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# The Symmetry of Three-Beam Scattering Equations: Inversion of Three-Beam Diffraction Patterns from Centrosymmetric Crystals

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## Abstract

It is shown that for a centrosymmetric crystal, and within the range of validity of the three-beam approximation, the phases as well as the magnitudes of the three structure amplitudes can be measured uniquely and directly from the geometry of the intensity distributions in the discs of a convergent-beam diffraction pattern. In fact, the solution is given in terms of three distances measured on the diffraction pattern. It is further shown that the inversion is independent of thickness. Three proofs are given, each illustrating a different aspect of the physical processes involved. In the first, the fundamental symmetry of the diffraction process is shown to be that of the special unitary group of order three and the Gell-Mann representation is used to construct three sub-algebras, in terms of which the explicit solution is written. SU(3) is shown to have particular significance in crystallography, namely, that it is the group of lowest order with symmetries that can be analysed to yield structural phase. The second and longer method involves the projection of the scattering matrix into the spaces of the eigenvectors. Unlike the first method, this makes use of a basis; however, it is not necessary to calculate explicitly either the eigenvectors or the eigenvalues. The third method, based on the Bloch-wave expansion, shows that the system is characterized by three lines, which are ruled on one of the dispersion surfaces, and that all of the information in the system is embodied in these lines. Although this theory is scalar and developed here for electron diffraction, it can apply equally to the right circular component of the wave function of X-rays. Some brief remarks are made on the practicability of this method based on preliminary experiments that indicate that phase is the easiest of the parameters to measure.

## 1. Introduction

It has been known theoretically for some time that, in the three-beam approximation and for centrosymmetric crystals, both the magnitudes and the phases of $V(\mathbf{g})$, $V(\mathbf{h})$ and $V(\mathbf{h}-\mathbf{g})$ can be determined directly and uniquely from the geometry of the intensity distributions in the discs of convergent-beam electron diffraction patterns (Moodie, 1979). [$V(\mathbf{g})$, $V(\mathbf{h})$ and $V(\mathbf{h}-\mathbf{g})$ are the Fourier coefficients of the crystal potential, which are referred to here as the structure amplitudes.]

The original proof was lengthy and complicated and never published in full. Subsequently, a less involved proof based on a projector-operator formalism (Hurley, Johnson, Moodie, Rez & Sellar, 1978) was outlined at the XV Congress of the IUCr in Bordeaux (Moodie, 1990) along with an extension to the noncentrosymmetric case. It is the main purpose of the present communication to present a full but compact proof in which the symmetries inherent in the equations of high-energy dynamical electron diffraction are exploited by an appeal to some of the elementary properties of Lie groups and Lie algebras. This method exposes the fundamental mathematical structure of the system and so offers both economy of effort and the prospect of generalization to noncentrosymmetric crystals and to a greater number of beams.

Since additional physical insights can be gained from different models, proofs are also outlined in terms of Dirac-projector operator and Bloch-wave formalisms.

## 2. Outline of the technique

In the two-beam approximation, the wave function of the diffracted beam $\langle\mathbf{g}|$ is given by

$$\langle\mathbf{g}|\mathbf{S}|0\rangle = \exp\{i\pi\zeta z\}i\sigma V(\mathbf{g})\frac{\sin[(\pi\zeta)^2+\sigma^2V(\mathbf{g})V(\bar{\mathbf{g}})]^{1/2}z}{[(\pi\zeta)^2+\sigma^2V(\mathbf{g})V(\bar{\mathbf{g}})]^{1/2}},$$

where $\zeta$ is the excitation error,

$$\mathbf{S}\equiv\exp\left\{i\begin{pmatrix}0 & \sigma V(\bar{\mathbf{g}})\\ \sigma V(\mathbf{g}) & 2\pi\zeta\end{pmatrix}z\right\}$$

is the relevant scattering matrix and $\sigma$ is the interaction constant (Cowley & Moodie, 1992). Since in the wave function the structure amplitude of the diffracted beam, $V(\mathbf{g})$, is always multiplied by the structure amplitude of the coupling beam, $V(\bar{\mathbf{g}})$, no phase information can be recovered from the two-beam diffraction pattern.

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In the three-beam approximation, however, triple products of structure amplitudes, those of both diffracted beams, $V(\mathbf{g})$ and $V(\mathbf{h})$, with the coupling beam, $V(\mathbf{h}-\mathbf{g})$, necessarily form part of the wave function so that phase information is certainly contained in the diffraction pattern. What is required is a method for extracting it. The method that is described in this paper involves the decoupling of the scattering equations in such a way as to identify certain loci of $\zeta$ in the three-beam convergent-beam pattern along which the intensity distribution $I(\zeta)$ is of two-beam form; that is, to identify certain loci of $\zeta$ for which, for some beam(s) $\mathbf{q}$,

$$\langle \mathbf{q}|S|0\rangle = \exp\{i\alpha z\}iA(\sin \beta z)/\beta.$$

The distribution of intensity along these loci is thus centrosymmetric with respect to the excitation error $\zeta$, $I(\zeta) = I(-\zeta)$, and this allows them in practice to be uniquely identified. $\alpha$, $A$ and $\beta$ are determined in terms of the three-beam parameters so that, although the intensity distribution along the loci mimics that of a two-beam system, all of the information characterizing the three-beam system is retained and, in particular, is made accessible through the simplicity of the two-beam form.

It is shown that the values of $\zeta$ at two specific and directly measurable points along the loci are sufficient to determine $|V(\mathbf{g})|$, $|V(\mathbf{h})|$, $|V(\mathbf{h}-\mathbf{g})|$ and the sign of $V(\mathbf{g})V(\mathbf{h})V(\mathbf{h}-\mathbf{g})$; that is, to invert the diffraction pattern. In addition, it is shown that the geometry on which the inversion depends is independent of crystal thickness.

