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Notes on the normalizer of a finite subgroup of $GL(n, d, \mathbb{Z})$ in $GL(n, d, \mathbb{Z})$

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A finite algorithm for calculating a finite set of generators for the normalizer of a finite subgroup G of $GL(n, d, \mathbb{Z})$ in $GL(n, d, \mathbb{Z})$ is presented. It is based on an algorithm for the normalizer of a finite subgroup G in $GL(n, \mathbb{Z})$, which has been developed recently by Opgenorth. The normalizer of G in $GL(n, d, \mathbb{Z})$ plays a role for superspace groups analogous to the role that the normalizer of G in $GL(n, \mathbb{Z})$ plays for n-dimensional space groups. It is important for calculating superspace groups with the Zassenhaus algorithm and is needed for testing equivalence of superspace groups.

1. Introduction

The importance of space groups for solid-state physics is well known. Thus they are well studied and for low dimensions [up to $n = 4$, see Brown *et al.* (1977)] there exist complete lists of all possible space groups and their properties. For higher dimensions, computer programs have been developed (Opgenorth *et al.*, 1998). A common way to calculate all types of space group of a given dimension or, more specifically, to calculate all inequivalent types of space group for a given point group P, is to use the Zassenhaus algorithm (Zassenhaus, 1947; Brown, 1969) or an extension algorithm (Janssen *et al.*, 1969; Fast & Janssen, 1971). This requires the knowledge of the normalizer of a finite subgroup $G \subset GL(n, \mathbb{Z})$ (G is isomorphic to the point group P) in the group $GL(n, \mathbb{Z})$, the group of integer $n \times n$ matrices. In fact, only a set of generators of the normalizer of G in $GL(n, \mathbb{Z})$ is required. Although this normalizer is in general an infinite group, it is long known that it possesses a finite set of generators (Siegel, 1943). However, it was only recently that a finite algorithm for this task was found (Opgenorth *et al.*, 1998; Opgenorth, 2000), which is based on the theory of G-perfect forms.

The interest of higher-dimensional space groups ($n > 3$) for physics lies in the fact that they can be used to describe the symmetry of quasiperiodic systems. In physics, however, the physical three-dimensional space plays a special role, which implies that additional requirements have to be imposed on the n-dimensional space groups. For example, consider incommensurately modulated systems. They are characterized by a three-dimensional periodic basis structure, whose symmetry can be described by ordinary three-dimensional space groups, and by one or more (incommensurate) modulation wave vectors. Their diffraction pattern consists of main reflections (due to the basis structure) and satellite reflections due to the modulation. The symmetry operations have to respect this special structure of main reflections and satellites, which leads to restrictions on the possible symmetry operations of the n-dimensional space group.

This leads to the definition of so-called superspace groups (Janner & Janssen, 1979). It can be shown that the matrices corresponding to the point-group elements with respect to a standard basis have a special block structure, which reflects the partition of the $n + d$-dimensional superspace into the n-dimensional physical space V_E and the d-dimensional internal space V_I or, alternatively, the distinction of main reflections and satellites. In fact, the point group of these superspace groups is isomorphic to a finite subgroup of the group $GL(n, d, \mathbb{Z})$ (see below; Janner & Janssen, 1979). Thus, a reformulation of certain concepts like equivalence of space groups and adaptions of algorithm are required for superspace groups (Janner & Janssen, 1979). In particular, for calculating the possible superspace groups for a given superpoint group or for testing the equivalence of superspace groups, we need to know the normalizer of a finite subgroup $G \subset GL(n, d, \mathbb{Z})$ in $GL(n, d, \mathbb{Z})$ instead of $GL(n + d, \mathbb{Z})$.

In the present article, we describe an algorithm for finding the normalizer of a finite subgroup $G \subset GL(n, d, \mathbb{Z})$ in $GL(n, d, \mathbb{Z})$, which is based on Opgenorth's normalizer algorithm for $GL(n, \mathbb{Z})$ (Opgenorth *et al.*, 1998; Opgenorth, 2000).

