International Tables for Crystallography (2006). Vol. F, Section 11.3.2.3, p. 219.

$$\begin{aligned} F\mathbf{S}/\mathbf{S}\cdot\mathbf{d}_3 &= (F\mathbf{S}\cdot\mathbf{d}_1/\mathbf{S}\cdot\mathbf{d}_3)\mathbf{d}_1 + (F\mathbf{S}\cdot\mathbf{d}_2/\mathbf{S}\cdot\mathbf{d}_3)\mathbf{d}_2 + F\mathbf{d}_3 \\ &= (X - X_0)\mathbf{d}_1 + (Y - Y_0)\mathbf{d}_2 + F\mathbf{d}_3, \end{aligned}$$

which leads to a diffraction spot recorded at detector coordinates

$$\begin{aligned} X &= X_0 + F\mathbf{S}\cdot\mathbf{d}_1/\mathbf{S}\cdot\mathbf{d}_3, \\ Y &= Y_0 + F\mathbf{S}\cdot\mathbf{d}_2/\mathbf{S}\cdot\mathbf{d}_3. \end{aligned}$$

11.3.2.3. *Standard spot shape*

A reciprocal-lattice point crosses the Ewald sphere by the shortest route only if the crystal happens to be rotated about an axis perpendicular to both the diffracted and incident beam wave vectors, the 'β-axis' $\mathbf{e}_1 = \mathbf{S}\times\mathbf{S}_0/|\mathbf{S}\times\mathbf{S}_0|$, as introduced by Schutt & Winkler (1977). Rotation around the fixed axis $\mathbf{m}_2$, as enforced by the rotation camera, thus leads to an increase in the length of the shortest path by the factor $1/|\mathbf{e}_1\cdot\mathbf{m}_2|$. This has motivated the introduction of a coordinate system $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, specific for each reflection, which has its origin on the surface of the Ewald sphere at the terminus of the diffracted beam wave vector $\mathbf{S}$,

$$\mathbf{e}_1 = \mathbf{S}\times\mathbf{S}_0/|\mathbf{S}\times\mathbf{S}_0|, \quad \mathbf{e}_2 = \mathbf{S}\times\mathbf{e}_1/|\mathbf{S}\times\mathbf{e}_1|,$$
$$\mathbf{e}_3 = (\mathbf{S}+\mathbf{S}_0)/|\mathbf{S}+\mathbf{S}_0|.$$

The unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ are tangential to the Ewald sphere, while $\mathbf{e}_3$ is perpendicular to $\mathbf{e}_1$ and $\mathbf{p}^* = \mathbf{S} - \mathbf{S}_0$. The shape of a reflection, as represented with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, then no longer contains geometrical distortions resulting from the fixed rotation axis of the camera and the oblique incidence of the diffracted beam on a flat detector. Instead, all reflections appear as if they had followed the shortest path through the Ewald sphere and had been recorded on the surface of the sphere.

A detector pixel at X', Y' in the neighbourhood of the reflection centre X, Y, when the crystal is rotated by φ' instead of φ, is mapped to the profile coordinates $\varepsilon_1, \varepsilon_2, \varepsilon_3$ by the following procedure:

$$\begin{aligned} \mathbf{S}' &= [(X' - X_0)\mathbf{d}_1 + (Y' - Y_0)\mathbf{d}_2 + F\mathbf{d}_3] \\ &\quad \times \{\lambda\cdot[(X' - X_0)^2 + (Y' - Y_0)^2 + F^2]^{1/2}\}^{-1} \\ \varepsilon_1 &= \mathbf{e}_1\cdot(\mathbf{S}' - \mathbf{S})180/(|\mathbf{S}|\pi), \\ \varepsilon_2 &= \mathbf{e}_2\cdot(\mathbf{S}' - \mathbf{S})180/(|\mathbf{S}|\pi) \\ \varepsilon_3 &= \mathbf{e}_3\cdot[D(\mathbf{m}_2, \varphi' - \varphi)\mathbf{p}^* - \mathbf{p}^*]180/(|\mathbf{p}^*|\pi) \simeq \zeta\cdot(\varphi' - \varphi) \\ \zeta &= \mathbf{m}_2\cdot\mathbf{e}_1. \end{aligned}$$

ζ corrects for the increased path length of the reflection through the Ewald sphere and is closely related to the reciprocal Lorentz correction factor

$$L^{-1} = |\mathbf{m}_2\cdot(\mathbf{S}\times\mathbf{S}_0)|/(|\mathbf{S}|\cdot|\mathbf{S}_0|) = |\zeta\cdot\sin\angle(\mathbf{S}, \mathbf{S}_0)|.$$