## 3. Inversion directly from inherent dynamical symmetries

### 3.1. *Defining equations*

The starting point is Tournarie's (1962) semi-reciprocal equation for the forward elastic scattering of fast electrons,

$$\mathrm{d}|u\rangle/\mathrm{d}z = i\mathbf{M}_0|u\rangle, \quad |u\rangle_{z=0} \equiv |0\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

with the formal solution in the projection approximation (Sturkey, 1962),

$$|u\rangle = \exp\{i\mathbf{M}_0 z\}|0\rangle \equiv \mathbf{S}|0\rangle.$$

For $N$-beam scattering, the fundamental symmetry is therefore that of $U(N)$, the unitary group of order $N$. This group can always be factored into the less complicated groups $U(1)$ and SU($N$), so that

$$\mathbf{S} = \exp\{i\mathbf{M}_0 z\} = \exp\{i\eta z\}\mathbf{E}\exp\{i\mathbf{M}_s z\},$$

with $\mathbf{E}$ the unit matrix, $\exp\{i\eta z\}\mathbf{E}$ in $U(1)$ and $\exp\{i\mathbf{M}_s z\}$ in SU($N$), the special unitary group of order $N$. $\eta$ is chosen to make $\mathbf{M}_s$ traceless.

In the present work, $N = 3$, so that the group to be analysed is SU(3), a much more complicated mathematical entity than SU(2), the group of the two-beam approximation. This additional complexity is to be expected in view of the greater physical content of the system and, above all, because of the influence of structural phase on the distribution of scattered intensity. SU(3) in fact has the particular significance in crystallography that it is the group of lowest order with symmetries that embody and can be analysed to yield structural phase.

The analysis takes the form of determining for what angles of incidence the three-beam approximation has an intensity distribution with two-beam form, a course of action that is suggested by the fact that SU(2) can form a subgroup of SU(3). The possibility of achieving this is explored by determining what functional relationships must be imposed on the diagonal terms of the scattering matrix in order that it describes a system with the symmetry of SU(2). There is of course no *a priori* reason to believe that this will be possible, but a necessary condition is that $\langle \mathbf{g}|\mathbf{M}_0^2|0\rangle/V(\mathbf{g})$ should be real (Moodie & Fehlmann, 1993). While this condition can be satisfied to various approximations in a number of noncentrosymmetric space groups (Moodie & Whitfield, 1994), it cannot in general be satisfied in $P1$ even in the three-beam approximation. In the first instance, therefore, only the centrosymmetric case will be considered, that is, the discrete symmetry of inversion associated with the space group of the crystal will be combined with the continuous symmetries of SU(3) associated with the scattering equations.

There are well established methods for determining whether a crystal is centrosymmetric (Goodman & Lehmpfuhl, 1968) and therefore whether the technique described in this paper is applicable. (These methods derive from the fact that Friedel's law is broken in dynamical scattering.)

### 3.2. *Conditions for equivalent two-beam forms*

If at least one diffracted beam is of two-beam form, independent of thickness and of any relationships between the structure amplitudes induced by symmetries other than that of a centre of inversion, then, for some beam $\langle \mathbf{q}|$, and with $\alpha$, $\beta$ and $A$ real but otherwise arbitrary,

$$\langle \mathbf{q}|\mathbf{S}|0\rangle = \exp\{i\alpha z\}iA(\sin \beta z)/\beta.$$

Thus, $\exp\{-i\alpha z\}\langle \mathbf{q}|\mathbf{S}|0\rangle$ is required to be antisymmetric in $z$ and hence $\langle \mathbf{q}|\mathbf{M}^{2n}|0\rangle$ must be zero for all positive integral $n$, for at least one $\langle \mathbf{q}|$ and with $\mathbf{M}$ defined by

$$\exp\{-i\alpha z\}\langle\mathbf{q}|\mathbf{S}|0\rangle = \langle\mathbf{q}|\exp\{-i\alpha z\}\mathbf{E}\exp\{i\mathbf{M}_0 z\}|0\rangle$$
$$= \langle\mathbf{q}|\exp\{i\mathbf{M}z\}|0\rangle.$$

Explicitly,

$$\mathbf{M} = \begin{pmatrix} -\alpha & \sigma V(\mathbf{g}) & \sigma V(\mathbf{h}) \\ \sigma V(\mathbf{g}) & 2\pi\zeta_{\mathbf{g}} - \alpha & \sigma V(\mathbf{h}-\mathbf{g}) \\ \sigma V(\mathbf{h}) & \sigma V(\mathbf{h}-\mathbf{g}) & 2\pi\zeta_{\mathbf{h}} - \alpha \end{pmatrix}.$$

Now,

$$\exp\{i\mathbf{M}z\} = \exp\{i(\eta-\alpha)z\}\mathbf{E}\exp\{i\mathbf{M}_s z\}$$

with

$$\eta = (2\pi/3)(\zeta_{\mathbf{g}} + \zeta_{\mathbf{h}}).$$

$\mathbf{M}_s$ is symmetric and traceless, belongs to the algebra su(3) and can therefore be expanded in, say, the Gell-Mann bases (Gell-Mann, 1962) (Appendix *A*). The Lie algebra of order $N$ is spanned by $N^2-1$ bases so that eight are in general required in su(3). Since $\mathbf{M}_s$ derives from a centrosymmetric structure, however, it is symmetric rather than Hermitian and consequently only the five bases of the 'centrosymmetric' anti-commutator sub-algebra are required, namely, $\lambda_1$, $\lambda_4$, $\lambda_6$, $\lambda_3$, $\lambda_8$ (using conventional notation, Appendix *A*). The first three relate to potential energy and the last two, which are diagonal, to kinetic energy. The symmetries of the system are then summarized as

$$\lambda_i\lambda_j + \lambda_j\lambda_i \equiv \{\lambda_i, \lambda_j\} = (4/3)\delta_{ij}\mathbf{E} + 2d_{ijk}\lambda_k,$$

where $d_{ijk}$ are the structure constants of the anti-commutator sub-algebra, given by

$$d_{ijk} = \tfrac{1}{4}\mathrm{tr}(\{\lambda_i, \lambda_j\}\lambda_k)$$

and listed in Appendix *A*. Thus,

$$\mathbf{M}_s = {}_1a_1\lambda_1 + {}_1a_4\lambda_4 + {}_1a_6\lambda_6 + {}_1a_3\lambda_3 + {}_1a_8\lambda_8$$

and

$$\mathbf{M}_s^{2n} = {}_{2n}a_1\lambda_1 + {}_{2n}a_4\lambda_4 + {}_{2n}a_6\lambda_6 + {}_{2n}a_3\lambda_3 + {}_{2n}a_8\lambda_8,$$

where the ${}_na_i$ incorporate the structural and orientational parameters of the three-beam system, for example, ${}_1a_1 = \sigma V(\mathbf{g})$. If we write $\sum_5 {}_{2n}a_i\lambda_i$ for the summation over the five bases, the condition for antisymmetry that leads to a two-beam form is that $\alpha$ must satisfy

$$\left\langle \mathbf{q}\left|\left[(\eta-\alpha)\mathbf{E} + \sum_5 {}_1a_i\lambda_i\right]^{2n}\right|0\right\rangle = 0$$

for at least one $\langle\mathbf{q}|$.