Let us first recall some definitions and facts for superspace groups which are indispensable in the following [see Janner & Janssen (1979) for a detailed discussion of superspace groups]. We have already mentioned that the superpoint groups are isomorphic to finite subgroups of $GL(n, d, \mathbb{Z})$, the group of matrices of the form

$$\Gamma = \begin{pmatrix} \Gamma_E & 0 \\ \Gamma_M & \Gamma_I \end{pmatrix} \qquad (1)$$

with $\det \Gamma = \pm 1$, where Γ_E, Γ_I and Γ_M are integer $n \times n$, $d \times d$ and $d \times n$ matrices, respectively. It can be shown (Janner &

Janssen, 1979) that Γ_M can be expressed as $\Gamma_M = \sigma\Gamma_E - \Gamma_I\sigma$, where the $d \times n$ matrix σ is independent of the group element $\Gamma \in G$ (Janner & Janssen, 1979). This matrix σ is not unique but may be replaced by any matrix $\sigma + \sigma'$, where σ' satisfies the equations $\sigma'\Gamma_E - \Gamma_I\sigma' = 0$ for all $\Gamma \in G$. This freedom can be exploited to choose a rational matrix for σ (Janner & Janssen, 1979). The matrices Γ_E form a group of integer matrices too. It is a finite subgroup of $GL(n, \mathbb{Z})$, which we denote by G_E. Similarly, the matrices Γ_I form a subgroup of $GL(d, \mathbb{Z})$, which we denote by G_I.

Note, however, that G is in general not a direct product of these two groups G_E and G_I but only a subdirect product of G_E and G_I. A subdirect product G of two groups G_1 and G_2 is a subgroup of the direct product $G_1 \otimes G_2$ such that for each element $g_1 \in G_1$ there exists an element $g_2 \in G_2$ such that $g = (g_1, g_2)$ is an element of G, and for any $g_2 \in G_2$ there exists $g_1 \in G_1$ such that $g = (g_1, g_2) \in G$. Subdirect products have an important property: Define $N_1 \subseteq G_1$ as the group of all elements $g_1 \in G_1$ such that $(g_1, e_2) \in G$, where e_2 is the unit element of G_2. Analogously define N_2. Then N_i is a normal subgroup of G_i and the following relation holds: $G/N_1 \sim G/N_2$, where $\sim$ denotes an isomorphism.

We are now ready to study the normalizer of G in $GL(n, d, \mathbb{Z})$.

2. Properties of the normalizer

Owing to the structure of the elements of $GL(n, d, \mathbb{Z})$, any element S of the normalizer $\mathcal{N}$ of G in $GL(n, d, \mathbb{Z})$ can be written as

$$S = \begin{pmatrix} S_E & 0 \\ S_M & S_I \end{pmatrix}, \tag{2}$$

where S_E, S_I and S_M are integer $n \times n$, $d \times d$ and $d \times n$ matrices, respectively. In order that S is in fact an element of the normalizer $\mathcal{N}$ of G, the matrix $S\Gamma S^{-1}$ must be an element of G for any matrix $\Gamma \in G$. This condition reads explicitly

$$S\Gamma S^{-1} = \begin{pmatrix} S_E\Gamma_E S_E^{-1} & 0 \\ S_M\Gamma_E S_E^{-1} + S_I\Gamma_M S_E^{-1} - S_I\Gamma_I S_I^{-1} S_M S_E^{-1} & S_I\Gamma_I S_I^{-1} \end{pmatrix} \in G. \tag{3}$$

