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3D Image Reconstruction
Determination of Pattern Orientation [1]

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Abstract:

The problem of determining the euler angles of a randomly oriented 3-D object from its 2-D Fraunhofer diffraction patterns is discussed. This problem arises in the reconstruction of a positive semi-definite 3-D object using oversampling techniques. In such a problem, the data consists of a measured set of magnitudes from 2-D tomographic images of the object at several unknown orientations. After the orientation angles are determined, the object itself can then be reconstructed by a variety of methods using oversampling, the magnitude data from the 2-D images, physical constraints on the image and then iteration to determine the phases.

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1 Introduction and Motivation

In these notes, part of the problem of reconstructing an image from the measured magnitude of its fourier transform is discussed [1]. The full problem involves reconstructing the unknown Fourier phases based on general properties of the image such as positivity and finite extent [2]. Experimental measurements have shown the usefulness of this "over sampling" approach [3, 4].

In a companion paper [5], we discuss the fitting of multiple transforms and images of a single three dimensional object in which each image pattern has been rotated by a known Euler angles. Here we will discuss the determination of the Euler angles in each pattern from measured properties in the set of patterns. Our treatment will be modelled after a treatment of robotic vision by Xu and Sugimoto [6]. Other references that have treated this problem are [7, 8, 9, 10, 11]. First we will introduce the object description and then define the Euler angle set and the corresponding rotation matrix to be used. During the discussion of the determination of the orientation of each pattern from properties of the 2-D image patterns, several (perhaps too many) examples will be given.

2 Object Definition

For simplicity, several notational abbreviations will be introduced. The image source, which in 3-dimensions could just as well be termed an object, will be defined on a cartesian x-y-z lattice with unit spacing and $N = 2I + 1$ lattice points in each dimension. Thus the coordinate point $\vec{r} = (i, j, k)$ and a volume integral then becomes,

$$\int d^3r \ v[\vec{r}] = \sum_{i=-I}^{i=I} \sum_{j=-I}^{j=I} \sum_{k=-I}^{k=I} v[i, j, k] \tag{1}$$

$$\equiv \sum_{\vec{r}} v[\vec{r}] \ . \tag{2}$$

It will be convenient in many circumstances to split this integral into a longitudinal integral along z (which will eventually be defined by the fixed beam axis) and a transverse 2-dimensional integral over $\vec{r}_\perp = (x, y)$. Thus

$$\int d^2\vec{r}_\perp \ dz \ v[\vec{r}] = \sum_{r_\perp} \sum_{z} v[\vec{r}] \ . \tag{3}$$

This problem deals with diffraction images of an object oriented at arbitrary angles and positions. The rotation of a vector is written as

$$\vec{r}' = \vec{R}^T \cdot \vec{r}, \tag{4}$$

where the rotation matrix $\vec{R}^T$ is discussed in more detail in Appendix A. Thus an object which is rotated about the origin is written as

$$v_R[\vec{r}] \;=\; v[\vec{R}^T\,\vec{r}] \;. \tag{5}$$

It may be convenient in certain circumstances to center the object at the coordinate origin,

$$\int d^3r\ \vec{r}\ v[\vec{r}] \;=\; 0 \;. \tag{6}$$

A general rotation will take the points off the lattice. The values of $v[\vec{r}]$ could then be extracted by interpolation.

For later use we also note the relation and the notation ($\mathbf{l} = \vec{R}\cdot\vec{k}$)

$$\begin{aligned} l_x &= R(x,x)k_x + R(x,y)k_y + R(x,z)k_z \\ l_y &= R(y,x)k_x + R(y,y)k_y + R(y,z)k_z \\ l_z &= R(z,x)k_x + R(z,y)k_y + R(z,z)k_z \;. \end{aligned}$$

3 Rotation Determination—Example

In this section an example will be given in which the relative rotation angles between fourier transform patterns will be determined. The fourier pattern from a source rotated by R will be written as

$$\begin{aligned} F_R[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp\cdot\vec{r}]\ v[\vec{R}^T r] \\ F_R[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp\cdot\vec{R}\cdot\vec{r}]\ v[\vec{r}] \;. \end{aligned} \tag{7}$$

Write $\vec{k}_\perp = \; k(c,s,0)$ so that

$$\begin{aligned} \vec{k}_\perp\cdot\vec{R}\cdot\vec{r} = \; k\Big(& c \quad [R(x,x)\,x + R(x,y)\,y + R(x,z)\,z] \\ & + \; s \quad [R(y,x)\,x + R(y,y)\,y + R(y,z)\,z]\Big) \;. \end{aligned} \tag{8}$$

