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# On the factor systems of the Shubnikov space groups

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**Abstract.** The procedure of Backhouse for the determination of a complete set of inequivalent factor systems of the symmorphic Shubnikov space groups of type I is generalized for all Shubnikov space groups of types I and III. The results are used to obtain a method for the construction of a set of inequivalent factor systems of the Shubnikov space groups of types II and IV.

## 1. Introduction

In the quantum mechanical description of a physical system an essential role is played by the projective unitary (PU) and projective unitary–antiunitary (PUA) representations of the symmetry group of the system, as is well known from the results of Wigner (1939) and Bargmann (1954). PU and PUA representations of Shubnikov space groups have been used in the theory of an electron in a crystalline potential when a uniform static magnetic field is present (see e.g. Brown 1964, Opechowski and Tam 1969, Tam 1969). A natural consequence of dealing with PU and PUA representations is the study of their factor systems. In this paper we will study the factor systems of the Shubnikov space groups. Backhouse (1970) has given a method to derive a complete set of inequivalent factor systems of the symmorphic space groups, and Bradley (1973) used this method to tabulate these factor systems. Here we will extend the method of Backhouse both to the non-symmorphic space groups and to the Shubnikov space groups of type III. The results will then be used to discuss the factor systems of the Shubnikov space groups of types II and IV. We will only treat the three-dimensional Shubnikov space groups here; the extension to the case of $n$ dimensions however is straightforward.

## 2. Preliminaries

A detailed description of the Shubnikov space groups has been given by Bradley and Cracknell (1972). They are subdivided into four types as follows.

- Type I: the ordinary space groups.
- Type II: the grey space groups; they contain the time-reversal operator.
- Type III: the black and white space groups based on ordinary Bravais lattices.
- Type IV: the black and white space groups based on black and white Bravais lattices.

A factor system of a magnetic or non-magnetic group $G$ with non-magnetic subgroup $G_0$ is defined to be a mapping $\sigma\colon G\times G\to U(1)$ which satisfies

$$\sigma(g_1, g_2)\sigma(g_1g_2, g_3)=\sigma(g_1, g_2g_3)\sigma^{g_1}(g_2, g_3) \qquad \forall g_1, g_2, g_3\in G \tag{2.1}$$

and

$$\sigma(e, g)=\sigma(g, e)=1 \qquad \forall g\in G \tag{2.2}$$

where $e$ denotes the identity of $G$ and $\lambda^g$ is defined by

$$\lambda^g=\begin{cases}\lambda & \text{if } g\in G_0\\ \lambda^* & \text{if } g\notin G_0.\end{cases} \tag{2.3}$$

Two factor systems $\sigma$ and $\sigma'$ of $G$ are called equivalent if there exists a mapping $c\colon G\to U(1)$ such that

$$\sigma'(g_1, g_2)=\sigma(g_1, g_2)\frac{c(g_1)c^{g_1}(g_2)}{c(g_1g_2)} \qquad \forall g_1, g_2\in G. \tag{2.4}$$

Now let $G$ be a Shubnikov space group of type I or III, $H$ its subgroup of translations and $G_0$ its non-magnetic subgroup. If $G$ is of type I then $G=G_0$ and if $G$ is of type III then $G_0$ is a subgroup of $G$ of index two which contains $H$. The Shubnikov point groups $K$ and $K_0$ are defined by $G/H$ and $G_0/H$ respectively. The identities of $H$ and $K$ will be denoted by $\boldsymbol{e}$ and $E$ respectively.

Elements of $G$ will be denoted by $(\boldsymbol{t},R)$ where $\boldsymbol{t}\in H$ and $R\in K$. We define $(\boldsymbol{t}, R)$ by its action on space–time:

$$(\boldsymbol{t}, R)(\boldsymbol{x}; t)=(R\boldsymbol{x}+\boldsymbol{t}+\boldsymbol{t}_R; \epsilon_R t) \tag{2.5}$$

where $\epsilon_R$ is defined by

$$\epsilon_R=\begin{cases}1 & \text{if } R\in K_0\\ -1 & \text{if } R\notin K_0\end{cases} \tag{2.6}$$

and $\boldsymbol{t}_R$ is a fixed non-primitive translation associated with $R$. The multiplication of elements of $G$ is now given by

$$(\boldsymbol{t}, R)(\boldsymbol{t}', R')=(\boldsymbol{t}+R\boldsymbol{t}'+\boldsymbol{m}(R, R'), RR') \tag{2.7}$$

where the mapping $\boldsymbol{m}\colon K\times K\to H$ is given by

$$\boldsymbol{m}(R, R')=\boldsymbol{t}_R+R\boldsymbol{t}_{R'}-\boldsymbol{t}_{RR'}. \tag{2.8}$$

In the sequel we shall write $\lambda^R$ as a shorthand symbol for $\lambda^{(\boldsymbol{e},R)}$.