Thus we infer that S_E has to be an element of the normalizer $\mathcal{N}_E(G_E)$ of G_E in $GL(n, \mathbb{Z})$, and analogously S_I must be an element of the normalizer $\mathcal{N}_I(G_I)$ of G_I in $GL(d, \mathbb{Z})$. However, these are not the only restrictions for S_E and S_I. Additional restrictions arise from the fact that G is not a direct product of the groups G_E and G_I but only a subdirect product of G_E and G_I. Choosing an element Γ with $\Gamma_E = I_n$, where I_n is the n-dimensional unit matrix, we readily infer that S_I has to be an element of the normalizer $\mathcal{N}_I(N_I)$ of the normal subgroup $N_I \lhd G_I$ in $GL(d, \mathbb{Z})$. Analogously, S_E must be an element of the normalizer $\mathcal{N}_E(N_E)$ of the normal subgroup $N_E \lhd G_E$ in $GL(n, \mathbb{Z})$. Furthermore, let $\varphi_G : G_E/N_E \to G_I/N_I$ be the canonical isomorphism of the two quotient groups G_E/N_E and G_I/N_I and let $\gamma_E(S_E)$ and $\gamma_I(S_I)$ be the automorphisms of G_E/N_E and G_I/N_I, respectively, which are induced by the conjugations $\Gamma_E \to S_E\Gamma_E S_E^{-1}$ and $\Gamma_I \to S_I\Gamma_I S_I^{-1}$, respectively. Then the following diagram has to commute:

$$\begin{array}{ccc} G_E/N_E & \xrightarrow{\varphi_G} & G_I/N_I \\ {\scriptstyle \gamma_E(S_E)}\downarrow & & \downarrow{\scriptstyle \gamma_I(S_I)} \\ G_E/N_E & \xrightarrow{\varphi_G} & G_I/N_I \end{array} \tag{4}$$

or, in other words, the equation

$$\varphi_G\gamma_E(S_E) = \gamma_I(S_I)\varphi_G \tag{5}$$

must be satisfied. Note that all conditions on the matrices S_E and S_I obtained so far are only necessary conditions and are in general not sufficient. In particular, the fact that S_E and S_I fulfil all the conditions derived so far does not guarantee that an appropriate matrix S_M exists for such a pair (S_E, S_I). Nevertheless, it is useful to introduce a special name for such pairs (S_E, S_I). Let us agree that a pair (S_E, S_I) is called admissible if $S_E \in \mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$, $S_I \in \mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$, and if (5) is satisfied. Note that the set of admissible pairs forms a group if we define group multiplication in the natural way. This group, which we shall denote by $\mathcal{S}$, is in general not a direct product but only a subdirect product of $\mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$ and $\mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$.

In order to get some information about S_M, we exploit the fact that Γ_M can be written as $\Gamma_M = \sigma\Gamma_E - \Gamma_I\sigma$, where the $d \times n$ matrix σ is independent of the group element $\Gamma \in G$ (Janner & Janssen, 1979). Hence we obtain the equation

$$\begin{aligned} (S_M + S_I\sigma)\Gamma_E S_E^{-1} - S_I\Gamma_I S_I^{-1}(S_M + S_I\sigma)S_E^{-1} \\ = \sigma S_E\Gamma_E S_E^{-1} - S_I\Gamma_I S_I^{-1}\sigma, \end{aligned} \tag{6}$$

which is equivalent to the condition

$$(S_M + S_I\sigma)S_E^{-1} = \sigma + \tau, \tag{7}$$

where τ is a $d \times n$ matrix satisfying the equation

$$\tau S_E\Gamma_E S_E^{-1} - S_I\Gamma_I S_I^{-1}\tau = 0 \tag{8}$$

for all group elements $\Gamma \in G$. Moreover, since S_E and S_I are elements of the normalizers of G_E and G_I in $GL(n, \mathbb{Z})$ and $GL(d, \mathbb{Z})$, respectively, and, since they have to satisfy (5), this reduces to the condition that

$$\tau\Gamma_E - \Gamma_I\tau = 0 \tag{9}$$

has to be satisfied for all $\Gamma \in G$. Thus we have derived the following representation of S_M:

$$S_M = \sigma S_E - S_I\sigma + \tau S_E. \tag{10}$$

Note that in general neither σ nor τ are integer matrices and may even be irrational. However, one can always choose σ to be rational such that all matrix entries have a denominator which is a divisor of the order of the group G. With such a choice of σ, τ is a matrix with rational entries whose denominators are divisors of $|G|$.

