invariant quantities which are independent of the choice of origin. $(\varphi+\mathbf{H}.\mathbf{r}_\kappa)$ satisfies this condition, but it takes a very different form from the invariants found in elastic diffraction, the simplest of which involves a sum of three phases (*e.g.* Bird, James & Preston, 1987). $(\varphi+\mathbf{H}.\mathbf{r}_\kappa)$ arises naturally in inelastic scattering theory because many such processes are localized about the atomic sites $\mathbf{r}_\kappa$. It follows that in addition to thermal diffuse scattering, X-ray production and energy loss spectroscopy, phase-dependent two-beam effects should also be present in, for example, backscattered and channelling patterns (Marthinsen & Høier, 1986; Marthinsen, Anisdahl & Høier, 1987). Throughout the paper we have referred to our analysis being a two-beam theory, and in this context $(\varphi+\mathbf{H}.\mathbf{r}_\kappa)$ might be called a two-beam phase invariant. This, however, may be a little misleading.* Without an incident beam there could be no 'two-beam' Kikuchi pattern formation, so in this sense ours is a three-beam theory (one incident and two scattered beams), even though the incident beam is treated on a very different footing from the scattered beams and plays no significant role in the final results. Looked at this way, our results do not break the standard rule from elastic diffraction theory, that at least three beams are required to produce phase-dependent quantities.

## 4. Concluding remarks

The basic results of this paper are (2) and (4) which give the intensity distribution in a Kikuchi pattern. Both expressions show how structural information is carried in the pattern, provided a dependent-Bloch-wave theory is used. Equation (2) is valid in a general diffraction situation [with possible corrections from (5) and for absorption], such as the central region of a strong band. The weakest lines in the pattern may be analysed using the two-beam result (4). In a second paper (Bird & Wright, 1989) computational results based on (2) and (4) are presented for crystals with the non-centrosymmetric GaAs structure and comparison is made between theory and experimental patterns.

* We are grateful to a referee for pointing this out.

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# The Possible Translational Parts of (3 + *d*) Superspace Symmetry Operations

BY V. PETŘÍČEK

*Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance* 2, 180 40 *Praha* 8, *Czechoslovakia*

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## Abstract

A necessary condition for possible translational parts of $(3+d)$ superspace symmetry operations is derived. The general conditions are discussed especially for $(3+1)$ superspace symmetry operations and some examples illustrate the application.


## 1. Introduction

An electron density function of incommensurate crystals with an internal dimensionality $d$ can be described as a periodic function $\tilde{\rho}$ in $(3+d)$-dimensional space (de Wolff, 1974). The translational periodicity in $(3+d)$ superspace is characterized by

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a lattice $\Lambda$ spanned by $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_{3+d}$,

$$\begin{aligned} \mathbf{b}_i &= \mathbf{a}_i - \sum_{j=1}^{d} (\mathbf{q}_j \cdot \mathbf{a}_i)\mathbf{e}_j \quad (i=1,2,3) \\ \mathbf{b}_{i+3} &= \mathbf{e}_i \quad (i=1,2,\ldots,d) \end{aligned} \tag{1}$$

where $\mathbf{e}_i$ are additional vectors perpendicular to an external space $V_E$ and $\mathbf{q}_j$ are incommensurate modulation vectors:

$$\mathbf{q}_j = \sum_{i=1}^{3} \sigma_{ji}\mathbf{a}_i^* \tag{2}$$

where the vectors $\mathbf{a}_i^*, \mathbf{q}_j$ ($i=1,2,3$ and $j=1,\ldots,d$) are rational independent. This means that any linear combination with rational coefficients of these vectors only vanishes if all the coefficients are zero. In particular this implies (Janner, Janssen & de Wolff, 1983, hereafter referred to as I) that 'in every linear combination with integral coefficients of the rows of $\boldsymbol{\sigma}$ there is an irrational entry'.

