Contents

1 3-Dimensional plot

The 3-dimensional plot requires an interpolation in 2 dimensions. The theoretical values are calculated at the points of a rectangular grid of equidistant steps. The stepwidths in the two directions may be different. A second order equation in two variables x,y has coefficients of six terms x,x^2,y,y^2,xy, and a constant. 6 theoretical values determine a parabolic surface. The coordinates of the point the value of which will be interpolated should be inside the the coordinates used for the calculation of the parabolic surface. Four points are chosen as the corners of the rectangle with the point inside. Two further coordinates of the grid are choosen in a systematic way whithout further reference to the position of the point.

2 Quadratic interpolation

The quadratic equation in Ω and Θ

$$\mathbf{\Phi} = \alpha\Omega^2 + \beta\Omega + \gamma\Theta^2 + \delta\Theta + \eta\Omega\Theta + \varphi \tag{1}$$

approximates the theory around the experimental coordinates. The rectangular network of theoretical coordinates (Ω_b - Ω_e and Θ_b - Θ_e) has stepwidth of $d\Omega$ and $d\Theta$, such that there are $n_\Omega = (\Omega_b - \Omega_e)/d\Omega + 1$ points in Ω direction. The experimental point $(\Omega_{exp}, \Theta_{exp})$ is supposed to be inside the network. The integer numbers

$$\begin{aligned} j_\Omega &= int(\Omega_{exp} - \Omega_b)/d\Omega \\ j_\Theta &= int(\Theta_{exp} - \Theta_b)/d\Theta \end{aligned} \tag{2}$$

range from $0 \leq j_\Omega < n_\Omega$ and $0 \leq j_\Theta < n_\Theta$. The coordinates of the experimental point inside the rectangular $(j_\Omega, j_\Theta), (j_\Omega, j_\Theta + 1), (j_\Omega + 1, j_\Theta), (j_\Omega + 1, j_\Theta + 1)$ shown in Fig.1,a) are given by

$$
\begin{aligned}
\partial\Omega &= (\Omega_{exp} - \Omega_b) - j_\Omega \cdot d\Omega \\
\partial\Theta &= (\Theta_{exp} - \Theta_b) - j_\Theta \cdot d\Theta
\end{aligned}
$$

The coefficients $\alpha, ..., \varphi$ of Eq. 1 have to be solved for the rectanle of the experimental point. The coordinates of the 6 points of Fig.1,a) are from 1 to 6: (0,0), ($d\Omega$,0),($2d\Omega$,0),(0,$d\Theta$),($d\Omega$,$d\Theta$),(0,$2d\Theta$). Inserting these 6 points 6 simple equations are obtained for the determination of the coefficients.

$$
\begin{aligned}
\mathbf{\Phi_1} &= \varphi \\
\mathbf{\Phi_2} &= \alpha d\Omega^2 + \beta d\Omega + \varphi \\
\mathbf{\Phi_3} &= 4 \cdot \alpha d\Omega^2 + \beta d\Omega + \varphi \\
\mathbf{\Phi_4} &= \alpha d\Theta^2 + \beta d\Theta + \varphi \\
\mathbf{\Phi_5} &= 4 \cdot \alpha d\Theta^2 + \beta d\Theta + \varphi \\
\mathbf{\Phi_6} &= \alpha d\Omega^2 + \beta d\Omega + \gamma d\Theta^2 + \delta d\Theta + \eta d\Omega d\Theta + \varphi
\end{aligned} \tag{3}
$$

The values Φ_n n=1,...,6 are calculated from the theory. With $f_n = \mathbf{\Phi_n} - \varphi$ the coefficients are written as

$$
\begin{aligned}
\alpha &= -\frac{1}{2}(2f_2 - f_3)/d\Omega^2 \\
\beta &= -\frac{1}{2}(f_3 - 4f_2)/d\Omega \\
\gamma &= -\frac{1}{2}(2f_4 - f_6)/d\Theta^2 \\
\delta &= -\frac{1}{2}(f_6 - 4f_4)/d\Theta \\
\eta &= \left[\frac{1}{2}(2f_2 - f_3) + \frac{1}{2}(f_3 - 4f_2) + \frac{1}{2}(2f_4 - f_6) + \frac{1}{2}(f_6 - 4f_4)\right] /d\Omega d\Theta
\end{aligned} \tag{4}
$$