First define two patterns labelled by a and b

$$F_a[\vec{k}_\perp] \;=\; \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{R}_a \cdot \vec{r}]\; v[\vec{r}]$$
$$F_b[\vec{k}_\perp] \;=\; \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{R}_b \cdot \vec{r}]\; v[\vec{r}]\;. \tag{9}$$

Can one find lines in the $k_x - k_y$ plane along which the patterns are equal? Define a match line in each pattern with a tilt angle A where $c = \cos A$ and $s = \sin A$. Then $\vec{k}_\perp = k\,\vec{t}_\perp$, with $t_x = c$, $t_y = s$ and $t_z = 0$ with $(-K < k < K)$. Assume that the following relation holds

$$F_a(k\,\vec{t}_\perp^{\,a}) = F_b(k\,\vec{t}_\perp^{\,b}) \qquad \text{or explicitly} \qquad F_a(k\,c_a, k\,s_a) = F_b(k\,c_b, k\,s_b)\;, \tag{10}$$

where $c_a = \cos a$, $s_a = \sin a$, $c_b = \cos b$, and $s_b = \sin b$. Note that along these lines, both the magnitude and the phase of the patterns are separately equal. In the application to real data, only the magnitude of the patterns will be available.

The equality of the a and b transform patterns along this line then requires that the phases agree identically for all $\vec{r}$ and k. That is,

$$\vec{t}_\perp^{\,a} \cdot \vec{R}_a \;=\; \vec{t}_\perp^{\,b} \cdot \vec{R}_b \tag{11}$$
$$\vec{t}_\perp^{a} \;=\; \vec{t}_\perp^{b} \cdot (\vec{R}_b\; \vec{R}_a^T) \tag{12}$$
$$\equiv\; \vec{t}_\perp^{b} \cdot \vec{R}_{ba}\;. \tag{13}$$

Note that if the rotations are only in the x-y plane, then the z-component of Eq. [13] is identically satisfied since $R(x,z) = R(y,z) = 0$. Clearly, in this case, one pattern can be rotated into the other via a rotation around the z-axis.

For a general rotation, a partial solution is straightforward. Using the Euler angles as defined in Appendix A, Eq. [13] becomes

$$c_a \;=\; c_b R(x,x) + s_b R(y,x) \tag{14}$$
$$s_a \;=\; c_b R(x,y) + s_b R(y,y) \tag{15}$$
$$0 \;=\; c_b R(x,z) + s_b R(y,z)\;. \tag{16}$$

Now $R(x,z) = \sin\psi\,\sin\theta$ and $R(y,z) = \cos\psi\,\sin\theta$. If $\sin\theta \neq 0$, the last condition is $c_b \sin\psi + s_b\cos\psi = 0$, or $\sin(\psi + b) = 0$.

The first two conditions now are

$$c_a \;=\; c_b[\cos\psi\cos\phi - \cos\theta\sin\psi\sin\phi] - s_b[\sin\psi\cos\phi + \cos\theta\sin\phi\cos\psi] \tag{17}$$
$$=\; \cos\phi(c_b\cos\psi - s_b\sin\psi) = \;\cos\phi\;\cos(\psi + b) \tag{18}$$

$$s_a \;=\; c_b[\cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi] - s_b[\sin\psi\sin\phi - \cos\theta\cos\psi\cos\phi] \tag{19}$$
$$=\; \sin\phi(c_b\cos\psi\; - s_b\sin\phi\;) = \;\sin\phi\;\cos(\psi + b)\;. \tag{20}$$

Recall the previous condition, $\sin(\psi + b) = 0$. Therefore there are two discrete solutions,

$$\text{soln 1} \quad : \quad \psi = -b\ , \quad \phi = a \tag{21}$$
$$\text{soln 2} \quad : \quad \psi = \pi - b, \quad \phi = \pi + a\ . \tag{22}$$

The Euler angle θ is not determined by these conditions.