Now, as can be seen from the relation $d_{ijk} = \frac{1}{4}\mathrm{tr}(\{\lambda_i, \lambda_j\}\lambda_k)$, the only sub-algebras of the 'centrosymmetric' sub-algebra compatible with this condition are those spanned by $\lambda_6, \lambda_3, \lambda_8$; $\lambda_4, \lambda_3, \lambda_8$ and $\lambda_1, \lambda_3, \lambda_8$, and these generate the forms

$$\mathbf{M}_b^2 = \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & m_{23} \\ 0 & m_{32} & m_{33} \end{pmatrix},$$

$$\mathbf{M}_g^2 = \begin{pmatrix} m_{11} & 0 & m_{13} \\ 0 & m_{22} & 0 \\ m_{31} & 0 & m_{33} \end{pmatrix},$$

$$\mathbf{M}_h^2 = \begin{pmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}.$$

It is not, of course, yet established that the constraints imposed by any one of these forms are physically admissible, so it is necessary to analyse each separately.

### 3.3. *The form* $\mathbf{M}_b^2 = \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & m_{23} \\ 0 & m_{32} & m_{33} \end{pmatrix}$ *spanned by the bases* $\lambda_6, \lambda_3, \lambda_8$

Equating $m_{21}$ to zero gives

$$m_{21} = \sigma V(\mathbf{g})(2\pi\zeta_{\mathbf{g}} - 2\alpha) + \sigma^2 V(\mathbf{h})V(\mathbf{h}-\mathbf{g}) = 0,$$

*i.e.*

$$\alpha = \tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})].$$

Equating $m_{31}$ to zero gives

$$m_{31} = \sigma V(\mathbf{h})(2\pi\zeta_{\mathbf{h}} - 2\alpha) + \sigma^2 V(\mathbf{g})V(\mathbf{h}-\mathbf{g}) = 0,$$

*i.e.*

$$\alpha = \tfrac{1}{2}[2\pi\zeta_{\mathbf{h}} + \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})].$$

Thus, in order that the conditions $m_{21} = m_{31} = 0$ can be satisfied, a constraint is imposed, namely,

$$2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})$$
$$= 2\pi\zeta_{\mathbf{h}} + \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}).$$

This is physically admissible since it defines a real locus along which the form exists and specifies a real value for $\alpha$. Specifically, the locus is a line parallel to the bisector of the angle between the diffracted beams. The wave functions associated with this locus can be obtained by explicit calculation of the appropriate matrix elements. These are labelled with the subscript *b*. Thus,

$$\langle\mathbf{g}|\exp\{i\mathbf{M}z\}|0\rangle_b = \sum_{n=0}^{\infty} \sigma V(\mathbf{g})m_{11}^n(iz)^{2n+1}/(2n+1)!$$
$$= i\sigma V(\mathbf{g})(\sin m_{11}^{1/2}z)/m_{11}^{1/2}.$$

Similarly,

$$\langle\mathbf{h}|\exp\{i\mathbf{M}z\}|0\rangle_b = i\sigma V(\mathbf{h})(\sin m_{11}^{1/2}z)/m_{11}^{1/2}.$$

Further,

$$\langle 0|\exp\{i\mathbf{M}z\}|0\rangle_b = \cos m_{11}^{1/2}z - i\alpha(\sin m_{11}^{1/2}z)/m_{11}^{1/2}.$$

Now,

$$\begin{aligned} m_{11} &= [\alpha^2 + \sigma^2 V^2(\mathbf{g}) + \sigma^2 V^2(\mathbf{h})] \\ &= \{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2 + \sigma^2 V^2(\mathbf{g}) \\ &\quad + \sigma^2 V^2(\mathbf{h}), \end{aligned}$$

so that $2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) \equiv 2\pi\zeta_{\mathbf{b}}$ is the effective excitation error and $\sigma V(\mathbf{g}) + i\sigma V(\mathbf{h}) \equiv \sigma V(\mathbf{b})$ the effective potential in the equivalent two-beam form,

$$\begin{pmatrix} u(0) \\ u(1) \end{pmatrix} = \exp\{i\pi\zeta_{\mathbf{b}} z\}\mathbf{E} \times \exp\left\{ i \begin{pmatrix} -\pi\zeta_b & \sigma V^*(\mathbf{b}) \\ \sigma V(\mathbf{b}) & \pi\zeta_{\mathbf{b}} \end{pmatrix} z \right\} \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

where

$$u(1) = \langle \mathbf{g}|u\rangle_{\mathbf{b}} + i\langle \mathbf{h}|u\rangle_{\mathbf{b}}.$$

Thus,

$$\begin{aligned} u(1) &= \exp\{i\pi\zeta_{\mathbf{b}} z\} i\sigma V(\mathbf{b}) \sin[(\pi\zeta_{\mathbf{b}})^2 + \sigma^2 V(\mathbf{b})V^*(\mathbf{b})]^{1/2} z \\ &\quad \times [(\pi\zeta_{\mathbf{b}})^2 + \sigma^2 V(\mathbf{b})V^*(\mathbf{b})]^{-1/2}, \end{aligned}$$

so that, typically,

$$\begin{aligned} \langle \mathbf{g}|u\rangle_{\mathbf{b}} &= \exp\{i\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]z\} \\ &\quad \times i\sigma V(\mathbf{g}) \sin\left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2 \right. \\ &\quad \left. + \sigma^2 V^2(\mathbf{g}) + \sigma^2 V^2(\mathbf{h})\right)^{1/2} z \\ &\quad \times \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2 \right. \\ &\quad \left. + \sigma^2 V^2(\mathbf{g}) + \sigma^2 V^2(\mathbf{h})\right)^{-1/2}. \end{aligned}$$

In this form, therefore, the same two-beam intensity distribution exists along a locus in all three convergent-beam discs. Further, all of these loci are parallel to the bisector of the angle between the diffracted beams and displaced the same distances and in the same direction from the origins of the excitation errors. As it must be, this form is invariant under the interchange of **h** and **g**.

The effective excitation error contains a triple product of the structure amplitudes and so at the outset the distribution of intensity along the two-beam loci in the convergent-beam discs is seen to be dependent on structural phase in a directly interpretable way.