Inserting the relative coordinates $(\partial\Omega, \partial\Theta)$ together with the coefficients Eq. 4 into Eq. 1 the stepwidths cancel down such that with $\omega = \partial\Omega/d\Omega, \theta = \partial\Theta/d\Theta)$ the interpolated value becomes

$$
\mathbf{\Phi} = a\omega^2 + b\omega + c\theta^2 + d\theta + e\omega\theta + \varphi \tag{5}
$$

and

$$
\begin{aligned}
a &= -\frac{1}{2}(2f_2 - f_3) \\
b &= -\frac{1}{2}(f_3 - 4f_2) \\
g &= -\frac{1}{2}(2f_4 - f_6) \\
d &= -\frac{1}{2}(f_6 - 4f_4) \\
e &= \frac{1}{2}(2f_2 - f_3) + \frac{1}{2}(f_3 - 4f_2) + \frac{1}{2}(2f_4 - f_6) + \frac{1}{2}(f_6 - 4f_4)
\end{aligned}
\tag{6}
$$

The case of Fig. 1,a) is met for the majority of experimental points with positions inside the network of theoretical points. If the boundary is reached Fig. 1,b), the point number 6 as defined in a) is outside the network ($j_\Theta + 2 > n_\Theta$). Therefore the figure of 6 coordinates is arranged in a different way. Mirrowing Fig. b) by the Ω-border line the figure is the same as a) but the Θ-coordinate of the experimental point is $d\Theta - \partial\Theta$ or the reduced coordinate θ is replaced by $1 - \theta$. In case c) ($j_\Omega + 2 > n_\Omega$) the mirror line is the Ω-border line at Ω_e and the Ω-coordinate has to be replaced: $1 - \omega$. In case d) two mirror operations are necessary in order to obtain the situation of Fig. a) ($j_\Omega + 2 > n_\Omega$ and $j_\Theta + 2 > n_\Theta$) and both coordinates are replaced: $1 - \omega$,$1 - \theta$. The last case is only met for experimental points inside the rectangle at the corner of (Ω_e, Θ_e).