The rotation matrix for solution 1 is

$$\vec{R}_1(-b, \theta, a) = \begin{pmatrix} c_a c_b + \cos\theta s_a s_b & s_a c_b - \cos\theta c_a s_b & -s_b \sin\theta \\ c_a s_b - \cos\theta s_a c_b & s_a s_b + \cos\theta c_a c_b & +c_b \sin\theta \\ s_a \sin\theta & -c_a \sin\theta & \cos\theta \end{pmatrix} \tag{23}$$

while the rotation matrix for solution 2 is

$$\vec{R}_2(\pi - b, \theta, \pi + a) = \begin{pmatrix} c_a c_b + \cos\theta s_a s_b & s_a c_b - \cos\theta c_a s_b & +s_b \sin\theta \\ c_a s_b - \cos\theta s_a c_b & s_a s_b + \cos\theta c_a c_b & -c_b \sin\theta \\ -s_a \sin\theta & c_a \sin\theta & \cos\theta \end{pmatrix} . \tag{24}$$

Note that solution 1 is transformed into solution 2 by the replacement $\theta \to -\theta$ or equivalently, $\theta \to 2\pi - \theta$. This is a result of the Necker reversal property mentioned in Appendix A. Since the angle θ is not determined so far, the two solutions are equivalent. Solution 1 will be chosen to be the standard form of the solution.

The matching of two patterns along a line cannot determine the angle θ between the planes. Theta measures the angle of intersection and must be determined by comparing more than two patterns. The comparison of three nondegenerate patterns is sufficient to determine the rotations directly.

4 Some Examples

Consider several sequentially labelled patterns that arise from a target at some selected orientations. Recall that $\vec{R} = R(\psi, \theta, \phi)$ and define

$$\vec{R}_{11} = R(\,0,\ 0,\ 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \vec{R}_{21} = R(\,0, \pi/2,\ 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \tag{25}$$

$$\vec{R}_{31} = R(\pi/2, \pi/2, \pi/2) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \vec{R}_{41} = R(0, \pi/4, 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & f & f \\ 0 & -f & f \end{pmatrix} . \tag{26}$$

where $f = 1/\sqrt{2}$. These correspond to patterns taken along various axes of the object.

The patterns are then given explicitly by the transforms

$$F_1(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x x + k_y y] \tag{27}$$

$$F_2(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x x + k_y z] \tag{28}$$

$$F_3(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x z - k_y y] \tag{29}$$

$$F_4(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x x + f * k_y(y + z)] \ . \tag{30}$$

Thus it is clear that the first three patterns match along the lines

$$F_1(k, 0) = F_2(k, 0) \tag{31}$$

$$F_1(0, k) = F_3(0, -k) \tag{32}$$

$$F_2(0, k) = F_3(k, 0) \ . \tag{33}$$

Note also the matches along the lines

$$F_2(k, 0) = F_4(k, 0) \tag{34}$$

$$F_3(fk, -fk) = F_4(0, k) \ . \tag{35}$$

Now assume that all that is known is that the patterns match along the lines given by eqns[31 - 35]. Let pattern 1 define the standard orientation, that is, $R_1 = 1$. For later use define the shorthand

$$c_n = \cos\theta_n \qquad \text{and} \qquad s_n = \sin\theta_n \ . \tag{36}$$

Examining the first of these relations, Eq. [31], one sees that the lines of equality are given by $c_a = 1$ ($s_a = 0$) in pattern 1 and $c_b = 1$ ($s_b = 0$) in pattern 2. The rotation matrix then becomes

$$\vec{R}_{21} = R(0, \theta_{21}, 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{21} & s_{21} \\ 0 & -s_{21} & c_{21} \end{pmatrix} \ . \tag{37}$$

From Eq. [32] the angles are $c_a = c_b = 0$ and $s_a = -s_b = 1$ and therefore

$$\vec{R}_{31} = R(\pi/2, \theta_{31}, \pi/2) = \begin{pmatrix} -c_{31} & 0 & s_{31} \\ 0 & -1 & 0 \\ s_{31} & 0 & c_{31} \end{pmatrix} \ . \tag{38}$$

From Eq. [33], $c_a = s_b = 0$ and $s_a = c_b = 1$. The rotation matrix between from pattern 2 to pattern 3 is

$$\vec{R}_{32} = R(0, \theta_{32}, \pi/2) = \begin{pmatrix} 0 & 1 & 0 \\ -c_{32} & 0 & s_{32} \\ s_{32} & 0 & c_{32} \end{pmatrix} \ . \tag{39}$$

Now review the direct comparison of two patterns, F_a with F_b, neither of which are in the standard orientation:

$$\begin{aligned} F_a[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{r}]\ v[R_{a1}^T \vec{r}] \\ F_b[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{r}]\ v[R_{b1}^T \vec{r}]\ . \end{aligned} \tag{40}$$

In this case choose F_a to define a new standard orientation. In the second equation make the change of variable $\vec{r} \rightarrow\ R_{b1}R_{a1}^T\vec{r}$ and define $v[R_{a1}^T\vec{r}] = w[\vec{r}]$. Then

$$\begin{aligned} F_a[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{r}]\ w[\vec{r}] \\ F_b[\vec{k}_\perp] &= \sum_{\vec{r}} \exp[-i\vec{k}_\perp \cdot \vec{R}_{b1}\vec{R}_{a1}^T \cdot \vec{r}]\ w[\vec{r}]\ . \end{aligned} \tag{41}$$