In fact, if it is only necessary to determine the relative phases of the structure amplitudes, then no further analysis is required. It is sufficient to set up a three-beam condition, identify the two-beam locus in any beam, find the centre of the distribution and determine whether this point lies on the positive or negative side of the $\zeta_{\mathbf{g}}$ axis. This determines the sign of $V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})$. The other two beams can be used as checks, a first example of redundancy in the solution. Another three-beam condition is then set up and the process is repeated.

While the actual structure is centrosymmetric, the effective potential in the two-beam form, $\sigma V(\mathbf{b}) = \sigma V(\mathbf{g}) + i\sigma V(\mathbf{h})$, is noncentrosymmetric, pictorially because of the asymmetry induced by the effective excitation error, $2\pi\zeta_{\mathbf{b}} = 2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})$. This is a phase-dependent quantity so that the sign of the asymmetry can be considered as determining the sign of the structure amplitudes.

For complete inversion, that is the determination of the magnitudes as well as the signs of the structure amplitudes, information derived from the other forms is required. It will be found that the two-beam distributions associated with these forms derive from physical processes distinct from those described above.

### 3.4. *The form defined by* $\mathbf{M}_g^2 = \begin{pmatrix} m_{11} & 0 & m_{13} \\ 0 & m_{22} & 0 \\ m_{31} & 0 & m_{33} \end{pmatrix}$ *spanned by the bases* $\lambda_4, \lambda_3, \lambda_8$

Equating $m_{21}$ to zero gives

$$\alpha = \tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})],$$

while equating $m_{23}$ to zero gives

$$\alpha = \tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + 2\pi\zeta_{\mathbf{h}} + \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g})].$$

Thus, the constraint imposed in order that the conditions $m_{21} = m_{23} = 0$ are satisfied is

$$2\pi\zeta_{\mathbf{h}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}).$$

Again, this is physically admissible since it defines a real locus and specifies a real value for $\alpha$. Now, however, the locus is a line parallel to the $\zeta_{\mathbf{g}}$ axis. For this form, direct calculation shows that the locus is confined to the beam $\langle \mathbf{g}|$ and that the wave function, now labelled with the subscript **g**, is

$$\begin{aligned} \langle \mathbf{g}|u\rangle_{\mathbf{g}} &= \exp\{i\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]z\} \\ &\quad \times i\sigma V(\mathbf{g}) \sin\left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2 \right. \\ &\quad \left. + \sigma^2 V^2(\mathbf{g}) + \sigma^2 V^2(\mathbf{h}-\mathbf{g})\right)^{1/2} z \\ &\quad \times \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2 \right. \\ &\quad \left. + \sigma^2 V^2(\mathbf{g}) + \sigma^2 V^2(\mathbf{h}-\mathbf{g})\right)^{-1/2}. \end{aligned}$$

As with the locus '**b**', the effective excitation error depends on the phase of the structure amplitudes in a directly interpretable way and, again, if only the relative phase of the structure amplitudes is required, then only the centre of the two-beam distribution need be located. The displacement of the centre, while equal in magnitude, is opposite in sign to that of the first locus.

### 3.5. *The form defined by* $\mathbf{M}_h^2 = \begin{pmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}$ *and spanned by the bases* $\lambda_1, \lambda_3, \lambda_8$

On equating $m_{31}$ and $m_{32}$ successively to zero, the analysis proceeds in an analogous fashion to that for the previous form with results that are identical when **g** and **h** are interchanged. This is to be expected since **g** and **h** are arbitrary labels. Explicitly,

$$\langle \mathbf{h}|u\rangle_{\mathbf{h}} = \exp\{i\tfrac{1}{2}[2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})]z\} \times i\sigma V(\mathbf{h})\sin\left((\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})]\}^2 + \sigma^2 V^2(\mathbf{h}) + \sigma^2 V^2(\mathbf{h}-\mathbf{g})\right)^{1/2} z \times \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})]\}^2 + \sigma^2 V^2(\mathbf{h}) + \sigma^2 V^2(\mathbf{h}-\mathbf{g})\right)^{-1/2}.$$

## 4. Inversion

In the convergent-beam disc $\langle\mathbf{g}|$, the intersection of locus '**b**' with locus '**g**' defines the point $(G_1, G_2)$ with

$$G_1 = 2\pi\zeta_{\mathbf{g}} = \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}),$$
$$G_2 = 2\pi\zeta_{\mathbf{h}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}).$$

The coordinates of this point were determined by Gjønnes & Høier (1971) from the condition for confluence of two of the eigenvalues of $\mathbf{M}_0$. It will therefore be referred to as the Gjønnes–Høier point. The centre of the two-beam intensity distribution on locus **g** is given by

$$G_3 = 2\pi\zeta_{\mathbf{g}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}),$$

so that

$$\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}) = G_3 - G_2,$$
$$\sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}) = G_1 - G_2 + G_3,$$
$$\sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) = G_3$$

and the magnitudes of the structure amplitudes are given in terms of the directly measurable distances $G_1, G_2, G_3$ as

$$\sigma^2 V^2(\mathbf{g}) = (G_3 - G_2)(G_1 - G_2 + G_3),$$
$$\sigma^2 V^2(\mathbf{h}) = G_3(G_3 - G_2),$$
$$\sigma^2 V^2(\mathbf{h}-\mathbf{g}) = G_3(G_1 - G_2 + G_3).$$

Along with the sign of $G_3$, which phases the structure amplitude, this completes the inversion. The inversion therefore requires an analysis of the geometry of the pattern only, rather than a matching of the intensity distribution across $(\zeta_{\mathbf{g}}, \zeta_{\mathbf{h}})$.

There are numerous opportunities for checking the inversion. At any one thickness, the phase can be read separately from each of the three beams and the magnitudes of all the structure amplitudes can be obtained independently from either of the diffracted beams. In addition, the result is independent of thickness and, since each thickness generates independent data, extensive checking is possible.

The steps to inversion *via* the Lie algebra method are summarized in the flow diagram of Fig. 1.

## 5. Alternative derivations

The above calculations rely only on the symmetries intrinsic to the scattering equations. These are modelled by relationships among the subgroups of anticommutator Lie algebras. This involves little manipulation, and in particular does not require explicit calculation of eigenvalues or eigenvectors. Methods which do, while tending to be lengthy, nevertheless often offer those additional insights that derive from different, though ultimately equivalent, models.