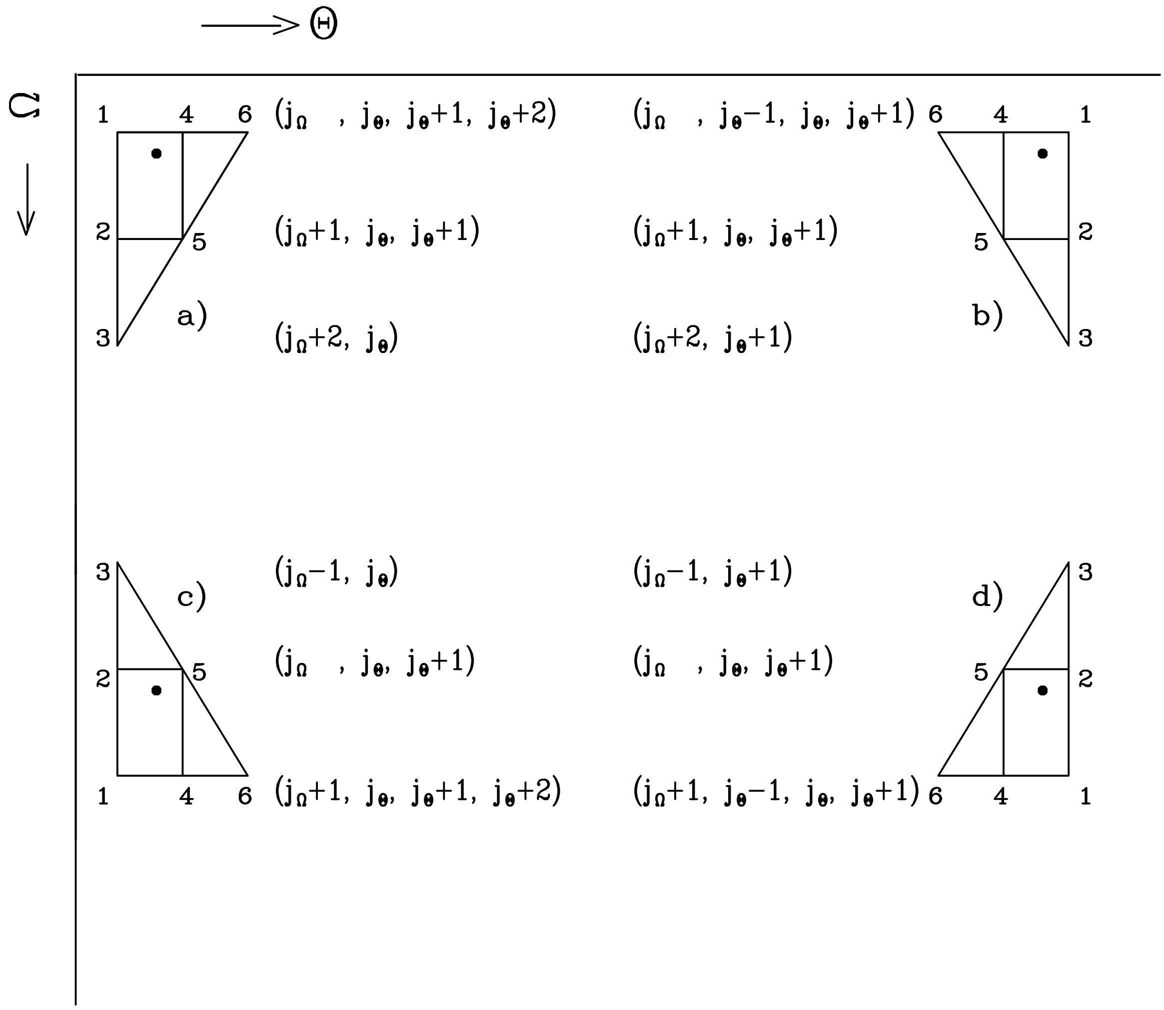

Figure 1: The interpolated theoretical value is obtained from 6 values in the neighborhood of the experimental point. The rectangle containing the eexperimental point is extended by two triangles depending on the position in the network of coordinates of theoretical points. At the upper bounderies for Θ and Ω of the network the triangles are added in different ways, case b), c), d). The integer values j_Ω, j_Θ of Eq. 2 belong to point 1 in a), to 4 in b), to 2 in c) and 5 in d). The coordinate numbers of all 6 points relative to j_Ω, j_Θ are listed in the figure.

3 The grid of theoretical values

There are 2 types of grid design corresponding to scan modes case 3) and case 4). Fig. 2 shows the grid for the scan mode of two independent Θ-, Ω loops. The Ω-angle is for the incident beam and Θ for the direction of the detector. The theoretical values are calculated with Ω as the inner loop and different Θ's in the outer loop. Counting the pairs of angles (Ω,Θ) the numbers attached to the pairs defining the grid are indicated in the figure. The Ω-loop runs over 6 equidistant values. The second Θ-loop starts with number 7, the third with 13, etc.
The red line in the figure marks the specular reflection case (Θ=Ω). An experimental point indicated by a dot defines the triangle highlighted in blue color. The corners are point numbers 9,11,21. It represents the standard triangle a) of Fig. 1.