Let $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{t}_3$ be basic translations of $H$. Then each element $\boldsymbol{t}$ of $H$ can be written as $\boldsymbol{t}=n_1\boldsymbol{t}_1+n_2\boldsymbol{t}_2+n_3\boldsymbol{t}_3$. In the sequel we shall identify $\boldsymbol{t}$ with the column vector with entries $n_1$, $n_2$ and $n_3$. Moreover each element $R$ of $K$ shall be identified with the $3\times3$ matrix which represents $R$ with respect to the basic vectors $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{t}_3$. These $3\times3$ matrices may be read off from table 3.2 of the book by Bradley and Cracknell (1972). The reciprocal lattice $H_0^*$ is spanned by $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ and $\boldsymbol{b}_3$ where $\boldsymbol{t}_i\,.\,\boldsymbol{b}_j=2\pi\delta_{ij}$. A vector $\boldsymbol{k}=\alpha_1\boldsymbol{b}_1+\alpha_2\boldsymbol{b}_2+\alpha_3\boldsymbol{b}_3$ of the first Brillouin zone of the reciprocal lattice shall be identified with the column vector with entries $\alpha_1$, $\alpha_2$ and $\alpha_3$.

The inner and outer products of two column vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ with elements $a_i$ and $b_i (i=1, 2, 3)$ respectively are defined and denoted as usual: $\boldsymbol{a}\,.\,\boldsymbol{b}=\Sigma_{i=1}^3 a_ib_i$ and $\boldsymbol{a}\times\boldsymbol{b}=\boldsymbol{c}$ where $c_i=a_jb_k-a_kb_j$ with $j=i+1 \pmod 3$ and $k=i+2 \pmod 3$.

## 3. The factor systems of Shubnikov space groups of type I and III

The aim of this section is to give a method to derive a complete set of inequivalent factor systems of $G$. Such a method has been given by Backhouse (1970) for the symmorphic space groups. Backhouse used a decomposition of factor systems of non-magnetic semi-direct product groups due to Mackey (1958). In a previous paper (van den Broek 1976b) we generalized this decomposition to factor systems of arbitrary magnetic and non-magnetic groups. Using the results of this paper we can state the following. Every factor system of $G$ is equivalent with a factor system $\omega$ of $G$ which decomposes as follows:

$$\omega((\boldsymbol{t}, R), (\boldsymbol{t}', R)) = \gamma(\boldsymbol{t}, R\boldsymbol{t}')\gamma(\boldsymbol{t}+R\boldsymbol{t}', \boldsymbol{m}(R, R'))\nu(R, R')\delta^*(R, R\boldsymbol{t}'). \tag{3.1}$$

Here $\gamma$ is a factor system of $H$, $\nu$ is a mapping from $K\times K$ into $U(1)$ and $\delta$ is a mapping from $K\times H$ into $U(1)$ with the following properties:

$$\nu(E, R) = \nu(R, E) = 1 \qquad \forall R \in K \tag{3.2}$$

$$\delta(E, \boldsymbol{t}) = \delta(R, \boldsymbol{e}) = 1 \qquad \forall R \in K, \forall \boldsymbol{t} \in H \tag{3.3}$$

$$\delta(R, \boldsymbol{t}+\boldsymbol{t}') = \delta(R, \boldsymbol{t})\delta(R, \boldsymbol{t}')\frac{\gamma^R(R^{-1}\boldsymbol{t}, R^{-1}\boldsymbol{t}')}{\gamma(\boldsymbol{t}, \boldsymbol{t}')} \qquad \forall R \in K, \forall \boldsymbol{t}, \boldsymbol{t}' \in H \tag{3.4}$$

$$\delta(RR', \boldsymbol{t}) = \delta(R, \boldsymbol{t})\delta^R(R', R^{-1}\boldsymbol{t})\frac{\gamma(\boldsymbol{m}(R, R'), \boldsymbol{t})}{\gamma(\boldsymbol{t}, \boldsymbol{m}(R, R'))} \qquad \forall R, R' \in K, \forall \boldsymbol{t} \in H \tag{3.5}$$

$$\frac{\nu(R, R')\nu(RR', R'')}{\nu(R, R'R'')\nu^R(R', R'')} = \frac{\gamma(R\boldsymbol{m}(R', R''), \boldsymbol{m}(R, R'R''))}{\gamma(\boldsymbol{m}(R, R'), \boldsymbol{m}(RR', R''))}\delta^*(R, R\boldsymbol{m}(R', R''))$$

$$\forall R, R', R'' \in K \tag{3.6}$$

Note that the mapping $P(R, \boldsymbol{t})$ from our previous paper now has been written as $\delta^*(R, R\boldsymbol{t})$. This is done in order to follow Backhouse as closely as possible.