A $(3+d)$-dimensional symmetry operation $\hat{S}$,

$$\hat{S}(\mathbf{r}_E, \mathbf{r}_I) = (\mathbf{r}'_E, \mathbf{r}'_I) \quad \text{and} \quad \tilde{\rho}(\mathbf{r}'_E, \mathbf{r}'_I) = \tilde{\rho}(\mathbf{r}_E, \mathbf{r}_I)$$

is described in matrix form with respect to the base $\mathbf{b}_1, \ldots, \mathbf{b}_{3+d}$ by

$$\begin{pmatrix} \boldsymbol{\Gamma}_E & \mathbf{0} \\ \boldsymbol{\Gamma}_M & \boldsymbol{\Gamma}_I \end{pmatrix}\begin{pmatrix} \mathbf{r}_E \\ \mathbf{r}_I \end{pmatrix} + \begin{pmatrix} \mathbf{s}_E \\ \mathbf{s}_I \end{pmatrix} = \begin{pmatrix} \mathbf{r}'_E \\ \mathbf{r}'_I \end{pmatrix} \tag{3}$$

where $\boldsymbol{\Gamma}_E$, $\boldsymbol{\Gamma}_M$ and $\boldsymbol{\Gamma}_I$ are $3\times3$, $d\times3$ and $d\times d$ matrices describing the rotational part of $\hat{S}$ and $\mathbf{s}_E$ and $\mathbf{s}_I$ are $3\times1$ and $(d\times1)$ columns describing the translational part of $\hat{S}$.

The property that a subset of the reflections (in this case the so-called main reflections) belongs to a reciprocal lattice (spanned by the $\mathbf{a}_i^*$) left invariant by the symmetry operations leads to

$$\boldsymbol{\Gamma}_M = \boldsymbol{\sigma}\boldsymbol{\Gamma}_E - \boldsymbol{\Gamma}_I\boldsymbol{\sigma}. \tag{4}$$

In accordance with I, we split $\boldsymbol{\sigma}$ in two parts $\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_r$, where

$$\boldsymbol{\sigma}_i\boldsymbol{\Gamma}_E - \boldsymbol{\Gamma}_I\boldsymbol{\sigma}_i = \mathbf{0} \tag{5a}$$

holds for all $\hat{S}$ from the superspace group and where the matrix $\boldsymbol{\sigma}_r$ is composed only of rational elements. Equation (4) can be rewritten

$$\boldsymbol{\Gamma}_M = \boldsymbol{\sigma}_r\boldsymbol{\Gamma}_E - \boldsymbol{\Gamma}_I\boldsymbol{\sigma}_r. \tag{5b}$$

The intrinsic rational increment $\boldsymbol{\tau}$ as defined by de Wolff, Janssen & Janner (1981) (hereafter referred to as II) for elements of a $(3+1)$-dimensional superspace group can be generalized by the equation

$$\boldsymbol{\tau} = \mathbf{s}_I - \boldsymbol{\sigma}_r\mathbf{s}_E \tag{6}$$

for elements of a $(3+d)$-dimensional superspace group and is again the most convenient parameter for characterizing the translational part of these elements. This can be illustrated by considering the translational part of the product $\hat{S}$ of two superspace group elements $\hat{S}^{(1)}$ and $\hat{S}^{(2)}$:

$$\mathbf{s}_E = \boldsymbol{\Gamma}_E^{(2)}\mathbf{s}_E^{(1)} + \mathbf{s}_E^{(2)} \tag{7a}$$

$$\mathbf{s}_I = \boldsymbol{\Gamma}_M^{(2)}\mathbf{s}_E^{(1)} + \boldsymbol{\Gamma}_I^{(2)}\mathbf{s}_I^{(1)} + \mathbf{s}_I^{(2)}. \tag{7b}$$

The expression (7$b$) can be rewritten by using (5$b$) and (6) into a more convenient form for the increments $\boldsymbol{\tau}$:

$$\boldsymbol{\tau} = \boldsymbol{\Gamma}_I^{(2)}\boldsymbol{\tau}^{(1)} + \boldsymbol{\tau}^{(2)}. \tag{8}$$

Equation (8) is analogous to (7$a$) and the calculation of the translational part is separated into external and internal subspace.

All possible translational parts of $(3+d)$ superspace symmetry operators can be derived from the simple requirements that $\hat{S}^n$, where $n$ is the order of the rotational part of $\hat{S}^n$, so that $\boldsymbol{\Gamma}^n = \mathbf{E}$ ($\mathbf{E}$ being the unit matrix), has to be some translational operator in $(3+d)$ superspace.

The next section contains a derivation of the necessary condition for the translational part of $(3+d)$ superspace symmetry operators and the last section contains the application of this method for $(3+1)$ superspace symmetry operators.

