Roper Scientific, Inc.

Tech Note

WinSpec Wavelength Calibration Using the Auto-Spectro Calibration Mode

WinSpec/32 wavelength calibration is based on the grating equation for Czerny-Turner or Ebert spectrographs (see Figure 1).

$$(\mathbf{m}/\mathbf{d})\lambda = \mathbf{sin}\ \alpha + \mathbf{sin}\ \beta, \text{ or } \lambda = (\mathbf{d}/\mathbf{m})(\mathbf{sin}\ \alpha + \mathbf{sin}\ \beta), \tag{1}$$

where: $\boldsymbol{\lambda}$ = wavelength at the center of the image plane,

m = diffraction order

d = distance between grooves (the inverse of grooves per mm), and

α, β = angles of the incident and exit beam relative to the grating normal.

The angles α and β are related to the inclusion angle, γ, and the rotational angle of the grating, ψ:

$$\alpha = \psi - \gamma/\mathbf{2}, \text{ and } \beta = \psi + \gamma/\mathbf{2}.$$

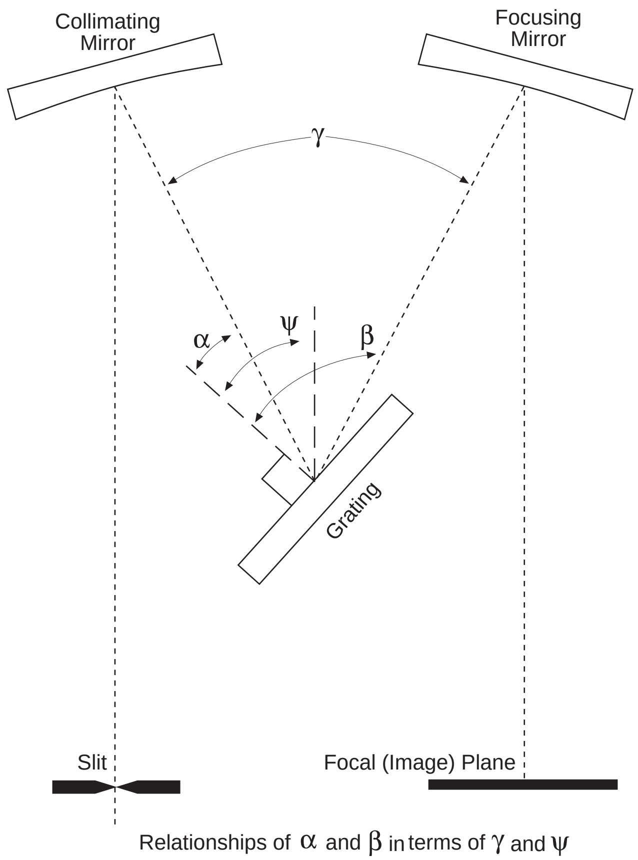
Thus the grating equation can be written as:

$$(\mathbf{m}/\mathbf{d})\ \lambda = \mathbf{sin}\ (\psi - \gamma/\mathbf{2}) + \mathbf{sin}\ (\psi + \gamma/\mathbf{2}) = \mathbf{2}\ \mathbf{sin}\ \psi\ \mathbf{cos}\ (\gamma/\mathbf{2}),$$

and the grating angle is given by:

$$\psi = \mathbf{asin}\ \{\mathbf{m}\lambda\ /\ (\mathbf{2d}\ \mathbf{cos}\ (\gamma/\mathbf{2}))\}. \tag{2}$$

Figure 1. Relationships of α and β in terms of ψ and γ.



Note that the wavelength at the **center** of the exit plane does not depend on the focal length, **f**. However, the wavelength at points off center depends on both the focal length and the detector angle, δ (the angle of the image plane relative to the plane perpendicular to the spectrograph focal axis at the center of the image plane; see Figure 2). For some wavelength λ' relatively close to λ (at the same grating angle),

$$\lambda' = (\mathbf{d}/\mathbf{m})(\mathbf{sin}\ \alpha + \mathbf{sin}\ \beta') = (\mathbf{d}/\mathbf{m})(\mathbf{sin}\ \alpha + \mathbf{sin}\ (\beta + \xi))$$
$$= (\mathbf{d}/\mathbf{m})\{\mathbf{sin}\ (\psi - \gamma/\mathbf{2}) + \mathbf{sin}\ (\psi + \gamma/\mathbf{2} + \xi)\}. \quad (3)$$

The angle ξ depends on the focal length **f**, the detector angle δ, and the distance of λ' from the center of the image plane, **nx**, where **n** is the number of pixels from the center and **x** is the pixel width; the relationship is given by:

$$\mathbf{tan}\ \xi = (\mathbf{nx\ cos}\ \delta) / (\mathbf{f} + \mathbf{nx\ sin}\ \delta), \text{ as shown in Figure 2.} \quad (4)$$

When the image plane is perpendicular, $\delta = 0$, and this reduces to:

$$\mathbf{tan}\ \xi = (\mathbf{nx} / \mathbf{f})$$

Using the known parameters of focal length **f**, detector angle δ, number of pixels from center **n**, and pixel width **x**, first calculate the angle ξ from equation **4**. The grating angle ψ can be calculated using the known parameters center wavelength λ, diffraction order **m**, grating grooves per mm **1/d**, and inclusion angle γ, from equation **2**. Finally, the wavelength at pixel **n** is calculated using equation **3**.