Accordingly, two alternative derivations will be outlined, one based on projection operators and one on Bloch waves.

In order to underline the relationship obtaining between the methods, as well as to define the notations, a few known results will first be summarized.

With eigenkets $|^j t\rangle$ and eigenvalues $\mu_j$,

$$\mathbf{M}_0|^j t\rangle = \mu_j|^j t\rangle, \quad \langle^i t|^j t\rangle = \delta_{ij}.$$

If $|^j t\rangle\langle^j t| \equiv \mathbf{P}_j$, then $\mathbf{P}_j^2 = |^j t\rangle\langle^j t|^j t\rangle\langle^j t| = \mathbf{P}_j$ and $\mathbf{P}_i\mathbf{P}_j = 0, i \neq j$.

Also,

$$\mathbf{M}_0\mathbf{P}_j = \mathbf{M}_0|^j t\rangle\langle^j t| = \mu_j|^j t\rangle\langle^j t| = \mu_j\mathbf{P}_j,$$

and so

$$f(\mathbf{M}_0)\mathbf{P}_j = f(\mu_j)\mathbf{P}_j.$$

If $f(x)$ can be expanded in a Taylor series, since $\sum_j \mathbf{P}_j = \mathbf{E}$, then

$$f(\mathbf{M}_0) = f(\mathbf{M}_0)\mathbf{E} = f(\mathbf{M}_0)\sum_j \mathbf{P}_j = \sum_j \mathbf{P}_j f(\mu_j) \quad \text{(Sylvester's theorem)}.$$

Hence,

$$\langle\mathbf{g}|\mathbf{S}|0\rangle = \sum_j \langle\mathbf{g}|^j t\rangle\langle^j t|0\rangle \exp\{i\mu_j z\}.$$

This latter result was obtained by Fujimoto (1959) by different methods.

An alternative form for $\mathbf{P}_j$ may be derived from the integral representation

$$\mathbf{S} = \exp(i\mathbf{M}_0 z) = (1/2\pi i)\oint[\exp(i\mu z)/(\mu\mathbf{E} - \mathbf{M}_0)]\,d\mu = \sum_{j=1}^{N} \mathbf{P}_j \exp(i\mu_j z)$$

with

$$\mathbf{P}_j = \prod_{\substack{l=1 \\ (l \neq j)}}^{N} (\mathbf{M}_0 - \mu_l\mathbf{E})/(\mu_j - \mu_l).$$

### 5.1. *Derivation by means of projection operators*

It is convenient to work with the traceless matrix $\mathbf{M}_s$ so that $\sum_{j=1}^{3}\mu_j = 0$ and

$$\langle \mathbf{g}|\mathbf{S}|0\rangle = \exp\{2\pi i[(\zeta_{\mathbf{g}} + \zeta_{\mathbf{h}})/3]z\}\sum_{j=1}^{3}\langle \mathbf{g}|\mathbf{P}_j|0\rangle \exp\{i\mu_j z\}.$$

A necessary condition that the wave function should be of two-beam form is that one of the $\langle \mathbf{g}|\mathbf{P}_j|0\rangle$ should be zero. In this way,

$$\langle \mathbf{g}|\mathbf{P}_3|0\rangle = \langle \mathbf{g}|\mathbf{M}_s^2|0\rangle - (\mu_1 + \mu_2)\sigma V(\mathbf{g}) = 0$$

and

$$\mu_3 = (2\pi/3)(2\zeta_{\mathbf{h}} - \zeta_{\mathbf{g}}) - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}).$$

In addition, since $\mathbf{P}_1 + \mathbf{P}_2 + \mathbf{P}_3 = \mathbf{E}$, $\langle \mathbf{g}|\mathbf{P}_1|0\rangle = -\langle \mathbf{g}|\mathbf{P}_2|0\rangle$ and, after some manipulation,

$$\langle \mathbf{g}|\mathbf{S}|0\rangle = \exp\{i\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\} \times i\sigma V(\mathbf{g})(\sin\beta z)/\beta,$$

where

$$\beta = \tfrac{1}{2}(\mu_1 - \mu_2).$$

There is yet no guarantee that any of these relations have physical validity. However, the root $\mu_3$ must satisfy the characteristic equation, so that

$$\begin{vmatrix} (-2\pi/3)(\zeta_{\mathbf{g}} + \zeta_{\mathbf{h}}) - \mu_3 & \sigma V(\mathbf{g}) & \sigma V(\mathbf{h}) \\ \sigma V(\mathbf{g}) & (2\pi/3)(2\zeta_{\mathbf{g}} - \zeta_{\mathbf{h}}) - \mu_3 & \sigma V(\mathbf{h}-\mathbf{g}) \\ \sigma V(\mathbf{h}) & \sigma V(\mathbf{h}-\mathbf{g}) & (2\pi/3)(2\zeta_{\mathbf{h}} - \zeta_{\mathbf{g}}) - \mu_3 \end{vmatrix} = 0.$$

This factorizes into

$$\begin{aligned}[2\pi\zeta_{\mathbf{g}} - 2\pi\zeta_{\mathbf{h}} &+ \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) \\ &- \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})] \\ \times [2\pi\zeta_{\mathbf{h}} &- \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) \\ &+ \sigma V(\mathbf{h})V(\mathbf{g})/V(\mathbf{h}-\mathbf{g})] = 0.\end{aligned}$$

Thus, $\zeta_{\mathbf{g}}$ and $\zeta_{\mathbf{h}}$ are constrained to lie on a degenerate hyperbola, that is, two intersecting straight lines, and these real loci ensure physical validity.

