Introduction to the use the UB matrix

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I. UB MATRIX FORMALISM

The purpose of using the UB matrix formalism is to map the scattering geometry in the laboratory frame to the reciprocal lattice of the sample. Assuming a right handed coordinate system for the lab frame, and a similar coordinate system tied to the crystal, the transformation between the two is a simple rotation, U.

The physics is described in reciprocal space by $\mathbf{Q} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}$ and energy transfer E. The B matrix (shown in section IV) is the transformation from h, k, l to a cartesian coordinate system tied to the sample.

$$\mathbf{Q}_c = 2\pi B \begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{1}$$

To orient the sample, the scattering instrument uses a goniometer with several rotation axes. The rotation of the sample can be described by

$$R = R_1(\Omega_1) \cdot R_2(\Omega_2) \cdot \ldots \cdot R_n(\Omega_n) \tag{2}$$

where the sample is attached to the rotation axis of R_n.

In the most general case, a rotation with angle Ω around a direction $\mathbf{u} = (u_x, u_y, u_z)$, with $u_x^2 + u_y^2 + u_z^2 = 1$, is described by

$$R(\Omega) = \begin{pmatrix} \cos(\Omega) + u_x^2(1-\cos(\Omega)) & u_x u_y(1-\cos(\Omega)) - u_z \sin(\Omega) & u_x u_z(1-\cos(\Omega)) + u_y \sin(\Omega) \\ u_y u_x(1-\cos(\Omega)) + u_z \sin(\Omega) & \cos(\Omega) + u_y^2(1-\cos(\Omega)) & u_y u_z(1-\cos(\Omega)) - u_x \sin(\Omega) \\ u_z u_x(1-\cos(\Omega)) - u_y \sin(\Omega) & u_z u_y(1-\cos(\Omega)) + u_x \sin(\Omega) & \cos(\Omega) + u_z^2(1-\cos(\Omega)) \end{pmatrix} \tag{3}$$

When all angles are 0, the rotation matrices are equal to the identity matrix, so the combined effect is still the unit matrix.

$$R(0) = I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4}$$

In the general case, when all angles of the goniometer are 0, the axes of the orthogonal crystal reciprocal lattice are not aligned with the axes of the cartesian laboratory frame. The transformation between these two can be described by a rotation matrix U. Then, our fundamental relations for transforming between $\mathbf{Q}_l$ (in laboratory frame) and $\mathbf{Q}$ (reciprocal lattice) are:

$$\mathbf{Q}_l = 2\pi R \cdot U \cdot B \begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{5}$$

$$\mathbf{Q}_l = \mathbf{k}_i - \mathbf{k}_f \tag{6}$$

$$E = \frac{\hbar^2}{2m}\left(k_i^2 - k_f^2\right) \tag{7}$$

Equation 6 is the momentum conservation for the lattice, where $\mathbf{k}_i, \mathbf{k}_f$ are the incident and final neutron vawevectors, while equation 7 is the energy transferred to the lattice.

By looking at equation 5, 6, and 7, we identify three modes of interacting with the UB matrix:

(a) We know $\mathbf{k}_i, \mathbf{k}_f, U, B$ and R. Then we can calculate h, k, l, E.

(b) We can calculate U and B if we have several reflections.

(c) We can rotate the goniometer so as to measure at a particular combination of h, k, l, and E in a specific detector.

II. CONVENTIONS

- a, b, c real lattice lengths (in Å)
- α, β, γ real lattice angles
- a^*, b^*, c^* reciprocal lattice lengths (in $Å^{-1}$). We are going to use crystallographic notations (no 2π in the definition of reciprocal lattice vectors)
- for any vector $\mathbf{v}$, v=$|\mathbf{v}|$, $\widehat{v}$=$\mathbf{v}/v$
- incident beam is along $\widehat{z}$ axis, with $\widehat{x}$ in the horizontal plane, and $\widehat{y}$ pointing up (Figure 1).
- the scattered beam makes an angle θ with the $\widehat{z}$ axis, and its projection on the $(\widehat{x}, \widehat{y})$ plane makes an angle ϕ with the $\widehat{x}$ axis (Figure 1).

From equation 6, $\mathbf{Q}_l$ can be written as

$$\mathbf{Q}_l = \begin{pmatrix} -k_f \sin(\theta)\cos(\phi) \\ -k_f \sin(\theta)\sin(\phi) \\ k_i - k_f \cos(\theta) \end{pmatrix} \tag{8}$$

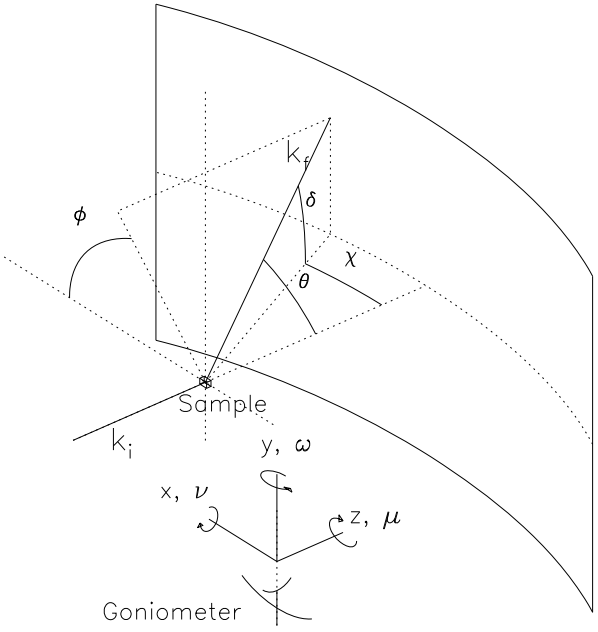

FIG. 1: Instrument geometry showing conventions for axis and angles. Details for goniometer axis are at the bottom

III. RECIPROCAL LATTICE

Note: for a more detailed description see International Tables for Crystallography (2006). Vol. B, ch. 1.1, pp. 2-9

This section will contain a description of the calculation of reciprocal lattice parameters. These are useful for calculating the B matrix, or for extracting real lattice parameters from the B matrix.