For short we write equation (3.1) as $\omega = (\gamma, \nu, \delta)$. For every factor system $\gamma$ of $H$ and every solution for $\delta$ and $\nu$ of the equations (3.2)–(3.6) the mapping $\omega$, defined by $\omega = (\gamma, \nu, \delta)$ is a factor system of $G$. Further, if $\omega = (\gamma, \nu, \delta)$ and $\omega' = (\gamma', \nu', \delta')$ then $\omega\omega' = (\gamma\gamma', \nu\nu', \delta\delta')$. Finally, a factor system $\omega = (\gamma, \nu, \delta)$ is equivalent with the trivial factor system if and only if there exist mappings $d: H \to U(1)$ and $e: K \to U(1)$ with $d(\boldsymbol{e}) = e(E) = 1$ such that $\gamma$, $\delta$ and $\nu$ can be written as

$$\gamma(\boldsymbol{t}, \boldsymbol{t}') = \frac{d(\boldsymbol{t})d(\boldsymbol{t}')}{d(\boldsymbol{t}+\boldsymbol{t}')} \tag{3.7}$$

$$\delta(R, \boldsymbol{t}) = \frac{d(\boldsymbol{t})}{d^R(R^{-1}\boldsymbol{t})} \tag{3.8}$$

$$\nu(R, R') = \frac{e(R)e^R(R')}{d(\boldsymbol{m}(R, R'))e(RR')}. \tag{3.9}$$

From this it follows that in order to get a complete set of inequivalent factor systems of $G$ we can restrict the factor systems of $H$ to a set of inequivalent ones. Such a set has been given by Backhouse (1970):

$$\gamma(\boldsymbol{t}, \boldsymbol{t}') = \exp(-2\pi i \boldsymbol{t}^{\mathrm{T}} A \boldsymbol{t}'). \tag{3.10}$$

Here $t^{\mathrm{T}}$ denotes the transpose of $t$ and $A$ is a matrix of the form

$$A=\begin{pmatrix} 0 & a_3 & -a_2 \\ -a_3 & 0 & a_1 \\ a_2 & -a_1 & 0 \end{pmatrix}$$

where $a_1, a_2, a_3 \in [0, \frac{1}{2})$. Then we can write

$$\frac{\gamma^R(R^{-1}\boldsymbol{t}, R^{-1}\boldsymbol{t}')}{\gamma(\boldsymbol{t}, \boldsymbol{t}')}=\exp[-2\pi \mathrm{i}\boldsymbol{t}^T(\epsilon_R R^{-1\mathrm{T}}AR^{-1}-A)\boldsymbol{t}']. \tag{3.11}$$

From equation (3.4) it follows that the left-hand side of equation (3.11) must be a factor system of $H$ which is equivalent to the trivial factor system. This is true if and only if

$$\epsilon_R R^{-1\mathrm{T}}AR^{-1}=A \quad (\mathrm{mod}\ \tfrac{1}{2}) \qquad \forall R\in K \tag{3.12}$$

since a factor system of a non-magnetic Abelian group is trivial if and only if it is symmetric. Let $\boldsymbol{a}$ be the vector with entries $a_1$, $a_2$ and $a_3$, then equation (3.12) can also be written as

$$\epsilon_R(\det R)R\boldsymbol{a}=\boldsymbol{a} \quad (\mathrm{mod}\ \tfrac{1}{2}) \qquad \forall R\in K. \tag{3.13}$$

From now on we suppose that $A$ satisfies equation (3.12). Then we can write

$$\epsilon_R R^{-1\mathrm{T}}AR^{-1}-A=B^R+N^R \tag{3.14}$$

where $N^R$ is an integer matrix and $B^R$ is a symmetric matrix. A particular solution of equation (3.4) is given by

$$\delta(R, \boldsymbol{t})=\exp(-\pi \mathrm{i}\boldsymbol{t}^{\mathrm{T}}B^R\boldsymbol{t}). \tag{3.15}$$

