DIFFRACTION GRATINGS IN SPECTROSCOPY

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Reference: Carroll, Bradley W. & Ostlie, Dale A. (2007), *An Introduction to Modern Astrophysics*, 2nd Edition; Pearson Education - Chapter 5, Problem 5.2.

Jenkins, Francis A. & White, Harvey E. (1957), *Fundamentals of Optics*, 3rd Edition; McGraw-Hill - Chapter 17.

One of the main sources of information about celestial objects is their spectrum. In the case of light from a star, the spectrum can tell us a lot about the composition of the star, and the Doppler shift can tell us the star's radial velocity.

Getting a detailed spectrum of a star is somewhat more involved than just passing its light through a prism, as Newton famously did to show that white light is composed of the colours of the rainbow. In practice, a *diffraction grating* is used to split starlight into its constituent spectral lines. A complete treatment of the physics of diffraction gratings is beyond the scope of this post, so if you're interested I'll refer you to any good textbook on optics. [My own reference, the book by Jenkins and White mentioned at the top, is quite dated now, but I doubt that the physics has changed in the intervening years.] I'll give a summary of the key concepts here.

A diffraction grating is basically a screen with a large number of closely-spaced parallel slits cut in it (actual gratings are usually made of glass with very fine lines ruled on them, but the principle is the same). Consider a grating with only 2 slits separated by a distance d. Monochromatic light of wavelength λ is shone onto the grating and diffracts through each of the slits. [Diffraction is the process by which a light wave spreads out after passing through a narrow gap. The same effect can be seen with water waves as they hit a narrow gap in a barrier; waves spread out in a semi-circular pattern beyond the gap.]

Now look at the light rays that leave the slits at an angle θ to the normal to the plane containing the slits. By drawing a diagram (see Fig 3.3 in Carroll & Ostlie, although in practice the two light rays leaving the slits are parallel and are focussed onto the detecting screen by a convex lens or concave mirror) we can see that the path difference between the two rays is $d\sin\theta$. If this path difference is an integral multiple of the wavelength, the two rays will reinforce each other and we'll see a bright fringe at that angle. On the other hand, if the path difference is an integral multiple of wavelengths plus half a wavelength, the two rays will destructively interfere, cancelling each other out, and we'll see a dark fringe. That is, the condition for bright fringes is

$$d \sin\theta = n\lambda \tag{0.1}$$

for n a non-negative integer.

Now suppose we have a diffraction grating with N slits. The same condition applies for light fringes, but because we're now adding up N rays instead of just 2, the intensity of the bright fringes is larger, and is in fact proportional to N^2. The actual formula for the intensity is

$$I = a^2 \frac{\sin^2 N\gamma}{\sin^2 \gamma} \tag{0.2}$$

where a is a constant, derived from the intensity passing through a single slit, and

$$\gamma = \frac{\pi d \sin\theta}{\lambda} \tag{0.3}$$

The bright fringes occur when $\gamma = n\pi$. This can be seen by finding the limit:

$$\lim_{\gamma\to n\pi} \frac{\sin N\gamma}{\sin\gamma} \tag{0.4}$$

This limit can be found using l'Hôpital's rule from calculus, which states that for two functions f and g where $f(x_0) = g(x_0) = 0$:

$$\lim_{x\to x_0} \frac{f(x)}{g(x)} = \lim_{x\to x_0} \frac{f'(x)}{g'(x)} \tag{0.5}$$

Therefore

$$\lim_{\gamma\to n\pi} \frac{\sin N\gamma}{\sin\gamma} = \lim_{\gamma\to n\pi} \frac{N\cos N\gamma}{\cos\gamma} = \pm N \tag{0.6}$$

$$\lim_{\gamma\to n\pi} \frac{\sin^2 N\gamma}{\sin^2\gamma} = N^2 \tag{0.7}$$

Because of the N in the upper sine, however, the numerator has many more zeroes than the denominator, meaning that whenever $N\gamma = m\pi$ but m is not a multiple of N, $I = 0$. Between any two bright fringes there will therefore be $N-1$ dark fringes and $N-2$ secondary 'brightish' fringes between these dark fringes. In practice, these secondary fringes are much fainter than the primary bright fringes and for large N they are effectively invisible.

It turns out that the number of slits N also determines the angular width of each primary maximum, according to

$$\Delta\theta_{width} = \frac{2\lambda}{Nd\cos\theta} \tag{0.8}$$

That is, the more slits, the sharper the spectral line for a given wavelength. Looked at another way, the smallest wavelength difference $\Delta\lambda$ that can be resolved is

$$\Delta\lambda = \frac{\lambda}{nN} \tag{0.9}$$

Not only does increasing the number slits increase the resolving power of the grating, but looking a higher order (larger n) lines allows greater resolution.

Example. The sodium D lines are commonly found in stellar spectra and have wavelengths of $\lambda_1 = 588.997$ nm and $\lambda_2 = 589.594$ nm. If light containing these two lines shines on a grating with 300 lines per millimetre, then

$$d = \frac{10^{-3}}{300} = 3.33\times10^{-6}\text{ m} \tag{0.10}$$

From 0.1 with $n = 2$ (second-order spectra) we have

$$\sin\theta_1 = \frac{2\left(588.997\times10^{-9}\right)}{3.33\times10^{-6}} = 0.3533982 \tag{0.11}$$

$$\theta_1 = 20.69531^\circ \tag{0.12}$$

$$\sin\theta_2 = \frac{2\left(589.594\times10^{-9}\right)}{3.33\times10^{-6}} = 0.3537564 \tag{0.13}$$

$$\theta_2 = 20.71725^\circ \tag{0.14}$$

The angle between the two lines is therefore

$$\Delta\theta_{Na} = \theta_2 - \theta_1 = 0.02194^\circ \tag{0.15}$$

From 0.9 we can work out how many lines need to be illuminated in order for these 2 lines to be resolved in second-order. For the wavelength in the formula, we'll use the average of the two wavelengths of the sodium D lines.

$$N = \frac{\lambda}{n\Delta\lambda} \tag{0.16}$$

$$= \frac{589.2955\times10^{-9}}{2\times0.597\times10^{-9}} \tag{0.17}$$

$$= 494 \tag{0.18}$$

Thus if only 2 mm of the grating were illuminated, we could resolve the lines, at least at second-order.

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