Suppose we have an orthonormal set of vectors $\widehat{i}, \widehat{j}, \widehat{k}$, such as

$$\mathbf{a} = a\widehat{i} \tag{9}$$

and $\mathbf{b}$ is in the plane of $\widehat{i}$ and $\widehat{j}$, and the angle between $\mathbf{a}$ and $\mathbf{b}$ is γ. Then

$$\mathbf{b} = b\cos(\gamma)\widehat{i} + b\sin(\gamma)\widehat{j} \tag{10}$$

For the **c** vector, it is slightly more complicated. We write

$$\mathbf{c} = c_i\hat{i} + c_j\hat{j} + c_k\hat{k} \tag{11}$$

In order to determine c_i, c_j, c_k we use

$$\cos(\beta) = \frac{\mathbf{a}\cdot\mathbf{c}}{a\ c} \tag{12}$$

$$\cos(\alpha) = \frac{\mathbf{b}\cdot\mathbf{c}}{b\ c} \tag{13}$$

$$c^2 = c_i^2 + c_j^2 + c_k^2 \tag{14}$$

In equation 12

$$\frac{\mathbf{a}\cdot\mathbf{c}}{a\ c} = \frac{a\ c_i}{a\ c} \tag{15}$$

so

$$c_i = c\cos(\beta) \tag{16}$$

In equation 13

$$\frac{\mathbf{b}\cdot\mathbf{c}}{b\ c} = \frac{b\cos(\gamma)\ c_i + b\sin(\gamma)\ c_j}{b\ c} \tag{17}$$

$$\cos(\alpha) = \cos(\gamma)\cos(\beta) + \sin(\gamma)\ c_j/c \tag{18}$$

so

$$c_j = c(\cos(\alpha) - \cos(\gamma)\cos(\beta))/\sin(\gamma) \tag{19}$$

From equation 14 we then get

$$c_k = cV_{\alpha\beta\gamma}/\sin(\gamma) \tag{20}$$

with

$$V_{\alpha\beta\gamma} = \sqrt{1 - \cos^2(\alpha) - \cos^2(\beta) - \cos^2(\gamma) + 2\cos(\alpha)\cos(\beta)\cos(\gamma)} \tag{21}$$

With these, we can now calculate the reciprocal lattice vectors:

$$\mathbf{a}^* = \frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}(\mathbf{b}\times\mathbf{c})} \tag{22}$$

$$\mathbf{b}^* = \frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}(\mathbf{b}\times\mathbf{c})} \tag{23}$$

$$\mathbf{c}^* = \frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}(\mathbf{b}\times\mathbf{c})} \tag{24}$$

It is easy to show that

$$\mathbf{a}(\mathbf{b}\times\mathbf{c}) = abcV_{\alpha\beta\gamma} \tag{25}$$

For further calculations in our problem, it is not necessary to explicitly write $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$, only their respective dot products. We will use the following identity:

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c}) \tag{26}$$

to derive the following:

$$\begin{aligned}
(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{a}\times\mathbf{b}) &= (\mathbf{a}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{b})-(\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{a}) \\
&= a^2b^2(1-\cos^2(\gamma)) && (27)\\
(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{a}) &= (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{a})-(\mathbf{a}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{c}) \\
&= a^2bc(\cos(\beta)\cos(\gamma)-\cos(\alpha)) && (28)\\
(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{b}\times\mathbf{c}) &= (\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c})-(\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{b}) \\
&= ab^2c(\cos(\gamma)\cos(\alpha)-\cos(\beta)) && (29)\\
(\mathbf{c}\times\mathbf{a})\cdot(\mathbf{c}\times\mathbf{a}) &= (\mathbf{c}\cdot\mathbf{c})(\mathbf{a}\cdot\mathbf{a})-(\mathbf{c}\cdot\mathbf{a})(\mathbf{c}\cdot\mathbf{a}) \\
&= a^2c^2(1-\cos^2(\beta)) && (30)\\
(\mathbf{c}\times\mathbf{a})\cdot(\mathbf{b}\times\mathbf{c}) &= (\mathbf{c}\cdot\mathbf{b})(\mathbf{a}\cdot\mathbf{c})-(\mathbf{c}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{a}) \\
&= abc^2(\cos(\alpha)\cos(\beta)-\cos(\gamma)) && (31)\\
(\mathbf{b}\times\mathbf{c})\cdot(\mathbf{b}\times\mathbf{c}) &= (\mathbf{b}\cdot\mathbf{b})(\mathbf{c}\cdot\mathbf{c})-(\mathbf{b}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{c}) \\
&= b^2c^2(1-\cos^2(\alpha)) && (32)
\end{aligned}$$

So we obtain:

$$\begin{aligned}
\mathbf{a}^*\mathbf{a}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{1-\cos^2(\alpha)}{a^2} && (33)\\
\mathbf{a}^*\mathbf{b}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{\cos(\alpha)\cos(\beta)-\cos(\gamma)}{ab} && (34)\\
\mathbf{a}^*\mathbf{c}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{\cos(\gamma)\cos(\alpha)-\cos(\beta)}{ac} && (35)\\
\mathbf{b}^*\mathbf{b}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{1-\cos^2(\beta)}{b^2} && (36)\\
\mathbf{b}^*\mathbf{c}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{\cos(\beta)\cos(\gamma)-\cos(\alpha)}{bc} && (37)\\
\mathbf{c}^*\mathbf{c}^* &= \frac{1}{V_{\alpha\beta\gamma}^2}\frac{1-\cos^2(\gamma)}{c^2} && (38)
\end{aligned}$$

The reciprocal lattice parameters are then given by

$$\begin{aligned}
a^* &= \frac{1}{V_{\alpha\beta\gamma}}\frac{\sin(\alpha)}{a} && (39)\\
b^* &= \frac{1}{V_{\alpha\beta\gamma}}\frac{\sin(\beta)}{b} && (40)\\
c^* &= \frac{1}{V_{\alpha\beta\gamma}}\frac{\sin(\gamma)}{c} && (41)\\
\cos(\alpha^*) &= \frac{\cos(\beta)\cos(\gamma)-\cos(\alpha)}{\sin(\beta)\sin(\gamma)} && (42)\\
\cos(\beta^*) &= \frac{\cos(\gamma)\cos(\alpha)-\cos(\beta)}{\sin(\gamma)\sin(\alpha)} && (43)\\
\cos(\gamma^*) &= \frac{\cos(\alpha)\cos(\beta)-\cos(\gamma)}{\sin(\alpha)\sin(\beta)} && (44)
\end{aligned}$$

IV. ORTHOGONAL BASIS AND THE B MATRIX

Note: for a more detailed description see International Tables for Crystallography (2006). Vol. B, ch. 1.1, pp. 2-9

Though a crystal may not have orthogonal basis vectors, such vectors facilitate rotation operations. This section describes how we define such a reference frame. The vectors written in this orthogonal basis are obtained by multiplying

the B matrix to $\begin{pmatrix} h \\ k \\ l \end{pmatrix}$ For an orthogonal set of basis vectors, one choice would be to project

$$\mathbf{Q}_c/(2\pi) \;=\; h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \tag{45}$$

on the following directions: (1) along $\mathbf{a}^*$, (2) in the $(\mathbf{a}^*, \mathbf{b}^*)$ plane, perpendicular to direction (1), and (3) in the direction perpendicular to (1) and (2). We will call these directions $\widehat{i^*}, \widehat{j^*}, \widehat{k^*}$.