Therefore for consistency, we must have $\vec{R}_{ba} = \vec{R}_{b1}\vec{R}_{a1}^T$. Since $\vec{R}_{a1}^T = \vec{R}_{1a}$, it is natural to interpret this condition in the form $\vec{R}_{ba} = \vec{R}_{b1}\vec{R}_{1a}$, i.e., in order to rotate from pattern a to pattern b, rotate first from pattern a to a standard orientation labelled 1, followed by 1 to b.

Apply this to the case $a = 2$ and $b = 3$ where $R_{32} = R_{31} \cdot R_{21}^T$, or

$$R(0, \theta_{32}, \pi/2) = R(\pi/2, \theta_{31}, \pi/2) \cdot R(0, -\theta_{21}, 0)\ , \tag{42}$$

or written explicitly

$$\vec{R}_{32} = \begin{pmatrix} 0 & 1 & 0 \\ -c_{32} & 0 & s_{32} \\ s_{32} & 0 & c_{32} \end{pmatrix} = \begin{pmatrix} -c_{31} & s_{31}s_{21} & s_{31}c_{21} \\ 0 & -c_{21} & s_{21} \\ s_{31} & c_{31}s_{21} & c_{31}c_{21} \end{pmatrix}\ . \tag{43}$$

The equality of the last two matrix forms for $\vec{R}_{23}$ demands that all the cosines vanish. The solutions are $s_{21} = s_{31} = s_{32} = \pm 1$. Therefore the planes for patterns 1, 2, and 3 intersect at right angles. The input angles for these examples were such that $s_{21} = s_{31} = s_{23} = 1$. The sign ambiguity corresponds to the obvious invariance of the pattern to reversing the direction of the beam.

In the next section, an analytic solution given in Appendix B for the θ angles will be demonstrated for more general cases.

5 Even More Examples

Consider several sequentially labelled patterns that arise from a target at various orientations. Recall that $\vec{R} = R(\psi, \theta, \phi)$ and define

$$\vec{R}_{11} = R(\,0,\ 0,\ 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \vec{R}_{21} = R(\,0, \pi/2,\ 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \tag{44}$$

$$\vec{R}_{51} = R(0, \pi/2,\ \pi/2) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad \vec{R}_{61} = R(0, \pi/2, \pi/4) = \begin{pmatrix} f & f & 0 \\ 0 & 0 & 1 \\ f & -f & 0 \end{pmatrix} \tag{45}$$

$$\vec{R}_{71} = R(\pi/2, \pi/2, 0) = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \qquad \vec{R}_{81} = R(\pi/4, \pi/2, 0) = \begin{pmatrix} f & 0 & f \\ -f & 0 & f \\ 0 & -1 & 0 \end{pmatrix}, \tag{46}$$

where again $f = 1/\sqrt{2}$. The patterns are then given explicitly by

$$F_1(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x x + k_y y] \tag{47}$$

$$F_2(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x x + k_y z] \tag{48}$$

$$F_5(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x y + k_y z] \tag{49}$$

$$F_6(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x f(x+y) + k_y z] \tag{50}$$

$$F_7(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x z - k_y x] \tag{51}$$

$$F_8(k_x, k_y) = \int d^3r v(\vec{r}) \exp -i[+k_x f(z+x) + k_y f(z-x)]\ , \tag{52}$$

Some of the match lines of the patterns are

$$F_1(k, 0) = F_2(k, 0)) \tag{53}$$

$$F_1(0, k) = F_5(k, 0) \tag{54}$$

$$F_1(fk, fk) = F_6(k, 0) \tag{55}$$

$$F_1(k, 0) = F_7(0, -k) \tag{56}$$

$$F_1(k, 0) = F_8(fk, -fk)\ . \tag{57}$$

Other relations will be discussed later.