Because of crystal mosaicity and beam divergence, the intensity of a reflection is smeared around the diffraction maximum. The fraction of total reflection intensity found in the volume element $\mathrm{d}\varepsilon_1\mathrm{d}\varepsilon_2\mathrm{d}\varepsilon_3$ at $\varepsilon_1, \varepsilon_2, \varepsilon_3$ can be approximated by Gaussian functions:

$$\begin{aligned} &\omega(\varepsilon_1, \varepsilon_2, \varepsilon_3)\mathrm{d}\varepsilon_1\mathrm{d}\varepsilon_2\mathrm{d}\varepsilon_3 \\ &\quad = \frac{\exp(-\varepsilon_1^2/2\sigma_D^2)}{(2\pi)^{1/2}\sigma_D}\mathrm{d}\varepsilon_1\cdot\frac{\exp(-\varepsilon_2^2/2\sigma_D^2)}{(2\pi)^{1/2}\sigma_D}\mathrm{d}\varepsilon_2\cdot\frac{\exp(-\varepsilon_3^2/2\sigma_M^2)}{(2\pi)^{1/2}\sigma_M}\mathrm{d}\varepsilon_3. \end{aligned}$$

11.3.2.4. *Spot centroids and partiality*

The intensity of a reflection can be completely recorded on one image, or distributed among several adjacent images. The fraction R_j of total intensity recorded on image j, the 'partiality' of the reflection, can be derived from the distribution function $\omega(\varepsilon_1, \varepsilon_2, \varepsilon_3)$ as

$$\begin{aligned} R_j &= \int_{-\infty}^{\infty}\mathrm{d}\varepsilon_1\int_{-\infty}^{\infty}\mathrm{d}\varepsilon_2\int_{\zeta[\varphi_0+(j-1)\Delta_\varphi-\varphi]}^{\zeta(\varphi_0+j\Delta_\varphi-\varphi)}\mathrm{d}\varepsilon_3\,\omega(\varepsilon_1, \varepsilon_2, \varepsilon_3) \\ &= \{[1/(2\pi)^{1/2}\sigma_M]/|\zeta|\} \\ &\quad \times\int_{\varphi_0+(j-1)\Delta_\varphi}^{\varphi_0+j\Delta_\varphi}\exp[-(\varphi' - \varphi)^2/2(\sigma_M/|\zeta|)^2]\,\mathrm{d}\varphi' \\ &= \Big(\mathrm{erf}[|\zeta|(\varphi_0 + j\Delta_\varphi - \varphi)/(2)^{1/2}\sigma_M] \\ &\quad - \mathrm{erf}\{|\zeta|[\varphi_0 + (j-1)\Delta_\varphi - \varphi]/(2)^{1/2}\sigma_M\}\Big)/2. \end{aligned}$$

The integral is evaluated by using a numerical approximation of the error function, erf (Abramowitz & Stegun, 1972).

While the spot centroids in the detector plane are usually good estimates for the detector position of the diffraction maximum, the angular centroid about the rotation axis,

$$Z = \varphi_0 + \Delta_\varphi\cdot\sum_{j=-\infty}^{\infty}(j - 1/2)R_j \approx \varphi,$$

can be a rather poor guess for the true φ angle of the maximum. Its accuracy depends strongly on the value of φ and the size of the oscillation range Δ_φ relative to the mosaicity σ_M of the crystal. For a reflection fully recorded on image j, the value $Z = \varphi_0 + (j - 1/2)\cdot\Delta_\varphi$ will always be obtained, which is correct only if φ accidentally happens to be close to the centre of the rotation range of the image. In contrast, the φ angle of a partial reflection recorded on images j and $j+1$ is closely approximated by $Z = \varphi_0 + [j + (R_{j+1} - R_j)/2]\cdot\Delta_\varphi$. If many images contribute to the spot intensity, $Z(\varphi)$ is always an excellent approximation to the ideal angular position φ when the Laue equations are satisfied; in fact, in the limiting case of infinitely fine-sliced data, it can be shown that $\lim_{\Delta_\varphi\to 0} Z(\varphi) = \varphi$.

Most refinement routines minimize the discrepancies between the predicted φ angles and their approximations obtained from the observed Z centroids, and must therefore carefully distinguish between fully and partially recorded reflections. This distinction is unnecessary, however, if observed Z centroids are compared with their analytic forms instead, because the sensitivity of the centroid positions to the diffraction parameters is correctly weighted in either case (see Section 11.3.2.8).

11.3.2.5. *Localizing diffraction spots*

Recognition and refinement of the parameter values controlling the observed diffraction pattern begins with the extraction of a list of coordinates of strong spots occurring in the images. As implemented in *XDS*, this list is obtained by the following procedure. First, each pixel value is compared with the mean value and standard deviation of surrounding pixels in the same image and classified as a strong pixel if its value exceeds the mean by a given multiple (typically 3 to 5) of the standard deviation. Values of the strong pixels and their location addresses and image running numbers are stored in a hash table during spot search [for a discussion of the hash technique, see Wirth (1976)]. After processing a fixed number of images, or when the table is full, all strong pixels are labelled by a unique number identifying the spot to which they belong. By definition, any two such pixels which can be connected by direct strong neighbours in two or three dimensions (if there are adjacent images) belong to the same spot (equivalence class). The labelling is achieved by the highly efficient algorithm for the recording of equivalence classes developed by Rem (see Dijkstra, 1976). At the end of this procedure, the table is searched for spots that have no contributing strong pixel on the current or the previous image. These spots are complete and their centroids are