Using the same procedure as in the previous section, we obtain:

$$\mathbf{a}^* \;=\; a^*\widehat{i^*} \tag{46}$$

$$\mathbf{b}^* \;=\; b^*\cos(\gamma^*)\widehat{i^*} + b^*\sin(\gamma^*)\widehat{j^*} \tag{47}$$

$$\mathbf{c}^* \;=\; c^*\cos(\beta^*)\widehat{i^*} + c^*\frac{\cos(\alpha^*) - \cos(\beta^*)\cos(\gamma^*)}{\sin(\gamma^*)}\widehat{j^*} + c^*\frac{V^*_{\alpha\beta\gamma}}{\sin(\gamma^*)}\widehat{k^*} \tag{48}$$

with

$$V^*_{\alpha\beta\gamma} = \sqrt{1 - \cos^2(\alpha^*) - \cos^2(\beta^*) - \cos^2(\gamma^*) + 2\cos(\alpha^*)\cos(\beta^*)\cos(\gamma^*)} \tag{49}$$

From equations 39-44, and noting that the real lattice is the reciprocal of the reciprocal lattice, we can rewrite equation 48 as

$$\mathbf{c}^* = c^*\cos(\beta^*)\widehat{i^*} - c^*\sin(\beta^*)\cos(\alpha)\widehat{j^*} + \frac{1}{c}\widehat{k^*} \tag{50}$$

With these,

$$\begin{aligned}
\mathbf{Q}/(2\pi) \;&=\; h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \\
&=\; ha^*\widehat{i^*} + k(b^*\cos(\gamma^*)\widehat{i^*} + b^*\sin(\gamma^*)\widehat{j^*}) + l(c^*\cos(\beta^*)\widehat{i^*} - c^*\sin(\beta^*)\cos(\alpha)\widehat{j^*} + \frac{1}{c}\widehat{k^*}) \\
&=\; (ha^* + kb^*\cos(\gamma^*) + lc^*\cos(\beta^*))\widehat{i^*} + (kb^*\sin(\gamma^*) - lc^*\sin(\beta^*)\cos(\alpha))\widehat{j^*} + l\frac{1}{c}\widehat{k^*} \\
&=\; B\begin{pmatrix} h \\ k \\ l \end{pmatrix}
\end{aligned} \tag{51}$$

where

$$B = \begin{pmatrix} a^* & b^*\cos(\gamma^*) & c^*\cos(\beta^*) \\ 0 & b^*\sin(\gamma^*) & -c^*\sin(\beta^*)\cos(\alpha) \\ 0 & 0 & 1/c \end{pmatrix} \tag{52}$$

If we use equations 42-44 and their reciprocals, we obtain that

$$B^TB = G^* = \begin{pmatrix} a^*a^* & a^*b^*\cos(\gamma^*) & a^*c^*\cos(\beta^*) \\ a^*b^*\cos(\gamma^*) & b^*b^* & b^*c^*\cos(\alpha^*) \\ a^*c^*\cos(\beta^*) & b^*c^*\cos(\alpha^*) & c^*c^* \end{pmatrix} \tag{53}$$

G^* is the matrix of the metric tensor of the reciprocal lattice. Its inverse is the metric tensor of the direct basis

$$G = (G^*)^{-1} = \begin{pmatrix} a^2 & ab\cos(\gamma) & ac\cos(\beta) \\ ab\cos(\gamma) & b^2 & bc\cos(\alpha) \\ ac\cos(\beta) & bc\cos(\alpha) & c^2 \end{pmatrix} \tag{54}$$

V. PRACTICAL USES OF UB MATRIX FORMALISM

In order to discuss concrete examples of using UB matrices, we are going to use a standard goniometer similar to those used on triple axes spectrometers at HFIR. The first rotation (our R_1) is around a vertical axis ($\widehat{y}$), with an

angle ω. On top of this, there is the lower tilt axis, defined as a rotation around $\widehat{z}$, with angle μ, while the upper tilt is a rotation around $\widehat{x}$ with angle ν(Figure 1). The sample is attached to this axis. While it is possible to use the convention in Busing and Levy (1967), or Lumsden *et al.* (2005) and decompose the rotation about vertical axis into two components, it is easier to understand and implement UB matrix formalism without this step. The rotation matrices are

$$R_1(\omega) = \begin{pmatrix} \cos(\omega) & 0 & \sin(\omega) \\ 0 & 1 & 0 \\ -\sin(\omega) & 0 & \cos(\omega) \end{pmatrix} \tag{55}$$

$$R_2(\mu) = \begin{pmatrix} \cos(\mu) & -\sin(\mu) & 0 \\ \sin(\mu) & \cos(\mu) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{56}$$

$$R_3(\nu) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\nu) & -\sin(\nu) \\ 0 & \sin(\nu) & \cos(\nu) \end{pmatrix} \tag{57}$$

A. Calculate h, k, l components

In this case, we assume that we know the U and B matrices. Equation 8 yield the components of momentum transfer in the laboratory reference frame. Then using equations 5, 55, 56, and 57, we write

$$\mathbf{Q}_l = 2\pi R_1(\omega)R_2(\mu)R_3(\nu)UB \begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{58}$$

which yields

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = \frac{1}{2\pi} B^{-1}U^{-1}R_3^{-1}(\nu)R_2^{-1}(\mu)R_1^{-1}(\omega) \begin{pmatrix} -k_f \sin(\theta)\cos(\phi) \\ -k_f \sin(\theta)\sin(\phi) \\ k_i - k_f \cos(\theta) \end{pmatrix} \tag{59}$$

It is worth mentioning that any rotations described by equation 3 satisfies

$$R^{-1}(\Omega) = R(-\Omega) = R^T(\Omega) \tag{60}$$

An interesting use of equation 59 can help users of the MSlice program, or other software using the convention below. The horizontal plane is described by two non-collinear vectors $\mathbf{u}$ and $\mathbf{v}$, with ψ the angle from $\mathbf{k}_i$ to $\mathbf{u}$. If measurements were made with constant μ and ν tilts, ($\mu = \nu = 0$ for goniometers with only one vertical rotation axis), we can determine a ($\mathbf{u}$, $\mathbf{v}$) pair for any value of ψ. We choose $\mathbf{u}_{lab}$ to have length u_{lab} at angle ψ in the horizontal plane, and $\mathbf{v}_{lab}$ at 90°

$$\mathbf{u}_{lab} = \begin{pmatrix} u_{lab}\sin(\psi) \\ 0 \\ u_{lab}\cos(\psi) \end{pmatrix} \tag{61}$$

$$\mathbf{v}_{lab} = \begin{pmatrix} v_{lab}\cos(\psi) \\ 0 \\ -v_{lab}\sin(\psi) \end{pmatrix} \tag{62}$$

Changing the values of u_{lab} and v_{lab} will just change the magnitudes of $\mathbf{u}$ and $\mathbf{v}$ vectors, so for convenience we use $u_{lab} = v_{lab} = 1$. With these values plugged into equation 59, we one obtains the components of $\mathbf{u}$ and $\mathbf{v}$. To obtain numbers on the order of unity, we can normalize h, k, l components of these vectors, by dividing to the largest value. For example:

$$\mathbf{u} = \begin{pmatrix} 0.12 \\ 0.06 \\ 0 \end{pmatrix} \rightarrow \mathbf{u} = \begin{pmatrix} 0.12 \\ 0.06 \\ 0 \end{pmatrix} /0.12 = \begin{pmatrix} 1 \\ 0.5 \\ 0 \end{pmatrix} \tag{63}$$

Note that u_{lab}, v_{lab} might not have length 1 after this transformation.