Let us consider the case $\sigma = 0$ first. In this case, τ has to be an integer matrix, in particular the trivial solution of (9) gives $S_M = 0$. Then any matrix

$$S = \begin{pmatrix} S_E & 0 \\ 0 & S_I \end{pmatrix} \quad (11)$$

such that the two matrices $S_E \in \mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$ and $S_I \in \mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$ fulfil the condition (5) is an element of the normalizer $\mathcal{N}$ of G in $GL(n, d, \mathbb{Z})$, *i.e.* the necessary conditions on S_E and S_I stated above are also sufficient for this case. Furthermore, any matrix

$$S = \begin{pmatrix} S_E & 0 \\ \tau S_E & S_I \end{pmatrix} \quad (12)$$

such that the integer matrix τ satisfies $\tau\Gamma_E - \Gamma_I\tau = 0$ is an element of the normalizer of G in $GL(n, d, \mathbb{Z})$. The reverse statement that any element of the normalizer $\mathcal{N}$ can be written as in (12) has already been proved.

In order to find a finite set of generators for the normalizer $\mathcal{N}$, we make use of the fact that $\mathcal{N}$ is a semidirect product of the normal subgroup $\mathcal{N}_1$ consisting of the matrices

$$S = \begin{pmatrix} I_n & 0 \\ \tau & I_d \end{pmatrix}$$

and the subgroup $\mathcal{N}_2$ consisting of the matrices

$$S = \begin{pmatrix} S_E & 0 \\ 0 & S_I \end{pmatrix},$$

i.e. any element of the normalizer $\mathcal{N}$ can be written as

$$S = \begin{pmatrix} I_n & 0 \\ \tau & I_d \end{pmatrix} \begin{pmatrix} S_E & 0 \\ 0 & S_I \end{pmatrix} \quad (13)$$

$$= \begin{pmatrix} S_E & 0 \\ 0 & S_I \end{pmatrix} \begin{pmatrix} I_n & 0 \\ S_I^{-1}\tau S_E & I_d \end{pmatrix}. \quad (14)$$

Hence it is sufficient to find generators for the subgroups $\mathcal{N}_1$ and $\mathcal{N}_2$ separately. $\mathcal{N}_1$ is isomorphic to the free abelian group of integer matrices τ satisfying (9) and it is thus sufficient to find a basis for this (finitely generated) $\mathbb{Z}$-module. Generators for $\mathcal{N}_2$ can be found by taking into account that $\mathcal{N}_2$ is a subgroup of finite index of the direct product $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$. This follows from the fact that the orbit of G under the action of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ (where action is defined as conjugation) is finite, which itself is a consequence of the invariance of the finite group $G_E \otimes G_I \supseteq G$ under $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$. By Schreier's theorem (Magnus *et al.*, 1966), a set of generators of $\mathcal{N}_2$ can be calculated from the set of generators g_i of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ and the left coset representatives r_j of $\mathcal{N}_2$ in $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ by means of

$$\{\overline{g_i r_j}^{-1} g_i r_j\}, \quad (15)$$

where $\overline{g_i r_j}$ denotes the coset representative corresponding to element $g_i r_j$.