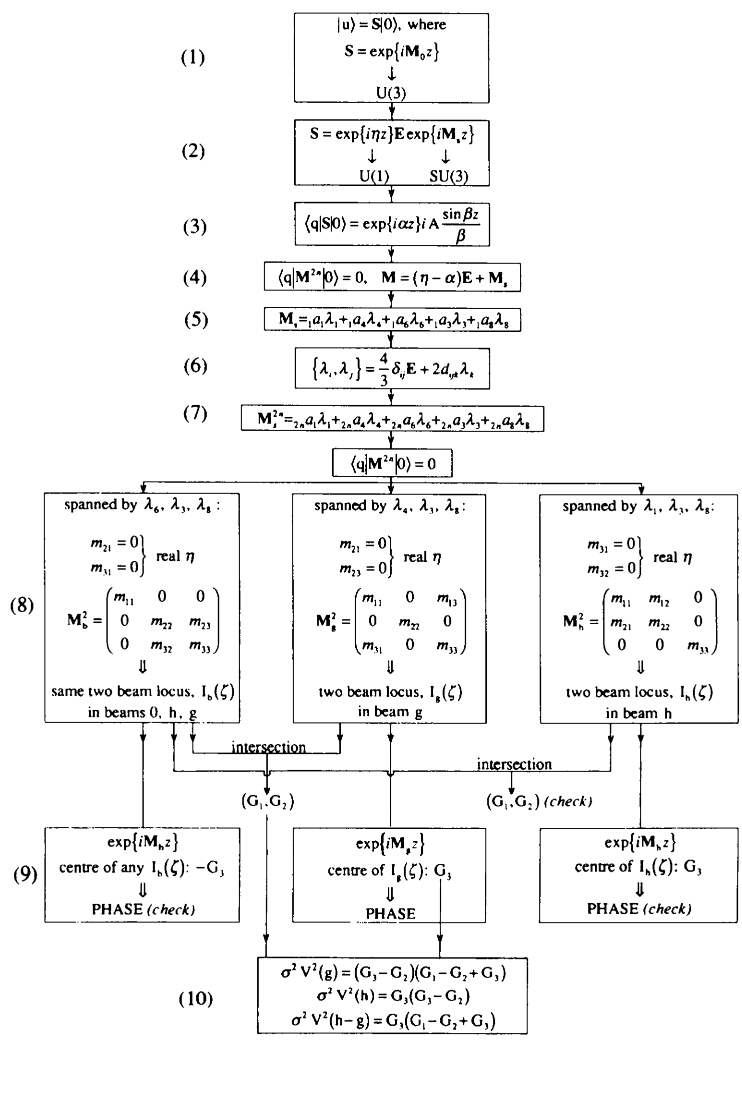


Fig. 1. Flow diagram for inversion by Lie algebra method. (1) Defining equations and symmetry, U(3). (2) Factorization into $U(1)$ and SU(3). (3) General form of two-beam equation. (4) Condition that $\langle \mathbf{q}|\mathbf{S}|0\rangle$ is antisymmetric in $z$. (5) Expansion into Gell-Mann representation. (6) The anticommutator symmetry of SU(3). (7) Expansion of even powers of $\mathbf{M}$ into Gell-Mann representation. (8) The three sub-algebras of su(3) defining the loci in each of the three beams. (9) Phase can be read off from each beam. (10) Structure amplitudes in terms of two points on the loci.

By comparing the coefficients of the characteristic equation with the corresponding elementary symmetric functions of the roots, $(\mu_1 - \mu_2)$ can be calculated and hence all of the previous results can be recovered.

Although lengthier calculations are involved in implementing this method than in implementing the previous one, explicit calculation of the eigenvalues and the eigenvectors can be avoided.

The steps to inversion *via* this projector-operator method are summarized in the flow diagram of Fig. 2.

5.2. *Bloch-wave approach*

Bloch introduced the functions that bear his name as the basis functions for a Lie group, specifically the translation group. Since the operators of this group commute with the Hamiltonian for a crystal in the one-body approximation, the form of the eigenfunctions is obtained immediately as $\exp\{i\mathbf{k}\cdot\mathbf{r}\}u(\mathbf{r})$, $u(\mathbf{r})$ having the periodicity of the crystal. In Bloch's vivid imagery, the orthonormal set takes the form of carrier waves modulated by the periodicities of the lattice and the momentum-space representation leads, by analogy with optics, to the equally graphic model of dispersion surfaces.

Independently of Bloch, Bethe constructed those functions in the course of his description of dynamical electron scattering. Having expanded the potential in the crystal in a Fourier series, he wrote the wave function as

$$\Psi(\mathbf{r}) = \sum_j {}^j\alpha \sum_{\mathbf{g}} {}^jC_{\mathbf{g}} \exp\{2\pi i({}^j\mathbf{k} + \mathbf{g})\cdot\mathbf{r}\}$$

using the notation conventional in this formulation (Hirsch, Howie, Nicholson, Pashley & Whelan, 1977).

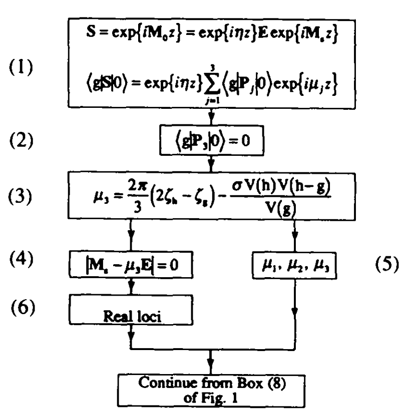


Fig. 2. Flow diagram for inversion by projection operator method. (1) Defining equations in terms of Dirac projector operators in a traceless matrix. (2) Condition for two-beam forms. (3) Third eigenvalue determined directly from condition (2). (4) Given $\mu_3$ is an eigenvalue, (4) must hold. (5) Calculation of other two eigenvalues from $\mu_3$. (6) Factorization of (4) to give real loci.

Here, ${}^j\alpha$ is the excitation amplitude of Bloch wave $j$ and ${}^jC_{\mathbf{g}}$ are the eigenvectors.

With the application of standard boundary conditions, ${}^j\alpha = {}^jC_0^*$ for a noncentrosymmetric crystal and ${}^j\alpha = {}^jC_0$ for a centrosymmetric crystal. Hence, the amplitude for beam $\mathbf{g}$ is

$$u(\mathbf{g}) = \sum_j {}^jC_0\, {}^jC_{\mathbf{g}} \exp\{2\pi i({}^j\mathbf{k} + \mathbf{g})_t z\}.$$

This is clearly the same relation as

$$\langle \mathbf{g}|\mathbf{S}|0\rangle = \sum_j \langle \mathbf{g}|{}^jt\rangle\langle {}^jt|0\rangle \exp\{i\mu_j z\}$$

and, indeed, it is a straightforward matter to cast the Bloch-wave treatment into eigenvalue form. In order to retain the more distinctive elements of the nomenclature of that formulation, the eigenvalue equation will now be written $\mathbf{M}_0|{}^jC\rangle = {}^j\gamma|{}^jC\rangle$.