1. Project onto different axes

In the previous formulas we projected $\mathbf{Q}_l$ onto an orthogonal basis in order to obtain the h, k, l components. But that is not always what the experimenter wants to see. What if we want to project $\mathbf{Q}_l$ onto different directions $\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$, for example (1,1,0), (1,-1,0), and (0,0,1)? That means finding h', k', l' such as

$$\begin{aligned} h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* &= h'\mathbf{W}_1 + k'\mathbf{W}_2 + l'\mathbf{W}_3 \\ &= h'(w_{11}\mathbf{a}^* + w_{12}\mathbf{b}^* + w_{13}\mathbf{c}^*) + k'(w_{21}\mathbf{a}^* + w_{22}\mathbf{b}^* + w_{23}\mathbf{c}^*) + l'(w_{31}\mathbf{a}^* + w_{32}\mathbf{b}^* + w_{33}\mathbf{c}^*) \end{aligned} \quad (64)$$

By grouping terms corresponding to the same reciprocal lattice basis vectors we obtain:

$$h = w_{11}h' + w_{21}k' + w_{31}l' \quad (65)$$
$$k = w_{12}h' + w_{22}k' + w_{32}l' \quad (66)$$
$$l = w_{13}h' + w_{23}k' + w_{33}l' \quad (67)$$

or in matrix form:

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \\ w_{13} & w_{23} & w_{33} \end{pmatrix} \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} = W \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} \quad (68)$$

If $\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$ are not coplanar, we can compute the inverse of W.

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} = W^{-1} \begin{pmatrix} h \\ k \\ l \end{pmatrix} \quad (69)$$

$$= \frac{1}{|W|} \begin{pmatrix} \begin{vmatrix} w_{22} & w_{32} \\ w_{23} & w_{33} \end{vmatrix} & \begin{vmatrix} w_{31} & w_{21} \\ w_{33} & w_{23} \end{vmatrix} & \begin{vmatrix} w_{21} & w_{31} \\ w_{22} & w_{32} \end{vmatrix} \\ \begin{vmatrix} w_{32} & w_{12} \\ w_{33} & w_{13} \end{vmatrix} & \begin{vmatrix} w_{11} & w_{31} \\ w_{13} & w_{33} \end{vmatrix} & \begin{vmatrix} w_{31} & w_{11} \\ w_{32} & w_{12} \end{vmatrix} \\ \begin{vmatrix} w_{12} & w_{22} \\ w_{13} & w_{23} \end{vmatrix} & \begin{vmatrix} w_{21} & w_{11} \\ w_{23} & w_{13} \end{vmatrix} & \begin{vmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{vmatrix} \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix} \quad (70)$$

One might notice that if we construct W from column vectors $\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$, W^{-1} can be written as

$$W^{-1} = \frac{1}{\mathbf{W}_1 \cdot (\mathbf{W}_2 \times \mathbf{W}_3)} \begin{pmatrix} \mathbf{W}_2 \times \mathbf{W}_3 \\ \mathbf{W}_3 \times \mathbf{W}_1 \\ \mathbf{W}_1 \times \mathbf{W}_2 \end{pmatrix} \quad (71)$$

where $\mathbf{W}_i \times \mathbf{W}_j$ are row vectors.

B. Determine UB matrix

The problem of determining U and B matrices is dependent of the amount of information available,

1. Evaluating U when two reflections are known

If the lattice parameters are known, the U matrix can be obtained from two reflections with known indices. Let's call these reflections $\mathbf{v}_1$ and $\mathbf{v}_2$, with components $v_{1h}, v_{1k}, v_{1l}, v_{2h}, v_{2k}$,and v_{2l}, and corresponding momentum transfers in the lab frame $\mathbf{Q}_1$ and $\mathbf{Q}_2$. We write equation 5 for the two reflections:

$$\mathbf{Q}_1 = 2\pi R(\Omega_1) UB \mathbf{v}_1 \quad (72)$$
$$\mathbf{Q}_2 = 2\pi R(\Omega_2) UB \mathbf{v}_2 \quad (73)$$

By dividing these equations by 2π, and multiplying the first one on the right with $R^{-1}(\Omega_1)$, and the second one with $R^{-1}(\Omega_2)$, we obtain:

$$\frac{1}{2\pi}R^{-1}(\Omega_1)\mathbf{Q}_1 = UB\mathbf{v}_1 \tag{74}$$

$$\frac{1}{2\pi}R^{-1}(\Omega_2)\mathbf{Q}_2 = UB\mathbf{v}_2 \tag{75}$$

U is just a rotation matrix, that nominally rotates $B\mathbf{v}_1$ and $B\mathbf{v}_2$ onto $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$ and $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$. However, in the real case, there are always some errors in determining angles, energies, or the lattice parameters are slightly different than what the experimenter uses as input. This means that the angle between $B\mathbf{v}_1$ and $B\mathbf{v}_2$ is slightly different than the angle between $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$ and $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$, and therefore finding U that satisfies simultaneously the equations above is impossible.

In order to overcome this problem, we are going to create two orthogonal coordinate systems, and let U be the rotation that transforms one into the other. For the reference frame of the sample, we create unit vectors $\widehat{t_{1c}}$ along $B\mathbf{v}_1$, $\widehat{t_{2c}}$ in the plane of $\widehat{t_{1c}}$ and $B\mathbf{v}_2$, and $\widehat{t_{3c}}$ perpendicular to $\widehat{t_{1c}}$ and $\widehat{t_{2c}}$.

$$\widehat{t_{1c}} = \frac{B\mathbf{v}_1}{|B\mathbf{v}_2|} \tag{76}$$

$$\widehat{t_{3c}} = \frac{(B\mathbf{v}_1)\times(B\mathbf{v}_2)}{|(B\mathbf{v}_1)\times(B\mathbf{v}_2)|} \tag{77}$$

$$\widehat{t_{2c}} = \widehat{t_{3c}}\times\widehat{t_{1c}} \tag{78}$$

In an identical fashion, we build three orthogonal unit vectors from $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$ and $R^{-1}(\Omega_1)\mathbf{Q}_1/(2\pi)$, labeled $\widehat{t_{1\nu}}, \widehat{t_{2\nu}}$ and $\widehat{t_{3\nu}}$. We used the index ν to indicate that this system is tied to the inner axis of the goniometer. The $\widehat{t_\nu}$ vectors must also be obtained by rotating the $\widehat{t_c}$ vectors by the U matrix.

$$\begin{aligned}\widehat{t_{1\nu}} &= U\widehat{t_{1c}}\\ \widehat{t_{2\nu}} &= U\widehat{t_{2c}}\\ \widehat{t_{3\nu}} &= U\widehat{t_{3c}}\end{aligned} \tag{79}$$

We can rewrite these equations as a single one using the matrix T_ν, that has columns $\widehat{t_{1\nu}}, \widehat{t_{2\nu}}, \widehat{t_{3\nu}}$ and T_c, that has columns $\widehat{t_{1c}}, \widehat{t_{2c}}, \widehat{t_{3c}}$:

$$T_\nu = UT_c \tag{80}$$

which immediately yields

$$U = T_\nu T_c^{-1} = T_\nu T_c^T \tag{81}$$

The consequence of this orthogonalization is that the direction of $\mathbf{v}_1$ "is taken to be exactly as observed while the observed secondary reflection defines the plane of the calculated secondary peak position but its exact location is taken to be consistent with the known lattice parameters." (M. Lumsden - Angle Calculations for Neutron Scattering Instruments) It is therefore recommended that the specification of which vector is the primary reflection is flexible, and allow for swapping of the two.

