} = \frac{d \cos(\phi - \theta)}{m} \quad (2-4)$$

The dispersion is often expressed as 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. (2-4), we get

$$\frac{d\lambda}{dy} = \frac{d \cos(\phi - \theta)}{mf} \quad (2-5)$$

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 $\cos(\phi - \theta) \approx 1$, then the dispersion in first order ($m = 1$) is according to Eqn. (2-5)

$$\frac{d\lambda}{dy} = \frac{833 \text{ nm}}{500 \text{ mm}} \cong 1.67 \frac{\text{nm}}{\text{mm}} \quad (2-6)$$

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 $(1.67 \text{ nm/mm}) (10 \mu\text{m}) = 0.0167 \text{ nm} \approx 0.17 \text{ angstroms}$. 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 angstroms. At a wavelength of 550 nm, a resolution of 0.03 nm gives a resolving power of

$$R \equiv \frac{\lambda}{\Delta\lambda} = \frac{550 \text{ nm}}{0.03 \text{ nm}} \approx 18,000 \quad (2-7)$$

This value is quite a bit less than the theoretical resolving power of the grating $R \equiv N m$ 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.