In the three-beam case, it is apparent that if one of the three Bloch waves is not excited, that is, if ${}^1C_0$ or ${}^2C_0$ or ${}^3C_0$ is zero, it may be possible to find a set of orientations for which the beams 0, $\mathbf{g}$ and $\mathbf{h}$ all have two-beam form.

In order to explore this possibility, the eigenvalue equation is expanded and $C_{\mathbf{h}}$ eliminated to give

$$[\sigma^2 V(\mathbf{g})V(\mathbf{h}) + \gamma\sigma V(\mathbf{h}-\mathbf{g})]C_0 = [\sigma^2 V(\mathbf{g})V(\mathbf{h}-\mathbf{g}) - \sigma V(\mathbf{h})(2\pi\zeta_{\mathbf{g}} - \gamma)]C_{\mathbf{g}},$$

$$[\sigma^2 V^2(\mathbf{h}) + \gamma(2\pi\zeta_{\mathbf{h}} - \gamma)]C_0 = [\sigma V(\mathbf{g})(2\pi\zeta_{\mathbf{h}} - \gamma) - \sigma^2 V(\mathbf{h})V(\mathbf{h}-\mathbf{g})]C_{\mathbf{g}}.$$

With ${}^3C_0 = 0$,

$$ {}^3\gamma = 2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) = 2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}).$$

Thus, the unexcited Bloch wave has the eigenvalue $2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})$ and the real locus shows that the condition ${}^3C_0 = 0$ is physically admissible.

If the conditions ${}^jC_{\mathbf{g}} = 0$, ${}^jC_0 \neq 0$ for $j = 1$, 2 or 3 can be shown to be admissible, then there will be a two-beam intensity distribution along a locus in beam $\mathbf{g}$ only.

With ${}^3C_{\mathbf{g}} = 0$,

$$ {}^3\gamma = -\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}) = \{2\pi\zeta_{\mathbf{h}} \pm [(2\pi\zeta_{\mathbf{h}})^2 + 4\sigma^2 V^2(\mathbf{h})]^{1/2}\}/2,$$

so that

$$2\pi\zeta_{\mathbf{h}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g})$$

is another real locus.

Since $\mathbf{g}$ and $\mathbf{h}$ are merely labels, it is only necessary to interchange them in order to obtain the results for the two-beam locus that exists in beam $\mathbf{h}$ alone.

All of the two-beam wave functions can now be calculated by straightforward elementary but lengthy algebra to recover the previous results. This lengthy manipulation is a recurrent difficulty encountered in the implementation of Bloch-wave methods, and one that can often be mitigated by a change in representation. It is not, for instance, necessary to calculate eigenvectors explicitly since only the products ${}^jC_{\mathbf{g}}{}^jC_0$ appear in the final wave function and ${}^jC_{\mathbf{g}}{}^jC_0 = \langle \mathbf{g}|{}^jC\rangle\langle {}^jC|0\rangle$, a matrix element of the projection operator $\mathbf{P}_j = |{}^jC\rangle\langle{}^jC|$. Here, the operator is written in the basis of the eigenvectors but other bases can be chosen or, indeed, other representations, for instance the integral representation,

$$(1/2\pi i)\oint[\exp(i\gamma z)/(\gamma\mathbf{E}-\mathbf{M}_0)]\,\mathrm{d}\gamma,$$

so that

$$u_{\mathbf{g}} = \sum_j \left\langle \mathbf{g}\left| \prod_{\substack{l=1\\ l\neq j}}^{N} (\mathbf{M}_0 - {}^l\gamma\mathbf{E})/({}^j\gamma - {}^l\gamma)\right|0\right\rangle \exp\{i{}^j\gamma z\}.$$

Now the frequently lengthy process of calculating eigenvectors in easily assimilable forms, as distinct from formal expressions, is replaced by matrix multiplication. Further, the eigenvalues are assembled as differences and symmetric functions so that, as in the present instance, explicit values may not be required.

In the Bloch-wave treatment, however, each eigenvalue ${}^j\gamma$ is pictorially the distance of the wave point on the branch $j$ of the dispersion surface from the centre of the Ewald sphere. In order to learn more about the geometry of inversion, explicit values were therefore calculated.

These are, with ${}^3\gamma$ the eigenvalue of the Bloch wave [unexcited for the locus given by (*a*) below]:

(*a*) For the line

$$\begin{aligned}
&2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})\\
&\quad = 2\pi\zeta_{\mathbf{h}} + \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}),\\
&{}^{1,2}\gamma = \tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\\
&\qquad \pm \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2\right.\\
&\qquad \left. + \sigma^2V^2(\mathbf{g}) + \sigma^2V^2(\mathbf{h})\right)^{1/2}\\
&{}^3\gamma = 2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}).
\end{aligned}$$

(*b*) For the line

$$\begin{aligned}
&2\pi\zeta_{\mathbf{h}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}),\\
&{}^{1,2}\gamma = \tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\\
&\qquad \pm \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{g}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})]\}^2\right.\\
&\qquad \left. + \sigma^2V^2(\mathbf{g}) + \sigma^2V^2(\mathbf{h}-\mathbf{g})\right)^{1/2}\\
&{}^3\gamma = -\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}).
\end{aligned}$$

(*c*) For the line

$$\begin{aligned}
&2\pi\zeta_{\mathbf{g}} = \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}),\\
&{}^{1,2}\gamma = \tfrac{1}{2}[2\pi\zeta_{\mathbf{h}} + \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})]\\
&\qquad \pm \left(\{\tfrac{1}{2}[2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h})]\}^2\right.\\
&\qquad \left. + \sigma^2V^2(\mathbf{h}) + \sigma^2V^2(\mathbf{h}-\mathbf{g})\right)^{1/2}\\
&{}^3\gamma = -\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}).
\end{aligned}$$

These relations describe the fundamental structure of the general centrosymmetric three-beam dispersion surfaces. The branch ${}^3\gamma$ has two lines, each of height $-\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g})$ relative to the centre of the Ewald sphere, running parallel to, but at different distances from, the $\zeta_{\mathbf{g}}$ and $\zeta_{\mathbf{h}}$ axes. A third line ruled on the surface runs parallel to the bisector of the angle between the other two and has a height given by $2\pi\zeta_{\mathbf{h}} - \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g})$. These lines characterize the system. The sections of branches ${}^2\gamma$ and ${}^1\gamma$ that contain the lines are hyperbolic. For all these branches, the eigenvalues are distinct except at the Gjønnes–Høier point,

$$\begin{aligned}
&\big(2\pi\zeta_{\mathbf{g}} = \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}),\\
&\ 2\pi\zeta_{\mathbf{h}} = \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}) - \sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g})\big),
\end{aligned}$$

where

$${}^2\gamma = {}^3\gamma = -\sigma V(\mathbf{g})V(\mathbf{h})/V(\mathbf{h}-\mathbf{g}).$$

At this point,

$${}^1\gamma = \sigma V(\mathbf{g})V(\mathbf{h}-\mathbf{g})/V(\mathbf{h}) + \sigma V(\mathbf{h})V(\mathbf{h}-\mathbf{g})/V(\mathbf{g}),$$

so that the centre of the hyperbola is displaced and this displacement, which again can be measured experimentally, completes the inversion in the Bloch-wave picture.