NOTE: Special care should be taken when using this procedure with monoclinic or triclinic lattices. For example, suppose we align on (1,0,0) and (0,1,0). In case of a wrong indexing, because they have the same length, (0,-1,0) might be confused with (0,1,0), resulting in the wrong U matrix.

As a corollary we outline a simplification of converting information from MSlice program to obtain the U matrix. The input contains lattice parameters $a, b, c, \alpha, \beta, \gamma$, which allow the calculation of the B matrix. The crystal orientation is specified by vectors $\mathbf{u}$ and $\mathbf{v}$, where $\mathbf{u}$ makes an angle ψ with respect to $\mathbf{k}_i$, and $\mathbf{u}\times\mathbf{v}$ points in the upward direction. With these conventions,

$$\begin{aligned}\widehat{t_{1\nu}} &= \begin{pmatrix}\sin(\psi)\\ 0\\ \cos(\psi)\end{pmatrix}\\ \widehat{t_{2\nu}} &= \begin{pmatrix}\cos(\psi)\\ 0\\ -\sin(\psi)\end{pmatrix}\end{aligned} \tag{82}$$

$$\widehat{t_{3\nu}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

The rest of the steps are identical to the procedure described before.

2. Evaluating U and B when three reflections are known

If one has three non-coplanar indexed reflections, one can determine U and B matrices. Similar to the previous procedure, we write

$$\frac{1}{2\pi} R^{-1}(\Omega_1)\mathbf{Q}_1 = UB\mathbf{v}_1 \tag{83}$$

$$\frac{1}{2\pi} R^{-1}(\Omega_2)\mathbf{Q}_2 = UB\mathbf{v}_2 \tag{84}$$

$$\frac{1}{2\pi} R^{-1}(\Omega_3)\mathbf{Q}_3 = UB\mathbf{v}_3 \tag{85}$$

Let's call Q_ν the matrix made up by the three columns of $\frac{1}{2\pi} R^{-1}(\Omega_i)\mathbf{Q}_i$, and V the matrix made up from the three column vectors $\mathbf{v}_i$. Then the above equations can be written in the matrix form:

$$Q_\nu = UBV \tag{86}$$

which yields

$$UB = Q_\nu V^{-1} \tag{87}$$

If the three reflections are coplanar, then the V matrix is singular, so the above equation has no solution.
If we used the fact that U is just a rotation, obeying equation 60, we can calculate now the lattice parameters from

$$(UB)^T(UB) = B^T U^T UB = B^T B \tag{88}$$

and equations 53 and 54. This allow calculation of B matrix and therefore U matrix as well.

3. Evaluating U and B using multiple reflections

The above procedure can be generalized to N non-coplanar indexed reflections, by using a standard least squares procedure. We define

$$\mathbf{q}_{\nu i} = \frac{1}{2\pi} R^{-1}(\Omega_i)\mathbf{Q}_i \tag{89}$$

so

$$\mathbf{q}_{\nu i} = UB\mathbf{v}_i \tag{90}$$

We can write this explicitly as

$$\begin{pmatrix} UB_{11} & UB_{12} & UB_{13} \\ UB_{21} & UB_{22} & UB_{23} \\ UB_{31} & UB_{32} & UB_{33} \end{pmatrix} \begin{pmatrix} v_{ih} \\ v_{ik} \\ v_{il} \end{pmatrix} - \begin{pmatrix} q_{\nu i1} \\ q_{\nu i2} \\ q_{\nu i3} \end{pmatrix} = 0 \tag{91}$$

or

$$\begin{pmatrix} F_{1i} \\ F_{2i} \\ F_{3i} \end{pmatrix} \equiv \begin{pmatrix} UB_{11}v_{ih} + UB_{12}v_{ik} + UB_{13}v_{il} - q_{\nu i1} \\ UB_{21}v_{ih} + UB_{22}v_{ik} + UB_{23}v_{il} - q_{\nu i2} \\ UB_{31}v_{ih} + UB_{32}v_{ik} + UB_{33}v_{il} - q_{\nu i3} \end{pmatrix} = 0 \tag{92}$$

The goal is to find out the UB matrix elements that verify the above equation for all reflections i. However, due to experimental errors, this is not a realistic goal. Instead, we are going to find the matrix that minimizes

$$F_1 \equiv \sum_{i=1}^{N} (F_{1i})^2, F_2 \equiv \sum_{i=1}^{N} (F_{2i})^2, F_3 \equiv \sum_{i=1}^{N} (F_{3i})^2 \tag{93}$$

We take partial derivatives of F_1, F_2, F_3 with respect to UB matrix elements and set them to 0. The first such equation is

$$\frac{\partial F_1}{\partial (UB_{11})} = 2\sum_{i=1}^{N}(UB_{11}v_{ih} + UB_{12}v_{ik} + UB_{13}v_{il} - q_{\nu i1})v_{ih} = 0 \tag{94}$$

which can be rewritten as

$$\left(\sum_{i=1}^{N} v_{ih}v_{ih}\right) UB_{11} + \left(\sum_{i=1}^{N} v_{ik}v_{ih}\right) UB_{12} + \left(\sum_{i=1}^{N} v_{il}v_{ih}\right) UB_{13} = \sum_{i=1}^{N} q_{\nu i1}v_{ih} \tag{95}$$

Similarly, taking the derivatives of F_1 with respect to UB_{12} and UB_{13}, we obtain three equations with three unknowns. We can write this in a matrix form as

$$\begin{pmatrix} (\sum_i v_{ih}v_{ih}) & (\sum_i v_{ik}v_{ih}) & (\sum_i v_{il}v_{ih}) \\ (\sum_i v_{ih}v_{ik}) & (\sum_i v_{ik}v_{ik}) & (\sum_i v_{il}v_{ik}) \\ (\sum_i v_{ih}v_{il}) & (\sum_i v_{ik}v_{il}) & (\sum_i v_{il}v_{il}) \end{pmatrix} \begin{pmatrix} UB_{11} \\ UB_{12} \\ UB_{13} \end{pmatrix} = \begin{pmatrix} \sum_i q_{\nu i1}v_{ih} \\ \sum_i q_{\nu i1}v_{ik} \\ \sum_i q_{\nu i1}v_{il} \end{pmatrix} \tag{96}$$