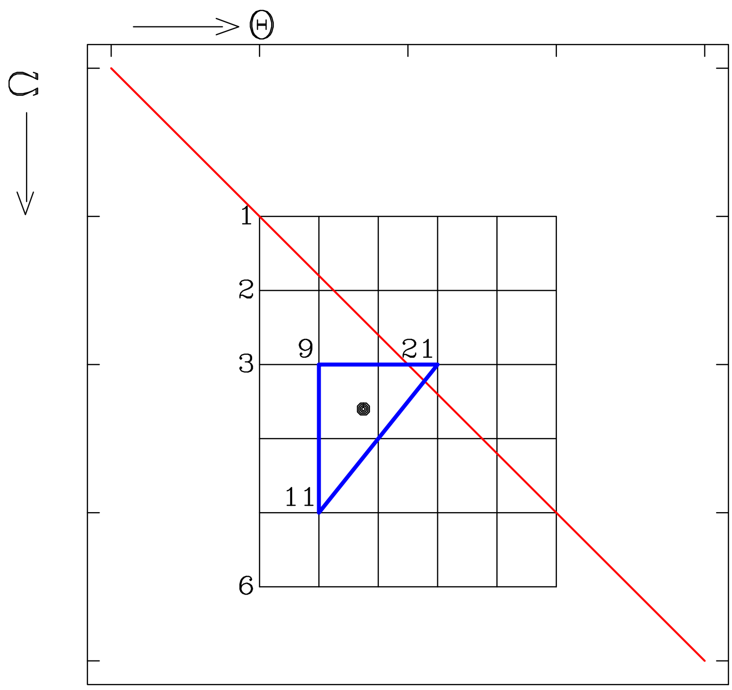

Figure 2: The grid of (Ω,Θ)- pairs as used for the calculation of theoretical values.The red line marks the specular reflection case (Θ=Ω). The grid points are counted as a results of the nested loops for Ω,Θ. The triangle in blue color is defined by an experimental point (black dot) - see section 2.

A second choice of the grid is shown in Fig. 3. The sequence of angular (Ω,Θ)-pairs are in the order as obtained from a Ω-2Θ-scan which probes the offspecular intensity in the direction orthonormal to the red colored line of specular reflections. In cases where different approximations of the theory are used when crossing the specular condition from low to high Ω-angles, this arrangement of the grid is more adequate than that of Fig. 2.

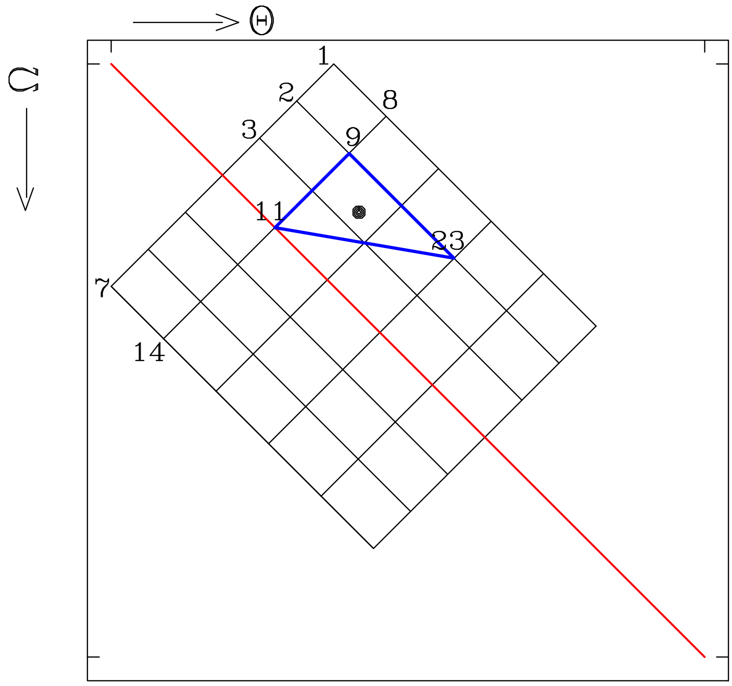

Figure 3: The grid of (Ω,Θ)- pairs as used for the calculation of theoretical values is oriented with respect to the red line which marks the specular reflection case $(\Theta{=}\Omega)$. The grid points are counted as a results of the nested loops for Ω,Θ as obtained for a Ω-2Θ-scan. The triangle in blue color is defined by an experimental point (black dot) - see section 2.

In order to use the same interpolation procedure as described in section 2 the experimental points are expressed in the coordinate sytem of the rotated grid with unit vectors $(\mathbf{e}_1, \mathbf{e}_2)$ as shown in Fig. 4. the following equations are obvious:

$$\begin{aligned}
\mathbf{e}_1 &= \frac{1}{\sqrt{2}}\left(\mathbf{e}_\Omega - \mathbf{e}_\Theta\right) \\
\mathbf{e}_2 &= \frac{1}{\sqrt{2}}\left(\mathbf{e}_\Omega + \mathbf{e}_\Theta\right)
\end{aligned} \tag{7}$$

The vector $\mathbf{q} = \omega\mathbf{e}_1 + \vartheta\mathbf{e}_2$ is the difference $\mathbf{q} = \mathbf{p} - \mathbf{r}_0$.

$$\begin{aligned}
\mathbf{r}_0 &= \Omega_b\mathbf{e}_\Omega + \Theta_b\mathbf{e}_\Theta \\
\mathbf{p} &= \Omega\mathbf{e}_\Omega + \Theta\mathbf{e}_\Theta
\end{aligned} \tag{8}$$

(Ω_b, Θ_b) are the coordinates of point number 1 of the grid.