Now assume that all that is known is that the patterns match along these lines. Let pattern 1 define the standard orientation, that is, $R_1 = 1$. For later use define the shorthand

$$c_n = \cos\theta_n \qquad \text{and} \qquad s_n = \sin\theta_n\ . \tag{58}$$

Examining the first of these relations, Eq. [53], one sees that $c_a = 1$ ($s_a = 0$) in pattern 1 and $c_b = 1$ ($s_b = 0$) in pattern 2. Therefore for the first solution, $\psi = \phi = 0$, with θ_2 undetermined. The rotation matrix is again

$$\vec{R}_{21} = R(0, \theta_{21}, 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{21} & s_{21} \\ 0 & -s_{21} & c_{21} \end{pmatrix} . \tag{59}$$

From Eq. [54] one has $s_a = 1$ ($a = \pi/2$) and $c_b = 1$ ($b = 0$). From Eq. [55] $c_a = s_a = f$ ($a = \pi/4$) and $c_b = 1$ ($b = 0$). The rotation matrices in terms of the θ angles are $\vec{R}_{51} = R(0, \theta_{51}, \pi/2)$ and $\vec{R}_{61} = R(0, \theta_{61}, \pi/4)$, or

$$\vec{R}_{51} = \begin{pmatrix} 0 & 1 & 0 \\ -c_{51} & 0 & s_{51} \\ s_{51} & 0 & c_{51} \end{pmatrix} \quad \text{and} \quad \vec{R}_{61} = \begin{pmatrix} f & f & 0 \\ -fc_{61} & fc_{61} & s_{61} \\ fs_{61} & -fs_{61} & c_{61} \end{pmatrix} . \tag{60}$$

Continuing down the list, from Eq. [56] we have $c_a = 1$ ($a = 0$) and $s_b = -1$ ($b = -\pi/2$). From the next equality, Eq. [57], $c_a = 1$ ($a = 0$) and $c_b = -s_b = f$ ($b = -\pi/4$). The rotation matrices in terms of the undetermined θ angles are $\vec{R}_{71} = R(\pi/2, \theta_{71}, 0)$ and $\vec{R}_{81} = R(\pi/4, \theta_{81}, 0)$,

$$\vec{R}_{71} = \begin{pmatrix} 0 & c_{71} & s_{71} \\ -1 & 0 & 0 \\ 0 & -s_{71} & c_{71} \end{pmatrix} \quad \text{and} \quad \vec{R}_{81} = \begin{pmatrix} f & c_{81} & fs_{81} \\ -f & fc_{81} & fs_{81} \\ 0 & -s_{81} & c_{81} \end{pmatrix} . \tag{61}$$

Now the determination of the θ angles will be illustrated by considering separately the triplets R_1, R_2, R_6, R_1, R_2, R_6 and R_1, R_5, R_6. The analytic solutions for the θ angles given in Appendix B will also be used. The additional needed relations are

$$F_2(0, k) = F_5(0, k) \tag{62}$$
$$F_2(0, k) = F_6(0, k) \tag{63}$$
$$F_5(0, k) = F_6(0, k) . \tag{64}$$

Proceeding as before, Eq. [62] yields $s_a = 1$ in pattern 2 and $s_b = 1$ in pattern 5. Therefore the rotation matrices from pattern 2 to pattern 6 and from pattern 5 to pattern 6 are of the same form, i.e., $\vec{R}_{52} = R(-\pi/2, \theta_{52}, \pi/2)$,

$$\vec{R}_{52} = \begin{pmatrix} c_{52} & 0 & -s_{52} \\ 0 & 1 & 0 \\ s_{52} & 0 & c_{52} \end{pmatrix} . \tag{65}$$

Similarly, Eq. [63] yields $s_a = 1$ in pattern 2 and $s_b = 1$ in pattern 6. Therefore $\phi = -\psi = \pi/2$. Equation [64] yields $s_a = 1$ in pattern 5 and $s_b = 1$ in pattern 6. Thus $\phi = -\psi = \pi/2$ also in this case. Therefore the rotation matrices from pattern 2 to pattern 6 and from pattern 5 to pattern 6 are of the same form, i.e., $\vec{R}_{62} = R(-\pi/2, \theta_{62}, \pi/2)$ and $\vec{R}_{65} = R(-\pi/2, \theta_{65}, \pi/2)$,

$$\vec{R}_{62} = \begin{pmatrix} c_{62} & 0 & -s_{62} \\ 0 & 1 & 0 \\ s_{62} & 0 & c_{62} \end{pmatrix} \qquad \text{and} \qquad \vec{R}_{65} = \begin{pmatrix} c_{65} & 0 & -s_{65} \\ 0 & 1 & 0 \\ s_{65} & 0 & c_{65} \end{pmatrix} . \tag{66}$$

Now the analytic solution given in Appendix B will be used. First consider the triplet R_1, R_2, and R_5 with $R_{52} = R_{51} \cdot R_{21}^T$. Using the match line angles determined above, we have

$$R(-\pi/2, \theta_{62}, \pi/2) = R(0, \theta_{61}, \pi/4) \cdot R(0, -\theta_{21}, 0) . \tag{67}$$