Similar equations can be obtained for the other elements of the UB matrix by taking the partial derivatives of F_2 and F_3. We can write all together as

$$\begin{pmatrix} (\sum_i v_{ih}v_{ih}) & (\sum_i v_{ik}v_{ih}) & (\sum_i v_{il}v_{ih}) \\ (\sum_i v_{ih}v_{ik}) & (\sum_i v_{ik}v_{ik}) & (\sum_i v_{il}v_{ik}) \\ (\sum_i v_{ih}v_{il}) & (\sum_i v_{ik}v_{il}) & (\sum_i v_{il}v_{il}) \end{pmatrix} \begin{pmatrix} UB_{11} & U_{21} & U_{31} \\ UB_{12} & U_{22} & U_{32} \\ UB_{13} & U_{23} & U_{33} \end{pmatrix} = \begin{pmatrix} \sum_i q_{\nu i1}v_{ih} & \sum_i q_{\nu i2}v_{ih} & \sum_i q_{\nu i3}v_{ih} \\ \sum_i q_{\nu i1}v_{ik} & \sum_i q_{\nu i2}v_{ik} & \sum_i q_{\nu i3}v_{ik} \\ \sum_i q_{\nu i1}v_{il} & \sum_i q_{\nu i2}v_{il} & \sum_i q_{\nu i3}v_{il} \end{pmatrix} \tag{97}$$

Noting that the second matrix is $(UB)^T$, we obtain

$$UB = \begin{pmatrix} \sum_i q_{\nu i1}v_{ih} & \sum_i q_{\nu i2}v_{ih} & \sum_i q_{\nu i3}v_{ih} \\ \sum_i q_{\nu i1}v_{ik} & \sum_i q_{\nu i2}v_{ik} & \sum_i q_{\nu i3}v_{ik} \\ \sum_i q_{\nu i1}v_{il} & \sum_i q_{\nu i2}v_{il} & \sum_i q_{\nu i3}v_{il} \end{pmatrix}^T \left(\begin{pmatrix} (\sum_i v_{ih}v_{ih}) & (\sum_i v_{ik}v_{ih}) & (\sum_i v_{il}v_{ih}) \\ (\sum_i v_{ih}v_{ik}) & (\sum_i v_{ik}v_{ik}) & (\sum_i v_{il}v_{ik}) \\ (\sum_i v_{ih}v_{il}) & (\sum_i v_{ik}v_{il}) & (\sum_i v_{il}v_{il}) \end{pmatrix}^{-1} \right)^T \tag{98}$$

If the multiple reflections are coplanar, the matrix on the left of equation 97 is singular, so we cannot obtain the UB matrix. Getting the lattice parameters and the U matrix follow the same steps as for only three reflections.

We also must mention here that the most difficult problem with this procedure is the correct indexing of multiple peaks, but that is outside the scope of this document. For more information, you can check for example Steller, I., Bolotovsky, R. & Rossmann, M.G. (1997)

C. Rotate sample in a particular direction

The accessible parameter space for a given measurement depends on sample and instrument orientation. Therefore, it is necessary to establish a procedure to calculate the rotation angles for various instrument axes. Once the UB matrix is determined, there are usually two equivalent ways to define the input of the problem: specify direction of $\mathbf{h}$ or specify the direction of $\mathbf{k}_f$ for a particular $\mathbf{h}$. But in general this problem does not always have a unique solution. Here are a few reasons:

- There is no solution. This happens when there are not enough rotation axes, or have limited range. For example, consider a sample aligned with $\mathbf{a}^*$ and $\mathbf{b}^*$ in the horizontal plane of an instrument that has a goniometer with only one one rotation axis, around the vertical direction. There is no rotation that can bring $\mathbf{c}^*$ in the horizontal plane.
- There is an ambiguity in the input. For example, assume that we want a particular vector $\mathbf{h}$ to point along $\mathbf{k}_i$.If we find a solution, any rotation of the sample around $\mathbf{k}_i$ is also a solution. To overcome this problem, a new constraint is usually defined (like a second vector to be in the horizontal plane).
- A variation of the issue above, when there are too many rotation axes. Even when the sample orientation is known, there are multiple combination of instrument angles that yield the same rotation matrix. For example, consider a goniometer with a vertical rotation axis, and a sample environment that also have a vertical rotation axis. If we want to rotate the sample by let's say 60°, we can rotate the goniometer by 60°, the sample environment by 60°, both by 30°, one by 10, the other by 50°, and so on. In this case it is customary to fix one of the rotations

- The rotation matrix can be obtained by more than one way even with three axes. In the case of the goniometer that was described earlier, $R_1(180^\circ)R_2(180^\circ)R_3(180^\circ) = R_1(0^\circ)R_2(0^\circ)R_3(0^\circ)$. This is usually taken care by either the physical limits of the goniometer (tilts in the goniometer used on triple axis spectrometers are usually limited at $\pm 25^\circ$), or by convention (for example one of the angle is between $\pm 90^\circ$).

It is helpful to write out the rotation matrix for a goniometer with three axes. We are going to use always right handed rotations. There are different conventions for the angles, all rotations being products rotations around different axes. For Euler angles convention two rotations occur around the same axis (for example Z - X - Z), while for Tait-Bryan convention all axes are different (for triple axes spectrometers at HFIR it is Z - Y - X, while the goniometer described at the beginning of this section is Y - Z - X).

$$\begin{aligned} R(\omega,\mu,\nu) &= R_y(\omega)R_z(\mu)R_x(\nu) = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \\ &= \begin{pmatrix} \cos(\omega)\cos(\mu) & -\cos(\nu)\cos(\omega)\sin(\mu)+\sin(\nu)\sin(\omega) & \cos(\omega)\sin(\mu)\sin(\nu)+\cos(\nu)\sin(\omega) \\ \sin(\mu) & \cos(\mu)\cos(\nu) & -\cos(\mu)\sin(\nu) \\ -\cos(\mu)\sin(\omega) & \cos(\omega)\sin(\nu)+\cos(\nu)\sin(\mu)\sin(\omega) & \cos(\nu)\cos(\omega)-\sin(\mu)\sin(\nu)\sin(\omega) \end{pmatrix} \end{aligned} \tag{99}$$

For the rotation matrix using the other conventions see http://en.wikipedia.org/wiki/Euler_angles#Matrix_orientation

If we have the elements of the rotation matrix, from the equation 99 we can determine angles ω, μ, ν.

$$\sin(\mu) = R_{21} \tag{100}$$

$$\cos(\mu) = \sqrt{R_{11}^2 + R_{31}^2} \tag{101}$$

$$\sin(\nu) = -\frac{R_{23}}{\sqrt{R_{11}^2 + R_{31}^2}} \tag{102}$$

$$\cos(\nu) = \frac{R_{22}}{\sqrt{R_{11}^2 + R_{31}^2}} \tag{103}$$

$$\sin(\omega) = -\frac{R_{31}}{\sqrt{R_{11}^2 + R_{31}^2}} \tag{104}$$

$$\cos(\omega) = \frac{R_{11}}{\sqrt{R_{11}^2 + R_{31}^2}} \tag{105}$$

For the other conventions, the above equations are similar, just different subscripts for R elements, and maybe sine and cosine functions are interchanged. Note that by choosing the positive value for $\cos(\mu)$, we chose to have μ between $\pm 90^\circ$. This is a reasonable request for the type of goniometers used on spectrometers at HFIR and SNS.