Next we turn to the case $\sigma \neq 0$. It is always possible to find a transformation such that σ vanishes. However, this transformation is in general not an integer but only a rational transformation (Janner & Janssen, 1979). Nevertheless, it is instructive to perform this transformation. Explicitly, this transformation reads

$$\Gamma \to T^{-1}\Gamma T = \begin{pmatrix} \Gamma_E & 0 \\ 0 & \Gamma_I \end{pmatrix}, \quad (16)$$

where

$$T = \begin{pmatrix} E_n & 0 \\ X & E_d \end{pmatrix}, \quad (17)$$

$$X = (1/|G|) \sum_{\Gamma\in G} \Gamma_M \Gamma_E^{-1} = \sigma - (1/|G|) \sum_{\Gamma\in G} \Gamma_I \sigma \Gamma_E^{-1}. \quad (18)$$

Thus, finding the normalizer of G in $GL(n, d, \mathbb{Z})$ is equivalent to finding the normalizer of the transformed group $G^T := T^{-1}GT$ in the group $GL(n, d, \mathbb{Z})^T := T^{-1}GL(n, d, \mathbb{Z})T$. Note that $GL(n, d, \mathbb{Z})^T \neq GL(n, d, \mathbb{Z})$ in general, except if (and only if) T is an integer matrix. In this special case, G is arithmetically equivalent to G^T and the results of the preceding paragraphs can be immediately transferred. In particular, the normalizer is again a semidirect product.

Let assume now that T (and thus X) is not an integer matrix. Then the elements $S' = T^{-1}ST$ of $GL(n, d, \mathbb{Z})^T$ are in general not integer but rational matrices of the form

$$S' = \begin{pmatrix} S_E & 0 \\ S_M - XS_E + S_I X & S_I \end{pmatrix}. \quad (19)$$

From this, we infer that S_M may be represented as

$$S_M = XS_E - S_I X + \tau' S_E, \quad (20)$$

where τ' is a $d \times n$ rational matrix satisfying the equation

$$\tau'\Gamma_E - \Gamma_I\tau' = 0 \quad (21)$$

for all group elements $\Gamma \in G$. Note that this representation differs slightly from (10), where τ is not necessarily rational if σ is not. Thus, τ' usually differs from τ of (10). However, (20) is not an additional condition for S_M but rather a special case of (10), where the freedom in the choice of σ is used to choose a rational $\sigma = X$. Moreover, note that $|G|\tau'$ is an integer matrix, since S_M and $|G|X$ are integer matrices by definition.

In contrast to the case $\sigma = 0$, which corresponds to $X = 0$, (20) imposes non-trivial restrictions on the pairs (S_E, S_I). In general, an admissible pair (S_E, S_I), *i.e.* a pair (S_E, S_I) with $S_E \in \mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$, $S_I \in \mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$ satisfying the condition (5) does not automatically give rise to an element S of the normalizer $\mathcal{N}$ but the additional requirement that an appropriate τ' exists must be taken into account. If we define $\mathcal{S}'$ as the group of admissible pairs (S_E, S_I), for which an element S of the normalizer $\mathcal{N}$ exists, then $\mathcal{S}'$ is a subgroup of $\mathcal{S}$ of finite index. To prove this statement, we consider $\rho(S_E, S_I) = X - S_I X S_E^{-1}$. In order that $(S_E, S_I) \in \mathcal{S}'$, there must be a solution τ' of (21) such that $\rho(S_E, S_I) = \tau' \pmod{\mathbb{Z}}$. Now let us define an equivalence relation on the sets of ρ's as follows: $\rho(S_E, S_I)$ and $\rho(S'_E, S'_I)$ are called equivalent, in symbols $\rho(S_E, S_I) \sim \rho(S'_E, S'_I)$, if their difference $\rho(S_E, S_I) - \rho(S'_E, S'_I) = 0$ modulo an integer matrix and a matrix τ' satisfying (21). Then the ρ matrices of all elements $(S_E, S_I) \in \mathcal{S}'$ are equivalent to the 0 matrix. Moreover, consider the left cosets $(S_E, S_I)\mathcal{S}'$ in $\mathcal{S}$. Then we can readily prove that the ρ matrices corresponding to the elements of the left coset $(S_E, S_I)\mathcal{S}'$ are all equivalent. This is most easily seen if we consider the ρ matrix corresponding to the product $(S_E S'_E, S_I S'_I)$:

$$\rho(S_E S'_E, S_I S'_I) = \rho(S_E, S_I) + S_I \rho(S'_E, S'_I) S_E^{-1}. \qquad (22)$$