## 2. A necessary condition for a translational part of a (3+ d) superspace symmetry operator

Let the orders of $\boldsymbol{\Gamma}_E$ and $\boldsymbol{\Gamma}_I$ be $n$ and $m$, respectively. Equation (5$a$) for $\boldsymbol{\Gamma}^n$ has the form

$$\boldsymbol{\sigma}_i - \boldsymbol{\Gamma}_I^n\boldsymbol{\sigma}_i = \mathbf{0}$$

which leads, owing to the incommensurability of $\mathbf{q}$ vectors, to the conclusion that $\boldsymbol{\Gamma}_I^n = \mathbf{E}$; this means that the order $m = n/p$ where $p$ is an integer and that the operator $\hat{S}^n$ can be expressed as

$$\hat{S}^n = (\mathbf{E}|\{\boldsymbol{\Gamma}\}_n\mathbf{s}) \tag{9}$$

where

$$\{\boldsymbol{\Gamma}\}_n = \mathbf{E} + \boldsymbol{\Gamma} + \ldots + \boldsymbol{\Gamma}^{n-1} = \left(\begin{array}{c|c} \{\boldsymbol{\Gamma}_E\}_n & \mathbf{0} \\ \hline \boldsymbol{\sigma}_n\{\boldsymbol{\Gamma}_E\}_n - \{\boldsymbol{\Gamma}_I\}_n\boldsymbol{\sigma}_n & \{\boldsymbol{\Gamma}_I\}_n \end{array}\right). \tag{10}$$

The operator $(1/n)\{\boldsymbol{\Gamma}\}_n$, where $n$ is an order of $\boldsymbol{\Gamma}$, is a projection operator into an invariant subspace of $\boldsymbol{\Gamma}$. The requirement that the operator (9) should be some translational operator $(\mathbf{E}|(\mathbf{l}_E, \mathbf{l}_I))$, leads to

$$\{\boldsymbol{\Gamma}_E\}_n\mathbf{s}_E = n\mathbf{s}_E^0 = \mathbf{l}_E \tag{11a}$$

$$\begin{aligned} \boldsymbol{\sigma}_r\{\boldsymbol{\Gamma}_E\}_n\mathbf{s}_E - \{\boldsymbol{\Gamma}_I\}_n\boldsymbol{\sigma}_r\mathbf{s}_E + \{\boldsymbol{\Gamma}_I\}_n\mathbf{s}_I \\ = n\boldsymbol{\sigma}_r\mathbf{s}_E^0 - \{\boldsymbol{\Gamma}_I\}_n\boldsymbol{\sigma}_r\mathbf{s}_E + \{\boldsymbol{\Gamma}_I\}_n\mathbf{s}_I = \mathbf{l}_I, \end{aligned} \tag{11b}$$

where $\mathbf{s}_E^0$ is an intrinsic translational part of the three-dimensional symmetry operator. The first equation (11$a$) restricts these parts, as for three-dimensional symmetry operations in the usual space group. The second equation ($11b$) shows us the necessary connection between $\mathbf{s}_E^0$, $\boldsymbol{\sigma}_r$ and $\mathbf{s}_I$, which leads to some additional restrictions for $\mathbf{s}_E^0$ and $\mathbf{s}_I$. This condition can be simplified by using $\boldsymbol{\tau}$:

$$n\boldsymbol{\sigma}_r\mathbf{s}_E^0 + n\boldsymbol{\tau}^0 = \mathbf{l}_I \qquad (12)$$

where $\boldsymbol{\tau}^0 = (1/m)\{\boldsymbol{\Gamma}_I\}_m\boldsymbol{\tau}$ is the projection of $\boldsymbol{\tau}$ into the invariant subspace of the operator $\boldsymbol{\Gamma}_I$ in $d$-dimensional internal subspace.

Note that $\boldsymbol{\sigma}_r = \mathbf{0}$ leads to a complete splitting of conditions ($11a$) and (12) for $\mathbf{s}_E$ and $\mathbf{s}_I = \boldsymbol{\tau}$ into two independent ones.