Note that the equations 100-105 have a problem when $\sqrt{R_{11}^2 + R_{31}^2} = 0$. A more complete procedure to determine Euler angles is presented in the Appendix.

In the next few subsections we are going to present a few cases on how to calculate angles.

1. Define a horizontal plane from two vectors

This subsection assumes that the goniometer can rotate around three axes. There are two version of this case. In the first version, we require that the first vector points along $\mathbf{k}_i$, while in the second one we require that a particular (h,k,l,E) combination is measured.

Let's start with the first case. once again we are going to create an orthogonal set of vectors. If the required reflections in the horizontal plane are $\mathbf{v}_1$ and $\mathbf{v}_2$, we create unit vectors

$$\mathbf{t}_1 = \frac{UB\mathbf{v}_1}{|UB\mathbf{v}_1|} \tag{106}$$

$$\mathbf{t}_3 = \frac{(UB\mathbf{v}_1)\times(UB\mathbf{v}_2)}{|(UB\mathbf{v}_1)\times(UB\mathbf{v}_2)|} \tag{107}$$

$$\mathbf{t}_2 = \mathbf{t}_3 \times \mathbf{t}_1 \tag{108}$$

We create a 3×3 matrix T with each column i containing the components of $\mathbf{t}_i$. The rotation matrix transforms $\mathbf{t}_1$ into $\widehat{z}$, $\mathbf{t}_2$ into $\widehat{x}$, and $\mathbf{t}_3$ into $\widehat{y}$. We can write this in a matrix form as

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = RT \tag{109}$$

which immediately yields

$$R = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} T^{-1} \tag{110}$$

If we want to measure (h, k, l, E), in a detector at angle θ, and $\phi = 0$ or $\phi = \pi$, the first thing is to calculate θ. From equation 8, with $\phi = 0$ we obtain

$$Q_l^2 = k_i^2 + k_f^2 - 2k_i k_f \cos(\theta) \tag{111}$$

At the same time, we can calculate Q^2 from the lattice parameters

$$Q^2 = 4\pi^2 \begin{pmatrix} h & k & l \end{pmatrix} B^T B \begin{pmatrix} h \\ k \\ l \end{pmatrix} = 4\pi^2 \begin{pmatrix} h & k & l \end{pmatrix} G^* \begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{112}$$

Since the $\mathbf{Q}_l$ and $\mathbf{Q}$ are related by rotations only, their magnitude is the same, so

$$\cos(\theta) = \frac{k_i^2 + k_f^2 - Q^2}{2k_i k_f} \tag{113}$$

This equation has both a positive and a negative value for θ. Since θ is between 0 and π, the positive solution corresponds to $(\theta, \phi = 0)$, while the negative solution corresponds to $(|\theta|, \phi = \pi)$. Now we calculate $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ as above, but after rotation they will become $\begin{pmatrix} -k_f/Q \sin(\theta) \\ 0 \\ k_i/Q - k_f/Q \cos(\theta) \end{pmatrix}$, $\begin{pmatrix} k_i/Q - k_f/Q \cos(\theta) \\ 0 \\ k_f/Q \sin(\theta) \end{pmatrix}$, and $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ so

$$R = \begin{pmatrix} -k_f/Q \sin(\theta) & k_i/Q - k_f/Q \cos(\theta) & 0 \\ 0 & 0 & 1 \\ k_i/Q - k_f/Q \cos(\theta) & k_f/Q \sin(\theta) & 0 \end{pmatrix} T^{-1} \tag{114}$$

Note 1. It is possible to choose $\mathbf{v}_1$ and $\mathbf{v}_2$ to define a plane other than horizontal. In that case, the form of the matrix on the left hand side of equation 109 must be changed accordingly. **Note 2.** It is possible to ask that the scattering corresponding to a particular set h, k, l, E to be observed at an angle $\phi \neq 0$. The righter most matrix in equation 114 must be changed accordingly.

2. Shortest path to move $\mathbf{Q}$ towards a specified direction

If there is good detector coverage, someone might be interested to move a particular $\mathbf{Q}$ vector to point in a specified direction $\mathbf{v}$, irrespective of the orientation of the crystal around $\mathbf{v}$, using the smallest rotations from the current position. This is easily achievable by using equation 3, using the following equations:

$$\mathbf{u} = \frac{\mathbf{Q} \times \mathbf{v}}{|\mathbf{Q} \times \mathbf{v}|} \tag{115}$$

$$\sin(\Omega) = \frac{\mathbf{Q} \times \mathbf{v}}{|\mathbf{Q}||\mathbf{v}|} \tag{116}$$

$$\cos(\Omega) = \frac{\mathbf{Q} \cdot \mathbf{v}}{|\mathbf{Q}||\mathbf{v}|} \tag{117}$$

One can use $\mathbf{v}$ to point for example along beamline. This formula can be used if we just want to observe a particular h, k, l, E combination in a particular detector as well. In that case $\mathbf{v} = \mathbf{Q}_l$, with $\mathbf{Q}_l$ given by equation 8.

3. Single vertical axis goniometer

The sample environment for a significant number of time-of-flight spectrometers allows only rotation around the vertical axis. In this case it is convenient to use angles $-\pi < \chi < \pi$ and $-\pi/2 < \delta < \pi/2$, as shown in figure 1. The wavevector transfer in the laboratory frame can then be written as:

$$\mathbf{Q}_l = \begin{pmatrix} -k_f \cos(\delta)\sin(\chi) \\ -k_f \sin(\delta) \\ k_i - k_f \cos(\delta)\cos(\chi) \end{pmatrix} \tag{118}$$

There are few relevant cases for which we want to compute angles:
(1) if we know h, k, l, E, E_i we would like to compute χ, δ, and goniometer angle ω.
(2) if we know h, k, l, E and we want to measure in detectors at angle χ, we calculate E_i, δ, and ω.
(3) point h, k, l as close as possible to $\mathbf{k}_i$.
For simplicity, let's introduce $\mathbf{Q}_0$ as

$$\mathbf{Q}_0 = 2\pi UB \begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{119}$$

so

$$\mathbf{Q}_l = R_1(\omega)\mathbf{Q}_0 \tag{120}$$

with the rotation given by equation 55.