The general solution of equation (3.4) can therefore be written as

$$\delta(R, \boldsymbol{t})=\exp(-\pi \mathrm{i}\boldsymbol{t}^{\mathrm{T}}B^R\boldsymbol{t})\exp(2\pi \mathrm{i}\boldsymbol{k}(R)\cdot\boldsymbol{t}) \tag{3.16}$$

where $\boldsymbol{k}(R)$ is a vector with entries in the interval $[0, 1)$. Defining

$$C(R, R')=B^{RR'}-B^R-\epsilon_R R^{-1\mathrm{T}}B^{R'}R^{-1} \tag{3.17}$$

it is easy to show that $\exp(-\pi \mathrm{i}\boldsymbol{t}^{\mathrm{T}}C(R, R')\boldsymbol{t})$ is a unitary representation of $H$. Therefore we may write

$$\exp(-\pi \mathrm{i}\boldsymbol{t}^{\mathrm{T}}C(R, R')\boldsymbol{t})=\exp(-2\pi \mathrm{i}\boldsymbol{k}(R, R')\cdot\boldsymbol{t}) \tag{3.18}$$

where $\boldsymbol{k}(R, R')$ is defined by

$$[\boldsymbol{k}(R, R')]_i=\tfrac{1}{2}C_{ii}(R, R'). \tag{3.19}$$

Furthermore we have

$$\frac{\gamma(\boldsymbol{m}(R, R'), \boldsymbol{t})}{\gamma(\boldsymbol{t}, \boldsymbol{m}(R, R'))}=\exp[-2\pi \mathrm{i}(2\boldsymbol{a}\times\boldsymbol{m}(R, R'))\cdot\boldsymbol{t}]. \tag{3.20}$$

Substituting equations (3.16) and (3.20) in equation (3.5) now gives

$$\boldsymbol{k}(RR')-\boldsymbol{k}(R)-\epsilon_R R^{-1\mathrm{T}}\boldsymbol{k}(R')=\boldsymbol{k}(R, R')-2\boldsymbol{a}\times\boldsymbol{m}(R, R') \quad (\mathrm{mod}\ 1) \tag{3.21}$$

and equation (3.6) becomes with equations (3.16) and (3.10)

$$\frac{\nu(R,R')\nu(RR',R'')}{\nu(R,R'R'')\nu^R(R',R'')} = \exp[-2\pi i(\boldsymbol{m}^T(R',R'')R^TA\boldsymbol{m}(R,R'R'')-\boldsymbol{m}^T(R,R')A\boldsymbol{m}(RR',R'') - \tfrac{1}{2}\boldsymbol{m}^T(R',R'')R^TB^RR\boldsymbol{m}(R',R'')+\boldsymbol{k}(R)\cdot R\boldsymbol{m}(R',R''))]. \tag{3.22}$$

For each $A$ which satisfies equation (3.12) we have to solve $\boldsymbol{k}(R)$ and $\nu(R, R')$ from the equations (3.2), (3.3), (3.21) and (3.22). The requirement that these equations do have solutions is a further restriction on the possible matrices $A$. Suppose that for some $A$ one solution $\boldsymbol{k}_0(R)$ of equation (3.21) is known. Then the general solution of this equation is given by

$$\boldsymbol{k}(R)=\boldsymbol{k}_0(R)+\boldsymbol{h}(R) \tag{3.23}$$

where $\boldsymbol{h}(R)$ is the general solution of

$$\boldsymbol{h}(RR')-\boldsymbol{h}(R)-\epsilon_R R^{-1T}\boldsymbol{h}(R')=0 \pmod 1. \tag{3.24}$$

From the equations (3.7) and (3.8) it follows that two solutions $\boldsymbol{h}_1(R)$ and $\boldsymbol{h}_2(R)$ of equation (3.24) give rise to equivalent factor systems of $G$ if and only if we can write

$$\boldsymbol{h}_1(R)-\boldsymbol{h}_2(R)=\boldsymbol{k}-\epsilon_R R^{-1T}\boldsymbol{k} \pmod 1 \tag{3.25}$$

for some vector $\boldsymbol{k}$. Two solutions of this type will be called equivalent. So we have to find a complete set of inequivalent solutions of equation (3.24). This gives a set of solutions $\boldsymbol{k}(R)$ of equation (3.21) via equation (3.23). For each such solution $\boldsymbol{k}(R)$ we have to solve $\nu(R, R')$ from equation (3.22).

The requirement that equation (3.22) has solutions is a restriction on the allowed solutions of equation (3.24).