## 3. Application to (3 + 1)-dimensional superspace groups

The main simplification of expressions follows from the fact that $\boldsymbol{\Gamma}_I$ is $\pm1$ and that the matrices $\boldsymbol{\sigma}$, $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_r$ are replaced by row vectors $\mathbf{q}$, $\mathbf{q}_i$ and $\mathbf{q}_r$, respectively. Equation ($5a$) is now

$$\mathbf{q}_i = \mathbf{q}_i\boldsymbol{\Gamma}_E \quad \text{for } \boldsymbol{\Gamma}_I = 1 \qquad (13a)$$

$$(1/n)\mathbf{q}_i\{\boldsymbol{\Gamma}_E\}_n = \mathbf{0} \quad \text{for } \boldsymbol{\Gamma}_I = -1, \qquad (13b)$$

which means that $\mathbf{q}_i$ is from an invariant subspace of $\boldsymbol{\Gamma}_E$ for $\boldsymbol{\Gamma}_I = 1$ and $\mathbf{q}_i$ is perpendicular to this subspace for $\boldsymbol{\Gamma}_I = -1$. A similar simplification of (12) leads to the formulae

$$n(\mathbf{q}_r \, . \, \mathbf{s}_E^0) + n\tau = l_I \quad \text{for } \boldsymbol{\Gamma}_I = 1 \qquad (14a)$$

$$n(\mathbf{q}_r \, . \, \mathbf{s}_E^0) = l_I \quad \text{for } \boldsymbol{\Gamma}_I = -1. \qquad (14b)$$

Table 2 of II was derived under the assumption that various kinds of centring in planes or spaces containing the additional vector $\mathbf{e}$ are expressed through $\mathbf{q}_r$ without any change of the base (1), which means that $l_I$ from ($14a$) and ($14b$) has to be an integer.

Two examples were chosen to illustrate the application of these rules.

*Example* 1

Twofold screw axes along $x$, $y$ and $z$ in orthorhombic superspace groups $[\mathbf{q}_i = (0, 0, \gamma), \mathbf{q}_r = (\alpha, \beta, 0)]$. From ($13a$) and ($13b$) it follows that $\boldsymbol{\Gamma}_I = -1$, $-1$ and 1 for $(2_1)_x$, $(2_1)_y$ and $(2_1)_z$, respectively. Thus we have from ($14a$) and ($14b$) $\alpha = l_I^x$, $\beta = l_I^y$ and $2\tau = l_I^z$ for $(2_1)_x$, $(2_1)_y$ and $(2_1)_z$, respectively, which means that $(2_1)_x$ must not be combined with $\mathbf{q}_r$ described by $A$ $[\mathbf{q}_r = (\frac{1}{2}, 0, 0)]$ or $W$ $[\mathbf{q}_r = (\frac{1}{2}, \frac{1}{2}, 0)]$, $(2_1)_y$ with $B$ $[\mathbf{q}_r = (0, \frac{1}{2}, 0)]$ or $W$ and $\tau = 0$ or $\frac{1}{2}$ for $(2_1)_z$.

Table 1. *Values of $\tau$ for the operators of Example* 2

| Operator | $P$ | $A$ | $B$ | $W$ |
|---|---|---|---|---|
| $a_y$ | 1, $s$ | $q$ | 1, $s$ | $q$ |
| $a_z$ | $\bar{1}$ | — | $\bar{1}$ | — |
| $b_x$ | 1, $s$ | 1, $s$ | $q$ | $q$ |
| $b_z$ | $\bar{1}$ | $\bar{1}$ | — | — |
| $c_x$ | 1, $s$ | 1, $s$ | 1, $s$ | 1, $s$ |
| $c_y$ | 1, $s$ | 1, $s$ | 1, $s$ | 1, $s$ |
| $n_x$ | 1, $s$ | 1, $s$ | $q$ | $q$ |
| $n_y$ | 1, $s$ | $q$ | 1, $s$ | $q$ |
| $n_z$ | $\bar{1}$ | — | — | $\bar{1}$ |

*Example* 2

Glide planes $a$, $b$, $c$ and $n$ with the normal along $x$, $y$ and $z$ in orthorhombic superspace groups $[\mathbf{q}_i = (0, 0, \gamma), \mathbf{q}_r = (\alpha, \beta, 0)]$.

Possible $\tau$ values of these operators are given as a function of $\mathbf{q}_r$ in Table 1. A − sign means that the operator must not be combined with certain $\mathbf{q}_r$.

The results of the previous examples enable us to understand why some of the orthorhombic superspace groups do not exist.

The two-line symbol of (3 + 1) superspace groups as defined in II is very convenient for application of the equations ($14a$) and ($14b$) because $\mathbf{q}_r$, $\mathbf{s}_E^0$ and $\tau$ can be derived from them, at least for operators used in the Herman–Mauguin symbol. The method described in this paper enables us to make a simple checking of the correctness of symbols of a superspace group. These necessary equations can also be used during a process of generating the complete list of superspace groups. But on the other hand these conditions cannot substitute the determination process as was described in II because they are necessary but not sufficient conditions.

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