From Appendix B, Eq. [107],

$$A_1 = \pi/2 \qquad A_2 = \pi/2 \qquad A_3 = \pi/2 , \tag{68}$$

and then from Eqs. [108 - 113],

$$\theta_{52} = \pi/2 \qquad \theta_{51} = \pi/2 \qquad \theta_{21} = \pi/2 . \tag{69}$$

Now consider the triplet R_1, R_2, and R_6 with $R_{62} = R_{61} \cdot R_{21}^T$, or

$$R(-\pi/2, \theta_{62}, \pi/2) = R(0, \theta_{61}, \pi/4) \cdot R(0, -\theta_{21}, 0) . \tag{70}$$

From Appendix B,

$$A_1 = \pi/2 \qquad A_2 = \pi/4 \qquad A_3 = \pi/2 \tag{71}$$

$$\text{and hence} \quad \theta_{62} = \pi/4 \qquad \theta_{61} = \pi/2 \qquad \theta_{21} = \pi/2 . \tag{72}$$

Now consider the triplet R_1, R_5, and R_6 with $R_{65} = R_{61} \cdot R_{51}^T$ or

$$R(-\pi/2, \theta_{65}, \pi/2) = R(0, \theta_{61}, \pi/4) \cdot R(-\pi/2, -\theta_{51}, 0) , . \tag{73}$$

Again from Appendix B,

$$A_1 = +\pi/2 \qquad A_2 = -\pi/4 \qquad A_3 = \pi/2 \tag{74}$$

$$\text{and hence} \quad \theta_{65} = -\pi/4 \qquad \theta_{61} = +\pi/2 \qquad \theta_{51} = \pi/2 . \tag{75}$$

Thus the determination of the Euler angles are in agreement with the input, except for an expected Necker reversal.

There is one more example that should be examined, namely the relation between F_1, F_7 and F_8,

$$F_1(k, 0) = F_7(0, -k) \tag{76}$$

$$F_1(k, 0) = F_8(fk, -fk) \tag{77}$$

$$F_8(k_x, k_y) = F_7(f(k_x - k_y), f(k_x + k_y)) . \tag{78}$$

This relation implies that F_7 and F_8 are the same 2-D pattern but rotated by an angle of $\pi/4$, that is, for any β

$$F_7(k\cos\beta, k\sin\beta) \;=\; F_8(k\cos(\pi/4+\beta), k\sin(\pi/4+\beta)) \;. \tag{79}$$

Such a relation, true throughout the plane, will not be discovered in a search for a match line. Therefore, after a match line is found, one should check to see if there is another match line perpendicular to the one originally found. If so, then the patterns may match in a plane and this should be checked more generally. If the target has a symmetry, then there may be more than one isolated and distinct match line.

6 General Strategy

The data is presented as a set of N two dimensional patterns at unknown orientations. The first step is to determine the orientation angles using the match lines discussed previously. Choose two patterns, n and m, say, and their corresponding patterns

$$F_n(k_x, k_y) \;=\; M_n(k_x, k_y)\exp[-i\Phi(k_x, k_y)] \;, \tag{80}$$

Since only the magnitudes are measured, define a "match" energy as

$$E(n,m) \;=\; \int_{-K}^{K} dk\; [M_n(c_{mn}k, s_{mn}k) - M_m(c_{nm}k, s_{nm}k)]^2 \;, \tag{81}$$

where $c_{mn} = \cos(\alpha_{mn})$ and $s_{mn} = \sin(\alpha_{mn})$ with α_{mn} defining the angle of the match line in pattern n that matches a line in pattern m (similarly for α_{nm}.)

The rotation from pattern n to m is denoted by R_{mn}. Now find the minimum of $E(n,m)$ by varying over the angles α_{mn} and α_{nm}. At the true minimum, the match energy vanishes and the rotation matrix is given by

$$R_{mn}(\theta_{mn}) \;=\; R(-\alpha_{nm}, \theta_{mn}, \alpha_{mn}) \;, \tag{82}$$

where θ_{mn} remains undetermined.

The rotations are fully determined by requiring that triplets of patterns be consistent, i.e.,

$$R_{mn}(\theta_{mn}) \;=\; R_{mj}(\theta_{mj}) \cdot R_{jn}(\theta_{jn}) \;=\; R_{mj}(\theta_{mj}) \cdot R^T_{nj}(\theta_{nj}) \;\;. \tag{83}$$

In the previous examples, pattern j was chosen to be the "standard orientation", but this relation must hold for any $j \neq n, m$. In Appendix B, a closed form solution is given for the three θ angles in terms of the six match line angles. The rotation angles are in general overdetermined. This means that the solution should be quite robust even in the present of noise in the measured pattern signal magnitudes. **Suggested Algorithm:**

1. Order the M observed patterns so that those labelled 1 and 2 are the "best" experimentally measured patterns. Then determine the ψ and ϕ match line angles by minimizing the energy $E(1, 2)$.