Suppose for some solution $\boldsymbol{k}(R)$ of equation (3.21) one solution $\nu_0(R, R')$ of equation (3.22) is known. Then the general solution of this equation is given by

$$\nu(R,R')=\nu_0(R,R')\mu(R,R') \tag{3.26}$$

where $\mu$ runs through the factor systems of $K$ (which are well known, see Janssen 1972). From the equations (3.7), (3.8) and (3.9) it follows that two factor systems $\mu_1$ and $\mu_2$ give rise to equivalent factor systems of $G$ if and only if they are equivalent or they can be written as

$$\mu_1(R,R')=\exp(2\pi i\boldsymbol{k}\cdot\boldsymbol{m}(R,R')\mu_2(R,R') \tag{3.27}$$

for some vector $\boldsymbol{k}$ satisfying

$$R^T\boldsymbol{k}=\epsilon_R\boldsymbol{k} \pmod 1 \tag{3.28}$$

Let us now summarize how to obtain a complete set of inequivalent factor systems of $G$.

(i) Find the set of matrices $A$ which satisfy equation (3.12).
(ii) For each matrix $A$ of this set, find a particular solution of the equations (3.3) and (3.21), if a solution exists.
(iii) Find the inequivalent solutions of equation (3.24).
(iv) For each matrix $A$ from steps (i) and (ii) and each solution of (3.24) from step (iii) find a particular solution of the equations (3.2) and (3.22).

(v) Obtain a complete set of inequivalent factor systems of $K$ with the property that no elements of this set are related as in equation (3.27).

(vi) The factor systems are now obtained from the equations (3.1), (3.10), (3.16), (3.14), (3.23) and (3.26).

Some remarks on the different steps given above might be useful.

(i) This step needs a short and straightforward calculation, using equation (3.13).

(ii), (iv) These steps consist of finding one solution of a set of equations of the type

$$\sum_i n_i x_i = \lambda \quad (\text{mod } 1)$$

where $n_i \in \mathbb{Z}$ and $\lambda \in \mathbb{R}$.

The number of equations and the number of unknowns in both cases increases rapidly if the order of $K$ increases. Therefore in some cases the help of a computer may be necessary.

(iii) This step does not involve the non-primitive translations. Therefore the solution for the Shubnikov space groups of type I can be found from the tables of Bradley (1973). For Shubnikov space groups of type III one can start from Bradley's solution for the non-magnetic subgroup.

(v) Here we have to analyse factor systems of $K$ of the type

$$\sigma(R, R') = \exp(2\pi i \boldsymbol{k} \cdot \boldsymbol{m}(R, R')).$$

This may be done (if necessary) using the decomposition of factor systems (van den Broek 1976b).

Similar procedures could be constructed to obtain the inequivalent factor systems of the Shubnikov space groups of the types II and IV. There is, however, another possibility: one first determines the inequivalent factor systems of the non-magnetic subgroup with the procedure given above, or, in case this subgroup is symmorphic, these factor systems are obtained from the tables by Bradley (1973). The inequivalent factor systems of the Shubnikov space groups of the types II and IV may then be determined from the inequivalent factor systems of their non-magnetic subgroups. This will be described in the next two sections.

## 4. Factor systems of Shubnikov space groups of type II

Let $\bar{G}$ be a Shubnikov space group of type II and $G$ its unitary subgroup which is a type I Shubnikov space group. The notation of the elements of $G$ will be as in the previous sections and the inequivalent factor systems of $G$ are supposed to be known. Elements of $\bar{G}$ will be denoted by $((\boldsymbol{t}, R), \alpha)$ where $(\boldsymbol{t}, R) \in G$, $\alpha \in C_2 = \{e, T\}$ and $T$ denotes the time-reversal operator. We define $((\boldsymbol{t}, R), \alpha)$ by $((\boldsymbol{t}, R), e) = (\boldsymbol{t}, R)$ and $((\boldsymbol{t}, R), T) = (\boldsymbol{t}, R)T$. The inequivalent factor systems of $\bar{G}$ are obtained as follows (van den Broek 1976a, b, Bradley and Wallis 1974).