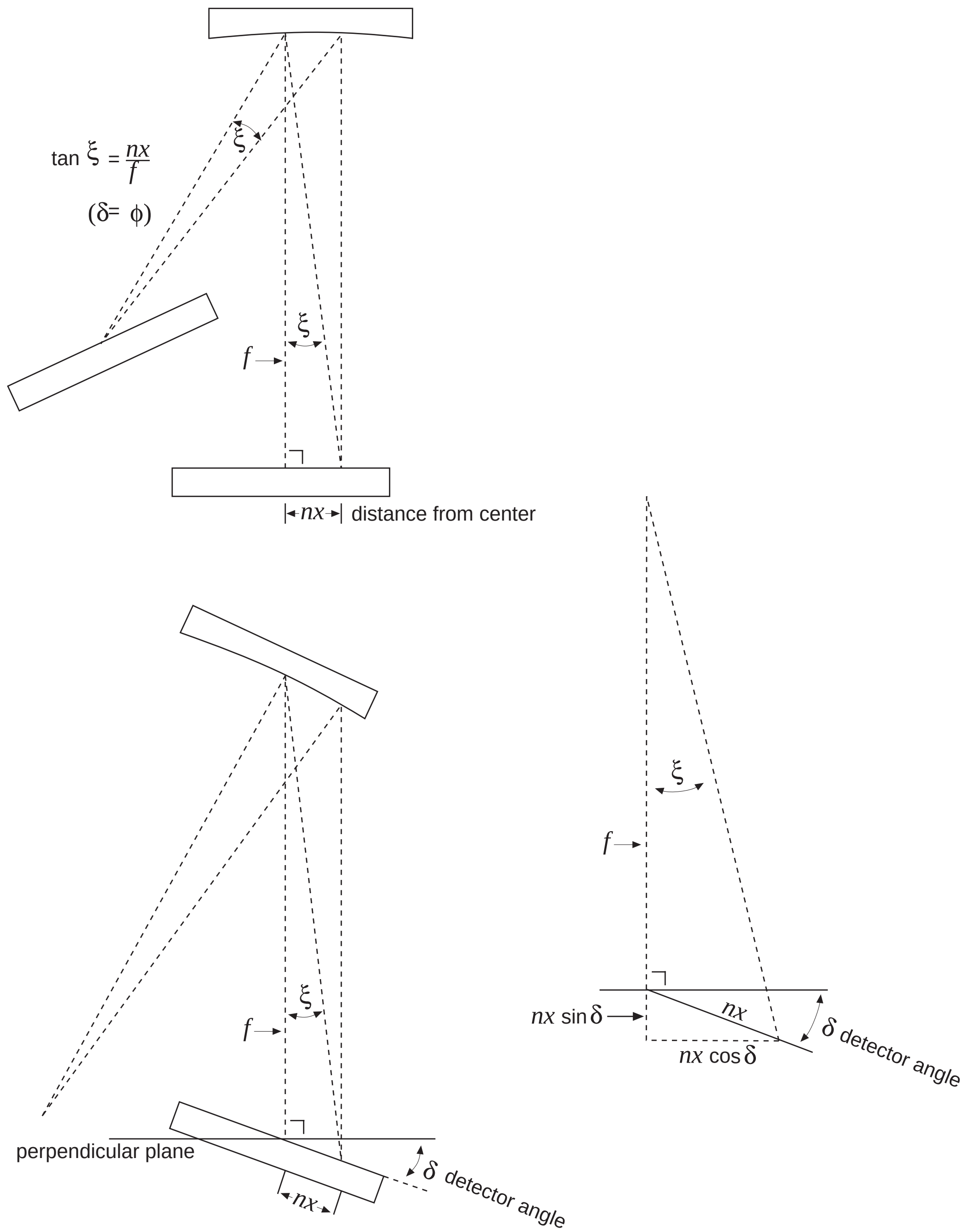


Figure 2. Relationship between ξ and the focal length, detector angle, and the distance of λ' from image plane.

WinSpec X Axis Auto Calibration

When "Calibration Usage" is set to "Auto Spectro" in WinSpec/32, the X Axis calibration is done in the following steps after a wavelength change. First the wavelength is calculated at each end of the array using the method above. Then these two points, plus the third center wavelength point, are automatically fit to a 2nd order polynomial using the wavelength calibration functions.