2. Repeat the angle determinations with the pair energies $E(1, m)$ and $E(2, m)$ for $2 < m \leq M$. The θ angles are then computed analytically for each triplet R_{21}, R_{m1} and R_{m2} $(m > 2)$ with the condition that θ_{21} has the same sign for every triplet. For more details, see Appendix C.

3. The angular determination can be both checked and improved statistically by minimizing other possible triplets, such as $E(l, k)$, $E(l, m)$, and $E(k, m)$ and then constructing R_{lk}, R_{lm} and R_{km}.

Now that the orientation of each pattern has been determined, one can proceed to reconstruct the 3-D charge distribution. At this point, there are three distinct paths that may be followed:

- Use the measured 2-D magnitudes, $M_n(k_x, k_y)$, their known orientations R_n, together with interpolation in order to construct the 3-D transform magnitude, $M(k_x, k_y, k_z)$. From this, via phase iteration, the 3-D charge distribution, $v(x, y, z)$ can be determined.

- Use each measured 2-D magnitude to construct by phase iteration the 2-D spatial distributions $v_n(x, y)$. These, together with their individual orientation, are then interpolated to achieve the 3-D distribution $v(x, y, z)$.

- Introduce a Hamiltonian (cost function) that uses each measured 2-D magnitude with its orientation as constraints on the 3-D spatial distribution $v(x, y, z)$. These M constraints together with additional constraint of positivity and finite extent of the object define the minimization problem to be solved.

These approaches will be discussed further in reference [5].

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Appendix A—Euler Rotation Matrix

The rotation of a vector will be written as

$$\vec{r}\,' = R\,\vec{r}, \tag{84}$$

or

$$r'(n) = \sum_m R(n,m)\; r(m), \tag{85}$$

where the rotation matrix $\vec{R}$ is (see Arfken [12])

$$\begin{pmatrix} +\cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & +\cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{pmatrix} . \tag{86}$$

The inverse rotation matrix $\vec{R}^{-1}$ is the transpose of the above

$$\begin{pmatrix} +\cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & +\sin\phi\sin\theta \\ +\cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & -\cos\phi\sin\theta \\ \sin\theta\sin\psi & +\sin\theta\cos\psi & +\cos\theta \end{pmatrix} . \tag{87}$$

For example, a rotation around the z-axis by the angle ϕ is achieved by setting $\sin\theta = 0$ and $\sin\psi = 0$ so that $\vec{R}$ becomes

$$\begin{pmatrix} +\cos\phi & +\sin\phi & 0 \\ -\sin\phi & +\cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} , \tag{88}$$

whereas a rotation around the y-axis by the angle θ is achieved by $\sin\phi = 1$ and $\sin\psi = -1$ which produces

$$\begin{pmatrix} +\cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ +\sin\theta & 0 & +\cos\theta \end{pmatrix} . \tag{89}$$

Note the relation

$$R(\psi \pm \pi, \theta, \phi \pm \pi) = R(\psi, -\theta, \phi) \;=\; R(\psi, 2\pi - \theta, \phi) \;. \tag{90}$$

This can be seen directly, or by defining the matrix

$$Q \;=\; \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{91}$$

and noting that

$$
\begin{aligned}
R(\psi,\theta,\phi) &= B(\psi)\cdot C(\psi)\cdot D(\phi) &(92)\\
\text{and}\quad D(\phi\pm\pi) &= Q\cdot D(\phi) &(93)\\
B(\psi\pm\pi) &= B(\psi)\cdot Q &(94)\\
Q\cdot C(\theta)\cdot Q &= C(-\theta) \;=\; C(2\pi-\theta)\ . &(95)
\end{aligned}
$$

Thus

$$
\begin{aligned}
R(\psi\pm\pi,\theta,\phi\pm\pi) &= B(\psi)\cdot Q\cdot C(\psi)\cdot Q\cdot D(\phi) &(96)\\
&= R(\psi,-\theta,\phi) \;=\; R(\psi,2\pi-\theta,\phi)\ . &(97)
\end{aligned}
$$

It also follows that if

$$
\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R(\psi,\theta,\phi)\cdot\begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad (98)
$$

then by multiplying by $-Q$ and using the above relations one sees that

$$
\begin{pmatrix} x' \\ y' \\ -z' \end{pmatrix} = R(\psi,-\theta,\phi)\cdot\begin{pmatrix} x \\ y \\ -z \end{pmatrix}\ . \qquad (99)
$$

This is termed the Necker reversal.