Clearly, the inversion could have started with the analysis of the algebraic geometry of the dispersion surfaces. The algebraic geometry of cubic surfaces has been extensively studied. The 27 lines ruled on cubic surfaces were discovered by Cayley & Salmon in 1849 (see, for instance, Henderson, 1911).

The steps to inversion using the Bloch-wave method are summarized in the flow diagram of Fig. 3.

## 6. Discussion

It emerges that the symmetries inherent in three-beam scattering from a centrosymmetric crystal are completely described by the group SU(3). One consequence of this is that three su(2) sub-algebras can be used to invert the system. In other words, three lines intersecting at a single point and ruled on one of the dispersion surfaces encapsulate all of the physical content of the system. Heavy redundancy in the solution suggests that an extension into the non-centrosymmetric case should be possible.

The symmetries of Lie groups depend continuously upon at least one parameter, so that the crystal orientations that exhibit these most clearly are very different from those sought in order to expose the symmetries of the crystallographic groups. In other words, the three-beam patterns required for inversion exhibit the symmetries of SU(3) rather than those of the space group.

There are two special cases of this analysis: the critical voltage and the intersecting Kikuchi line. In the former, the three beams lie on the same line so that the full symmetry of the system cannot be displayed and inversion is no longer possible. In this degenerate system, the loci coincide and the expressions reduce to the standard form for the critical voltage. The relationship between the critical-voltage method, the intersecting Kikuchi-line technique and hence the Gjønnes–Høier point has been discussed by Taftø & Gjønnes (1985).

The practicability of the inversion is currently under investigation. Preliminary experiments will be reported in separate publications; however, results obtained so far indicate that the quantity most readily determined is the phase. Once any of the two-beam loci has been identified, the displacement is easily detected.

Two main difficulties have been encountered in determining the structure amplitudes with accuracy. The first relates to the sufficiently accurate determination of the Bragg angle, that is, the origin of coordinates. The second arises because of the prevalence of $N$-beam scattering, which contributes a pseudopotential component even to apparently three-beam systems. Since the inversion is independent of thickness, some correction is possible but it is not yet clear how far this process can be extended. In any event, it would appear that, at least in favourable circumstances, structural centrosymmetric phase can be measured directly in convergent-beam diffraction.

This theory is, of course, scalar, but the equations defining X-ray dynamical scattering, when resolved into circularly polarized components, can be cast into a form isomorphic with those of electron diffraction (Moodie & Wagenfeld, 1975). Apart from numerical factors, the above analysis then applies to the right circular component of the wave function for X-rays. Since the wave functions of right- and left-handed components are complex conjugates, results for arbitrary polarization are readily obtainable. There is, however, a good deal of detail to be considered and this will be the subject of a separate publication.

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## APPENDIX *A*
## The Gell-Mann generators for SU(3)

Since SU(2) is a subgroup of SU(3), the first three generators can be obtained by direct extension of the Pauli matrices, the generators of SU(2),

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The remaining five are

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix},$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

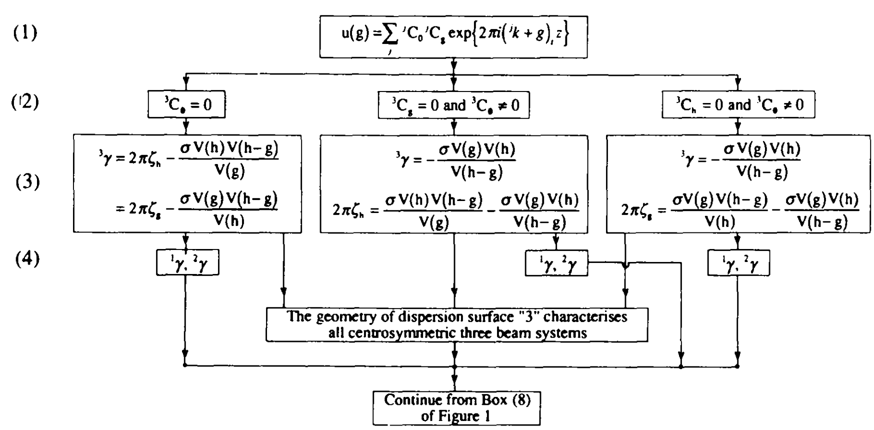


Fig. 3. Flow diagram for inversion by Bloch waves. (1) Defining equations. (2) Conditions for two-beam forms. (3) Loci and corresponding eigenvalues of branch three. (4) Remaining eigenvalues on branches one and two.

Table 1. *The symmetric structure constants of the anticommuting algebra of SU(3)*

| $ijk$ | $d_{ijk}$ | $ijk$ | $d_{ijk}$ |
|---|---|---|---|
| 118 | $1/3^{1/2}$ | 355 | $1/2$ |
| 146 | $1/2$ | 366 | $-1/2$ |
| 157 | $1/2$ | 377 | $-1/2$ |
| 228 | $1/3^{1/2}$ | 448 | $-1/(2\times 3^{1/2})$ |
| 247 | $-1/2$ | 558 | $-1/(2\times 3^{1/2})$ |
| 256 | $1/2$ | 668 | $-1/(2\times 3^{1/2})$ |
| 338 | $1/3^{1/2}$ | 778 | $-1/(2\times 3^{1/2})$ |
| 344 | $1/2$ | 888 | $-1/3^{1/2}$ |

$$\lambda_8 = \frac{1}{3^{1/2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

Structure constants for the anticommutator Lie algebra can be calculated from the relation $d_{ijk} = \mathrm{tr}(\{\lambda_i, \lambda_j\}\lambda_k)$. They are necessarily symmetric and are listed in Table 1. These and related matters are discussed, for instance, by Greiner & Müller (1992).

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