In the special case $(S'_E, S'_I) \in \mathcal{S}'$, we have $\rho(S'_E, S'_I) \sim 0$ and thus $\rho(S_E S'_E, S_I S'_I) \sim \rho(S_E, S_I)$, where we have taken into account that, with each solution τ' of (21), $S_I \tau' S_E^{-1}$ is also a solution of (21). Hence, the ρ matrices of elements of the same coset are equivalent. On the other hand, pairs (S_E, S_I) with equivalent matrices $\rho(S_E, S_I)$ belong to the same equivalence class $(S_E, S_I)\mathcal{S}'$, which we can readily infer from (22) and $\rho(S_E^{-1}, S_I^{-1}) = -S_I^{-1}\rho(S_E, S_I)S_E$. But this implies that the set of equivalence classes of ρ matrices is in one-to-one correspondence with the left cosets of $\mathcal{S}'$ in $\mathcal{S}$. Since the ρ matrices are rational matrices such that $|G|\rho(S_E, S_I)$ is an integer matrix, there is only a finite number of inequivalent ρ matrices, which proves that $\mathcal{S}'$ is a subgroup of finite index in $\mathcal{S}$. Thus we can again apply Schreier's theorem to obtain a finite set of generators of $\mathcal{S}'$, once a finite set of generators of $\mathcal{S}$ and the decomposition of $\mathcal{S}$ in left cosets of $\mathcal{S}'$ are known.

Note in passing that (22) in general does not define a group multiplication on the set $\mathcal{R}$ of equivalence classes of ρ matrices. However, if $\mathcal{S}'$ is a normal subgroup of $\mathcal{S}$, then (22) induces a multiplication law on the set $\mathcal{R}$ and $\mathcal{R}$ becomes a group, which is isomorphic to the quotient group $\mathcal{S}/\mathcal{S}'$.

It is now not difficult to find a set of generators for the normalizer $\mathcal{N}$. To this end, we first note that the set of matrices

$$S = \begin{pmatrix} I_n & 0 \\ S_M & I_d \end{pmatrix}$$

is not only a normal subgroup of $GL(n, d, \mathbb{Z})$ but is also invariant under the conjugation with the (rational) matrix T. Thus, these matrices form a normal subgroup of $GL(n, d, \mathbb{Z})^T$ too. In addition, the intersection of this group with the normalizer $\mathcal{N}$ is again the group $\mathcal{N}_1$, consisting of the matrices

$$S = \begin{pmatrix} I_n & 0 \\ \tau & I_d \end{pmatrix},$$

where τ is a $d \times n$ integer matrix satisfying (9). Moreover, $\mathcal{N}_1$ is a normal subgroup of $\mathcal{N}$ and the quotient group $\mathcal{N}/\mathcal{N}_1$ is isomorphic to $\mathcal{S}'$. Thus, $\mathcal{N}$ is an extension of $\mathcal{N}_1$ by $\mathcal{S}'$. Note, however, that it is in general not a semidirect product of these two groups. This special group structure allows us to find the generators of the normalizer $\mathcal{N}$ in two steps. As in the case $\sigma = 0$, we first calculate a set of generators of $\mathcal{N}_1$, which is a finite task as mentioned previously. Secondly, we obtain the remaining generators of $\mathcal{N}$ by determining for each generator $(S_E, S_I) \in \mathcal{S}'$ an appropriate matrix

$$S = \begin{pmatrix} S_E & 0 \\ XS_E - S_I X + \tau' S_E & S_I \end{pmatrix}.$$

Since the calculation of a finite set of generators of $\mathcal{S}'$ is a finite algorithm, too, a set of generators of $\mathcal{N}$ can be calculated in a finite number of steps. The results on the algebraic properties of the normalizer $\mathcal{N}$ can be summarized in the following theorem:

Theorem 1. Let G be a finite subgroup of $GL(n, d, \mathbb{Z})$ and G_E and G_I the corresponding groups describing the action of G in the physical and internal space, respectively. Let $\mathcal{N}_1$ be the group of integer matrices

$$S = \begin{pmatrix} I_n & 0 \\ \tau & I_d \end{pmatrix},$$

where τ satisfies (9), and let $\mathcal{S}$ be the group of all admissible pairs of G. Then the normalizer $\mathcal{N}$ of G in $GL(n, d, \mathbb{Z})$ is an extension of the (finitely generated) free abelian group $\mathcal{N}_1$ by a subgroup $\mathcal{S}' \subseteq \mathcal{S}$ of finite index in $\mathcal{S}$, which itself is a subgroup of finite index of the direct product of the normalizer of G_E in $GL(n, \mathbb{Z})$ and the normalizer of G_I in $GL(d, \mathbb{Z})$. Moreover, a pair $(S_E, S_I) \in \mathcal{S}$ is an element of $\mathcal{S}'$ if and only if the corresponding matrix $\rho(S_E, S_I) = X - S_I X S_E^{-1}$ differs only by an integer matrix from a solution τ' of (21).

Finally let us make some remarks on the connection of the normalizer $\mathcal{N} = N(G, GL(n, d, \mathbb{Z}))$ and $\mathcal{N}' = N(G, GL(n + d, \mathbb{Z}))$, the normalizer of G in $GL(n + d, \mathbb{Z})$. Clearly, $\mathcal{N} \subseteq \mathcal{N}'$, but in general $\mathcal{N} \neq \mathcal{N}'$. For instance, let G be the trivial subgroup of $GL(1, 1, \mathbb{Z})$ consisting only of the two-dimensional unit matrix. Then $\mathcal{N}$ is generated by the matrices

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

whereas $\mathcal{N}'$ is generated by

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

where the last one is obviously not an element of $GL(1, 1, \mathbb{Z})$. However, in some cases, the two normalizers $\mathcal{N}$ and $\mathcal{N}'$ may coincide. This occurs for instance if the matrix groups $\{\Gamma_E(\Gamma)\}$ and $\{\Gamma_I(\Gamma)\}$ are irreducible representations of G and there does not exist a permutation π of G such that the matrix representations $\{\Gamma_E(\Gamma)\}$ and $\{\Gamma_I(\pi(\Gamma))\}$ are equivalent. In fact, the weaker condition that $\{\Gamma_E(\Gamma)\}$ and $\{\Gamma_I(\pi(\Gamma))\}$ have no irreducible representations in common for any π is sufficient for $\mathcal{N} = \mathcal{N}'$, too.

3. An algorithm for finding the normalizer

From the discussion of the preceding section, we can formulate immediately a finite algorithm for computing a set of generators of the normalizer $\mathcal{N}$ (see Fig. 1).

Step 1: A basis of $d \times n$ integer matrices τ_i satisfying the equations

$$\tau_i \Gamma_E - \Gamma_I \tau_i = 0 \qquad (23)$$

is calculated and the matrices

$$S_i = \begin{pmatrix} I_n & 0 \\ \tau_i & I_d \end{pmatrix}$$

are constructed. These matrices are elements of the normalizer $\mathcal{N}$ and the set $Ge(\mathcal{N}_1) := \{S_i\}$ is a set of generators of $\mathcal{N}_1$.