Appendix B—Euler Matrix Solution

In the text, matrix equations of the following form must be solved for all the θ angles.

$$
R_{mn}(\theta_{mn}) \;=\; R_{mj}(\theta_{mj})\cdot R_{jn}(\theta_{jn}) \;=\; R_{mj}(\theta_{mj})\cdot R^T_{nj}(\theta_{nj})\ . \qquad (100)
$$

It will prove convenient to consider the other two equivalent forms of this relation

$$
\begin{aligned}
R_{mj}(\theta_{mj}) &= R_{mn}(\theta_{mn})\cdot R_{nj}(\theta_{nj}) &(101)\\
R_{nj}(\theta_{nj}) &= R^T_{mn}(\theta_{mn})\cdot R_{mj}(\theta_{mj})\ .\ . &(102)
\end{aligned}
$$

Following Arfken [12], the rotation matrix will be written as

$$
R(\psi,\theta,\phi) \;=\; Z(\psi)X(\theta)Z(\phi)\ ,\ . \qquad (103)
$$

where Z is a rotation around the z-axis and X is a rotation around the x-axis. The problem now becomes

$$
Z(\psi_{mn})X(\theta_{mn})Z(\phi_{mn}) = Z(\psi_{mj})X(\theta_{mj})Z(\phi_{mj})Z(-\phi_{nj})X(-\theta_{nj})Z(-\psi_{nj}) \qquad (104)
$$

or

$$X(\theta_{mn})Z(A_3) \;=\; Z(A_1)X(\theta_{mj})Z(A_2)X(-\theta_{nj}) \;, \tag{105}$$

where the last equation follows from [104] by using

$$Z(\beta)Z(\gamma) = \; Z(\beta+\gamma) \qquad \text{with} \qquad Z(0)=1, \tag{106}$$

and the definitions

$$A_1 = \psi_{mj} - \psi_{mn} \qquad A_2 = \phi_{mj} - \phi_{nj} \qquad A_3 = \phi_{mn} + \psi_{nj} \;. \tag{107}$$

By multiplying out selected matrix elements in Eqs. [100 - 102], the solutions are

$$\cos\theta_{mj} \;=\; +[\cos A_1 \cos A_2 - \cos A_3]/\sin A_1 \sin A_2 \tag{108}$$

$$\cos\theta_{nj} \;=\; -[\cos A_2 \cos A_3 - \cos A_1]/\sin A_2 \sin A_3 \tag{109}$$

$$\cos\theta_{mn} \;=\; -[\cos A_1 \cos A_3 - \cos A_2]/\sin A_1 \sin A_3 \;. \tag{110}$$

The relative signs of the θ angles are determined by other selected matrix elements

$$\sin A_1 \;\sin\theta_{mj} \;=\; \sin A_3 \;\sin\theta_{nj} \tag{111}$$

$$\sin A_2 \;\sin\theta_{nj} \;=\; \sin A_1 \;\sin\theta_{mn} \tag{112}$$

$$\sin A_3 \;\sin\theta_{mn} \;=\; \sin A_2 \;\sin\theta_{mj} \;\;. \tag{113}$$

One method of solution is to solve, for example, Eq. [108] for $\theta_{mj} > 0$, and then use Eqs. [112 & 113] to determine the other two angles. The Necker reversal is evident since the negative of the above angles is also a solution.

Here the general solution given above will be specialized to the case outlined in the algorithm. Matrix equations of the following form must be solved for all m values,

$$R_{m2}(\theta_{m2}) \;=\; R_{m1}(\theta_{m1}) \cdot R_{12}(\theta_{12}) \;=\; R_{m1}(\theta_{m1}) \cdot R^T_{21}(\theta_{21}) \;\;. \tag{114}$$

The solution is given in terms of the angles

$$A_1 = \psi_{m1} - \psi_{m2} \qquad A_2 = \phi_{m1} - \phi_{21} \qquad A_3 = \phi_{m2} + \psi_{21} \tag{115}$$

and explicitly by eqns[108 - 113].

The consistency of the solution requires that the data yield the *same* value of θ_{21} for *any* value of m. In order to guarantee the consistency of the signs of the rotation angles, one must simply solve for θ_{21} and choose its sign. From that solution, Eq. [111] and Eq. [113] then yield the angles θ_{m1} and θ_{m2} without ambiguity.

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