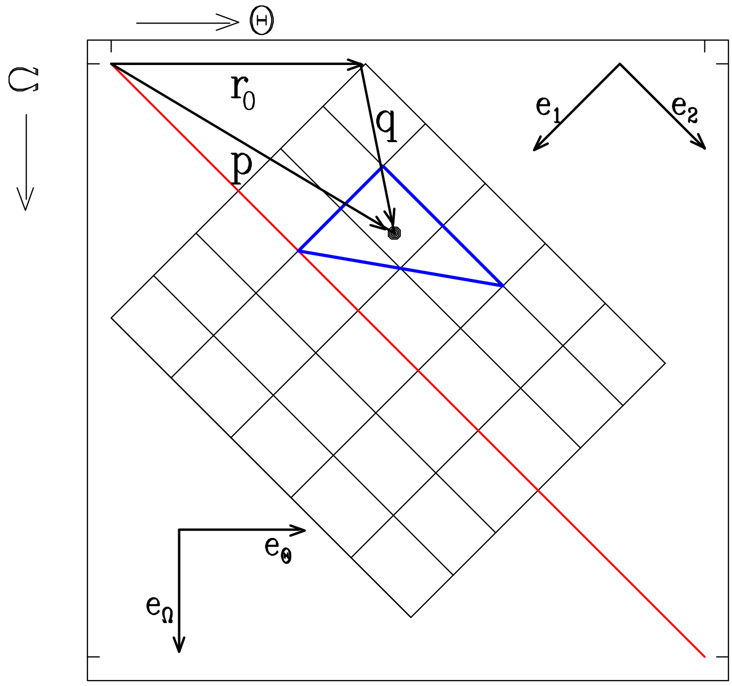

Figure 4: For the transformation of the experimental (Ω,Θ)- pairs to the coordinate system of the grid oriented to the specular reflection line (red colored) unit vectors $(\mathbf{e}_\Omega, \mathbf{e}_\Theta)$ and $(\mathbf{e}_1, \mathbf{e}_2)$ and vectors ($\mathbf{r}_0$, $\mathbf{p}$, $\mathbf{q}$) are defined (see text) .

The transformation is obtained as

$$\begin{aligned} \omega &= \frac{1}{\sqrt{2}}(\Omega - \Omega_0 - \Theta + \Theta_0) \\ \vartheta &= \frac{1}{\sqrt{2}}(\Omega - \Omega_0 + \Theta - \Theta_0) \end{aligned} \tag{9}$$

The stepwidth in the (ω, ϑ)-variables is obtained from the constuction of the loop $(\Omega_e = \Omega_b + d\Omega(n_\Omega - 1))$.

$$\begin{aligned} \Omega &= \Omega_b + d\Omega(k_\Omega - 1) + (i_\Theta - 1)d\Theta \\ \Theta &= 2\Omega_b + d\Omega(n_\Omega - 1) + (i_\Theta - 1)2d\Theta - \Omega \end{aligned} \tag{10}$$

The loop start at $k_\Omega = i_\Theta = 1$ with $(\Omega = \Omega_b, \Theta = \Omega_e)$ for point number 1. $k_\Omega = 2, i_\Theta = 1$ gives point number 2 with $\Omega = \Omega_b + d\Omega$ and $\Theta = \Omega_e - d\Omega$. Therefore, the stepwidth is $\sqrt{2}d\Omega$ in $\mathbf{e}_1$-direction. In $\mathbf{e}_2$-direction point 1 and point $n_\Omega + 1$ with $k_\Omega = 1, i_\Theta = 2$ have to be compared. The stepwidth becomes $\sqrt{2}d\Theta$.