The rotation around the vertical axis will not affect the vertical component of any vector. So angle δ is given by

$$\sin(\delta) = -\frac{Q_{0y}}{k_f} \tag{121}$$

For the range on δ that we have chosen, $\cos(\delta)$ is always positive

$$\cos(\delta) = \sqrt{1 - \sin^2(\delta)} \tag{122}$$

If we compare the $\widehat{z}$ components in equations 8 and 8

$$\cos(\delta)\cos(\chi) = \cos(\theta) = \frac{k_i^2 + k_f^2 - Q_0^2}{2k_i k_f} \tag{123}$$

so

$$\cos(\chi) = \frac{k_i^2 + k_f^2 - Q_0^2}{2k_i k_f \sqrt{1 - \sin^2(\delta)}} \tag{124}$$

This equation has two solutions

$$\chi = \pm \arccos\left(\frac{k_i^2 + k_f^2 - Q_0^2}{2k_i k_f \sqrt{1 - \sin^2(\delta)}} \right) \tag{125}$$

Once the value of χ is chosen, we can calculate ω. When the goniometer is at 0, the angle that the in-plane component makes with the $\widehat{z}$ axis is $\mathrm{atan2}(Q_{x0}, Q_{z0})$, while with the goniometer at ω, we want to point $\mathbf{Q}$ along $\mathbf{Q}_l$, so the angle between the in-plane component and the $\widehat{z}$ axis is $\mathrm{atan2}(Q_{xl}, Q_{zl})$. This yields

$$\omega = \mathrm{atan2}(Q_{xl}, Q_{zl}) - \mathrm{atan2}(Q_{x0}, Q_{z0}) \tag{126}$$

If we want to find the incident energy as a function of angle χ, we are going to use equations 7, 121, and 124.

$$k_i = \sqrt{k_f^2 + 2mE/\hbar^2} \tag{127}$$

$$k_i^2 + k_f^2 - Q_0^2 = 2k_i k_f \cos(\chi)\sqrt{1 - \sin^2(\delta)} \tag{128}$$

$$2k_f^2 + 2mE/\hbar^2 - Q_0^2 = 2k_f \sqrt{k_f^2 + 2mE/\hbar^2}\sqrt{1 - Q_{0y}^2/k_f^2}\cos(\chi) \tag{129}$$

$$2k_f^2 + 2mE/\hbar^2 - Q_0^2 = 2\sqrt{k_f^2 + 2mE/\hbar^2}\sqrt{k_f^2 - Q_{0y}^2}\cos(\chi) \tag{130}$$

By looking at equation 130, we observe that we can square it and obtain a quadratic equation in k_f^2. However, we must be aware of which one is the physical solution. Since both square roots are positive, we must choose the solution for which the sign of $2k_f^2 + 2mE/\hbar^2 - Q_0^2$ is the same as the sign of $\cos(\chi)$. With the correct solution for k_f^2, we can turn back to equation 7 to find E_i, and for the δ and ω angles, the procedure is identical as in the previous case.

For the last case, when we want $\mathbf{Q}$ to point as close as possible to $\mathbf{k}_i$, we can use equation 126, and plug in $Q_{x0} = 0$.

VI. ACKNOWLEDGEMENTS AND REFERENCES

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APPENDIX: METHOD FOR CALCULATING EULER ANGLES FROM A ROTATION MATRIX

In this section I will present a modified method to calculate Euler angles from the rotation matrix. It has the advantage that it can deal with matrix elements that are 0, and I will show a simple implementation for any choice of three axes. In equation 99, we first determine the inner most angle. For this convention,

$$\nu = \text{atan2}(-R_{23}, R_{22}) \tag{A.1}$$

If $\cos(\mu)$=0, then $R_{23} = R_{22} = 0$, and $\nu = 0$. Note that we can obtain a valid solution if we use $\nu = \text{atan2}(-R_{23}, R_{22}) + \pi$, by changing the sign of $\cos(\mu)$.

Once we determine ν, we write

$$\begin{aligned} R(\omega,\mu,\nu)R_x(\nu)^{-1} &= R_y(\omega)R_z(\mu) \\ &= \begin{pmatrix} \cos(\omega)\cos(\mu) & -\cos(\omega)\sin(\mu) & \sin(\omega) \\ \sin(\mu) & \cos(\mu) & 0 \\ -\sin(\omega)\cos(\mu) & \sin(\omega)\sin(\mu) & \cos(\omega) \end{pmatrix} \\ &= \begin{pmatrix} R'_{11} & R'_{12} & R'_{13} \\ R'_{21} & R'_{22} & R'_{23} \\ R'_{31} & R'_{32} & R'_{33} \end{pmatrix} \end{aligned} \tag{A.2}$$

From equations A.2, we immediately find

$$\mu = \text{atan2}(R'_{13}, R'_{33}) \tag{A.3}$$

$$\nu = \text{atan2}(R'_{21}, R'_{22}) \tag{A.4}$$

For $R = R_1(\Omega_1) \cdot R_2(\Omega_2) \cdot R_3(\Omega_3)$, we can write a general formula to determine $\Omega_1, \Omega_2, \Omega 3$ rotation angles, that considers what convention we use. We map X→0,Y→1, Z→2. We define parity 1 for combinations XY, YZ, ZX, and -1 for combinations YX, XZ, ZY. We introduce a coefficient TB, that is 0 if the first and last axis are the same, and 1 when all rotation axes are different. The values of all these numbers are shown in table I.

A compact way to write these values is shown below:

$$\text{TB} = 1 \text{ if (first + second + last == 3) else 0} \tag{A.5}$$

$$\text{par12} = 1 \text{ if ((last - second) \%3 == 1) else -1} \tag{A.6}$$

$$\text{par01} = 1 \text{ if ((second - first) \%3 == 1) else -1} \tag{A.7}$$

where $a\%3$ means a modulo 3. From here:

$$\begin{aligned}
\text{s3} &= (1 - \text{TB} - \text{TB par12})R[(\text{last} + \text{TB par12})\%3, (\text{last} - \text{par12})\%3] && \text{(A.8)}\\
\text{c3} &= (\text{TB} - (1 - \text{TB})\ \text{par12})R[(\text{last} + \text{TB par12})\%3, (\text{last} + \text{par12})\%3] && \text{(A.9)}\\
\Omega_3 &= \text{atan2}(\text{s3}, \text{c3}) && \text{(A.10)}\\
\text{R'} &= \text{R} \cdot \text{R}_3(-\Omega_3) && \text{(A.11)}\\
\text{s1} &= \text{par01}R'[(\text{first} - \text{par01})\%3, (\text{first} + \text{par01})\%3] && \text{(A.12)}\\
\text{c1} &= R'[\text{second}, \text{second}] && \text{(A.13)}\\
\text{s2} &= \text{par01}R'[\text{first}, 3 - \text{first} - \text{second}] && \text{(A.14)}\\
\text{c2} &= R'[\text{first}, \text{first}] && \text{(A.15)}\\
\Omega_2 &= \text{atan2(s2, c2)} && \text{(A.16)}\\
\Omega_1 &= \text{atan2(s1, c1)} && \text{(A.17)}
\end{aligned}$$

Convention	First axis (first)	Second axis (second)	Last axis (last)	Parity 0-1 (par01)	Parity 1-2 (par12)	TB convention (TB)
XYX	0	1	0	1	-1	0
XZX	0	2	0	-1	1	0
YXY	1	0	1	-1	1	0
YZY	1	2	1	1	-1	0
ZXZ	2	0	2	1	-1	0
ZYZ	2	1	2	-1	1	0
XYZ	0	1	2	1	1	1
XZY	0	2	1	-1	-1	1
YXZ	1	0	2	-1	-1	1
YZX	1	2	0	1	1	1
ZXY	2	0	1	1	1	1
ZYX	2	1	0	-1	-1	1

TABLE I: Symbols that describe different Euler conventions