Every factor system of $G$ is equivalent with a factor system $\sigma$ of $G$ which decomposes as follows:

$$\sigma(((\boldsymbol{t}, R), \alpha), ((\boldsymbol{t}, R'), \alpha')) = \Gamma((\boldsymbol{t}, R), (\boldsymbol{t}', R'))N(\alpha, \alpha')P(\alpha, (\boldsymbol{t}', R')) \quad (4.1)$$

where $\Gamma$ is a factor system of $G$ and $N$ and $P$ are mappings from $C_2 \times C_2$ and $C_2 \times G$, respectively, into $U(1)$ such that

$$N(e, e)=N(e, T)=N(T, e)=P(T, (\boldsymbol{e}, E))=1 \tag{4.2}$$

$$P(e, (\boldsymbol{t}, R))=1 \qquad \forall(\boldsymbol{t}, R)\in G \tag{4.3}$$

$$N^2(T, T)=1 \tag{4.4}$$

and

$$P(T, (\boldsymbol{t}, R)(\boldsymbol{t}', R')) = P(T, (\boldsymbol{t}, R))P(T, (\boldsymbol{t}', R'))\Gamma^2((\boldsymbol{t}, R), (\boldsymbol{t}', R')) \qquad \forall(\boldsymbol{t}, R), (\boldsymbol{t}', R')\in G. \tag{4.5}$$

On the other hand, if $N$ and $P$ satisfy these relations for some factor system $\Gamma$ of $G$, the mapping $\sigma$, defined by equation (4.1), is a factor system of $\bar{G}$.

From equation (4.5) it follows that $\Gamma$ must have the property that $\Gamma^2$ is equivalent with the trivial factor system. For such a $\Gamma$ we can write

$$\Gamma^2((\boldsymbol{t}, R), (\boldsymbol{t}', R'))=\frac{c_\Gamma((\boldsymbol{t}, R))c_\Gamma((\boldsymbol{t}', R'))}{c_\Gamma((\boldsymbol{t}, R)(\boldsymbol{t}', R'))}. \tag{4.6}$$

Then the solution of (4.5) is given by

$$P(T, (\boldsymbol{t}, R))=c_\Gamma^*((\boldsymbol{t}, R))D((\boldsymbol{t}, R)) \tag{4.7}$$

where $D$ runs through the unitary one-dimensional representations of $G$. The unitary one-dimensional representations of $G$ are given by:

$$D((\boldsymbol{t}, R))=\exp(2\pi i\boldsymbol{k}\,.\,\boldsymbol{t})\Delta(R) \tag{4.8}$$

where $\boldsymbol{k}$ is a vector from the first Brillouin zone of the reciprocal lattice with the properties:

(i) $R^{\mathrm{T}}\boldsymbol{k}=\boldsymbol{k} \pmod 1$.

(ii) The factor system $\mu(R, R')=\exp(2\pi i\boldsymbol{k}\,.\,\boldsymbol{m}(R, R'))$ of $K$ is equivalent with the trivial factor system,

and $\Delta$ is a one-dimensional projective representation of $K$ with factor system $\mu(R, R')$.

A factor system $\sigma=(\Gamma, N, P)$ of $\bar{G}$ is equivalent with the trivial factor system if and only if $\Gamma$ is equivalent with the trivial factor system of $G$, $N(T, T)=1$ and the unitary one-dimensional representation $D$ of $G$, determined by equation (4.7), is also the square of some unitary one-dimensional representation of $G$ (van den Broek 1976b).

Therefore we obtain a complete set of inequivalent factor systems of $\bar{G}$ in the following way:

(i) From a set of inequivalent factor systems of $G$ select those elements $\Gamma$ which have the property that $\Gamma^2$ is equivalent with the trivial factor system. Let us call this set $Q$.

(ii) For each $\Gamma\in Q$, find a mapping $c_\Gamma$: $G\to U(1)$ such that equation (4.6) holds.

(iii) Obtain the set of unitary one-dimensional representations of $G$, modulo the set of the squares of these representations. Let us call this set $S$.

(iv) The factor systems are now given by equation (4.1), where $\Gamma\in Q$, $N$ satisfies equations (4.2) and (4.4) and $P$ is given by equation (4.7), where $D\in S$.

## 5. Factor systems of Shubnikov space groups of type IV

Let $\bar{G}$ be a Shubnikov space group of type IV, $G$ its unitary subgroup, which is a type I Shubnikov space group, and let $\bar{H}$ be the black and white lattice of $\bar{G}$. $\bar{H}$ is given by $H$, the subgroup of translations of $G$ and an extra translation $\boldsymbol{t}_0$, with $2\boldsymbol{t}_0 \in H$, which occurs in $G$ in combination with the time-reversal operator. The notation of elements of $G$ will be as in the preceding sections. It is supposed that a complete set of inequivalent factor systems of $G$ is known and that these factor systems can be decomposed as in equation (3.1): $\Gamma = (\gamma, \nu, \delta)$. Let us denote this set by $Q$. We may assume that the trivial factor system of $G$ is contained in $Q$. Elements of $\bar{G}$ will be denoted by $((\boldsymbol{t}, R), \alpha)$ where $(\boldsymbol{t}, R) \in G$ and $\alpha \in C_2 = \{e, a\}$ with $a^2 = e$. We define $((\boldsymbol{t}, R), \alpha)$ by $((\boldsymbol{t}, R), e) = (\boldsymbol{t}, R)$ and $((\boldsymbol{t}, R), a) = (\boldsymbol{t} + R\boldsymbol{t}_0, R)T$ where $(\boldsymbol{t} + R\boldsymbol{t}_0, R)$ acts on space vectors in the usual way and $T$ denotes again the time-reversal operator. For the factor systems of $\bar{G}$ we can state the following (van den Broek 1976b). Every factor system of $\bar{G}$ is equivalent with a factor system $\sigma$ which decomposes as follows:

$$\sigma(((\boldsymbol{t}, R), \alpha)((\boldsymbol{t}', R'), \alpha'))$$
$$= \Gamma((\boldsymbol{t}, R), (\boldsymbol{t}', R')^\alpha)\Gamma((\boldsymbol{t}, R)((\boldsymbol{t}', R')^\alpha), n(\alpha, \alpha'))N(\alpha, \alpha')P(\alpha, (\boldsymbol{t}', R')) \quad (5.1)$$

where $(\boldsymbol{t}, R)^\alpha$ is given by $(\boldsymbol{t}, R)^e = (\boldsymbol{t}, R)$ and $(\boldsymbol{t}, R)^a = (\boldsymbol{t} + \boldsymbol{t}_0 - R\boldsymbol{t}_0, R)$, $n(\alpha, \alpha')$ is given by $n(e, e) = n(e, a) = n(a, e) = (\boldsymbol{e}, E)$ and $n(a, a) = (2\boldsymbol{t}_0, E)$, $\Gamma \in Q$ and $N$ and $P$ are mappings from $C_2 \times C_2$ and $C_2 \times G$ respectively into $U(1)$ with the properties

$$N(e, e) = N(e, a) = N(a, e) = P(a, (\boldsymbol{e}, E)) = 1 \quad (5.2)$$

$$P(e, (\boldsymbol{t}, R)) = 1 \qquad \forall (\boldsymbol{t}, R) \in G \quad (5.3)$$

$$P(a, (\boldsymbol{t}, R)(\boldsymbol{t}', R'))$$
$$= P(a, (\boldsymbol{t}, R))P(a, (\boldsymbol{t}', R'))\Gamma((\boldsymbol{t}, R)^a, (\boldsymbol{t}', R')^a)\Gamma((\boldsymbol{t}, R), (\boldsymbol{t}', R')) \quad (5.4)$$

$$P(a, (\boldsymbol{t}, R)^a)P^*(a, (\boldsymbol{t}, R))\Gamma((\boldsymbol{t} + 2\boldsymbol{t}_0 - 2R\boldsymbol{t}_0, R), (2\boldsymbol{t}_0, E))\Gamma^*((2\boldsymbol{t}_0, E), (\boldsymbol{t}, R)) = 1 \quad (5.5)$$

$$N^2(a, a) = P(a, 2\boldsymbol{t}_0). \quad (5.6)$$

For short we write equation (5.1) as $\sigma = (\Gamma, N, P)$. For every $\Gamma \in Q$ and every solution for $N$ and $P$ of the equations (5.2)–(5.6) the mapping $\sigma$, defined by $\sigma = (\Gamma, N, P)$ is a factor system of $\bar{G}$. Further, if $\sigma = (\Gamma, N, P)$ and $\sigma' = (\Gamma', N', P')$ then $\sigma\sigma' = (\Gamma\Gamma', NN', PP')$. Finally, a factor system $\sigma = (\Gamma, N, P)$ is equivalent with the trivial factor system if and only if $\Gamma$ is the trivial factor system and there exists a unitary one-dimensional representation $D$ of $G$ such that $P(a, (\boldsymbol{t}, R))$, which is now also a unitary one-dimensional representation of $G$, can be written as

$$P(a, (\boldsymbol{t}, R)) = D^2((\boldsymbol{t}, R))D((\boldsymbol{t}_0 - R\boldsymbol{t}_0, E)) \quad (5.7)$$

and further

$$N(a, a) = D((2\boldsymbol{t}_0, E)). \quad (5.8)$$

From equation (5.4) it follows that $\Gamma((\boldsymbol{t}, R)^a, (\boldsymbol{t}', R')^a)\Gamma((\boldsymbol{t}, R), (\boldsymbol{t}', R'))$ must be equivalent with the trivial factor system of $G$. If we take $R = R' = E$ it follows that $\gamma^2(\boldsymbol{t}, \boldsymbol{t}')$ must be equivalent with the trivial factor system of $H$. Taking $R = E$ in equation (5.5) gives $\gamma^2(\boldsymbol{t}, 2\boldsymbol{t}_0) = 1$. This means that there remain only two possible factor systems for $H$, as it should be, since $\bar{H}$ has only two inequivalent factor systems (van den Broek 1976b, Bradley and Wallis 1974). The non-trivial factor system of $H$ which is allowed is given by equation (3.10) where $a_i = \frac{1}{4}n_i$ if $2\boldsymbol{t}_0 = n_1\boldsymbol{t}_1 + n_2\boldsymbol{t}_2 + n_3\boldsymbol{t}_3$ and we suppose that $\boldsymbol{t}_0$ is chosen such that $n_1$, $n_2$ and $n_3$ are equal to 0 or 1.

From equation (5.4) it follows that

$$P(a, (\boldsymbol{t}, R)^a) = P(a, (\boldsymbol{t}_0 - R\boldsymbol{t}_0, E))P(a, (\boldsymbol{t}, R))\Gamma((\boldsymbol{t}_0 - R\boldsymbol{t}_0, E), (\boldsymbol{t}, R)^a) \times \Gamma((\boldsymbol{t}_0 - R\boldsymbol{t}_0, E), (\boldsymbol{t}, R)). \tag{5.9}$$

Substituting this equation in equation (5.5) gives, using $\Gamma = (\gamma, \nu, \delta)$:

$$P(a, (\boldsymbol{t}_0 - R\boldsymbol{t}_0, E)) = \gamma^*(\boldsymbol{t} + 2\boldsymbol{t}_0 - 2R\boldsymbol{t}_0, 2R\boldsymbol{t}_0)\gamma(2\boldsymbol{t}_0, \boldsymbol{t})\gamma((\boldsymbol{t}_0 - R\boldsymbol{t}_0, \boldsymbol{t} + \boldsymbol{t}_0 - R\boldsymbol{t}_0) \times \gamma^*(\boldsymbol{t}_0 - R\boldsymbol{t}_0, \boldsymbol{t})\delta(R, 2R\boldsymbol{t}_0). \tag{5.10}$$

Using the special form of $\gamma$ (equation (3.10)) and the fact that $\gamma^2(\boldsymbol{t}, 2\boldsymbol{t}_0) = 1$ for all $\boldsymbol{t} \in H$ we obtain after a short calculation that equation (5.10) reduces to

$$P(a, (\boldsymbol{t}_0 - R\boldsymbol{t}_0, E)) = \delta(R, 2R\boldsymbol{t}_0). \tag{5.11}$$

A complete set of inequivalent factor systems of $\bar{G}$ is now obtained as follows.

(i) Find the subset $Q_0$ of $Q$ of factor systems $\Gamma$ with the property that $\Gamma((\boldsymbol{t}, R)^a, (\boldsymbol{t}', R')^a)\Gamma((\boldsymbol{t}, R), (\boldsymbol{t}', R'))$ is equivalent with the trivial factor system of $\bar{G}$. A necessary condition for $\Gamma$ to belong to $Q_0$ is that $\gamma$ is one of the two allowed factor systems of $H$.

(ii) For each $\Gamma \in Q_0$, find a particular solution $P_0(a, (\boldsymbol{t}, R))$ of the equations (5.4) and (5.11), if one exists.

(iii) A set of factor systems of $\bar{G}$ is given by $\sigma = (\Gamma, N, P)$ where $\Gamma \in Q_0$, $P$ is given by equation (5.3) and $P(a, (\boldsymbol{t}, R)) = P_0(a, (\boldsymbol{t}, R))\Delta((\boldsymbol{t}, R))$ where $\Delta$ runs through the unitary one-dimensional representations of $G$ with the property that $\Delta((\boldsymbol{t}_0 - R\boldsymbol{t}_0, E)) = 1$ for each $R \in K$ and $N$ satisfies the equations (5.2) and (5.6).

(iv) Obtain from this set a set of inequivalent factor systems with the criterion given in the text following equation (5.6).

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