Step 2: A set of generators for the normalizers of G_E and G_I in $GL(n, \mathbb{Z})$ and $GL(d, \mathbb{Z})$ is calculated. A finite algorithm for doing this was found by J. Opgenorth (Opgenorth *et al.*, 1998; Opgenorth, 2000) and implemented in the computer package *CARAT* (Opgenorth *et al.*, 1998). A share package for GAP (The GAP Group, 1999) is also available.

Step 3: A set of generators for the group $\mathcal{S}$ of admissible pairs (S_E, S_I) is calculated. This can be performed in several ways.

In the first method, the left coset decomposition of the direct product of $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$ with respect to $\mathcal{S}$ is calculated:

$$\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I) = \sum_j r_j \mathcal{S}. \tag{24}$$

The coset representatives r_j can be found by exploiting the fact that there is a one-to-one correspondence between the cosets $r_j\mathcal{S}$ and the conjugated groups $r_j G r_j^{-1}$. The generators of $\mathcal{S}$ are then obtained from the generators of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ and the coset representatives r_j by means of Schreier's theorem mentioned previously. This algorithm is finite since both the number of coset representatives as well as the number of generators of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ are finite.

The second method makes use of the fact that a pair (S_E, S_I) is only admissible if $S_E \in \mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$ and $S_I \in \mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$. First the normal subgroups N_E and N_I are determined. Then the coset decompositions of $\mathcal{N}_E(G_E)$ into $\mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$ and $\mathcal{N}_I(G_I)$ into $\mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$ are calculated. Again the application of Schreier's theorem gives a set of generators for $\mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E)$ and $\mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$. Now $\mathcal{N}_E(G_E) \cap \mathcal{N}_E(N_E) \otimes \mathcal{N}_I(G_I) \cap \mathcal{N}_I(N_I)$ is decomposed into left cosets of $\mathcal{S}$, from which we can obtain the generators of $\mathcal{S}$ by another application of Schreier's theorem.

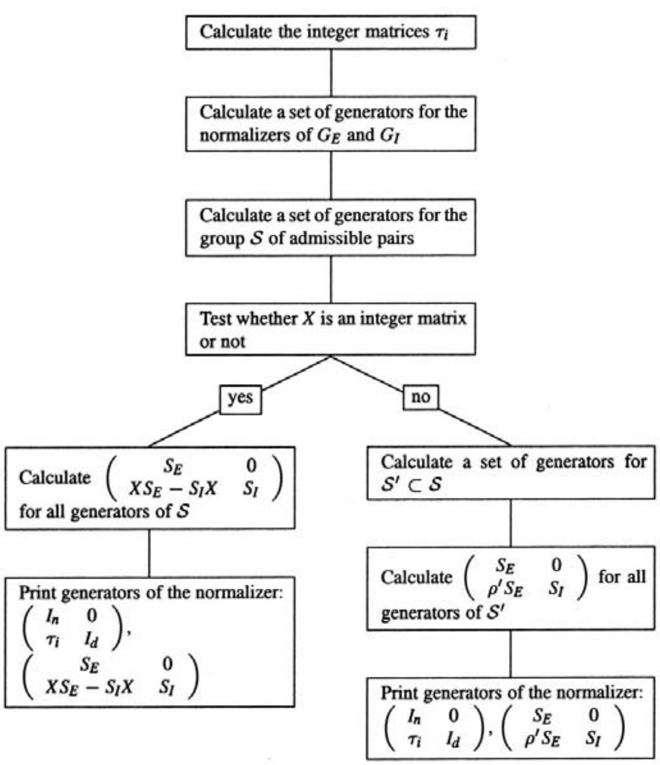

Figure 1
Algorithm for the normalizer.

Step 4: It is tested whether $X = \sigma - (1/|G|) \sum_{\Gamma \in G} \Gamma_I \sigma \Gamma_E^{-1}$ is an integer matrix or not. If X is an integer matrix, the matrices

$$S = \begin{pmatrix} S_E & 0 \\ XS_E - S_IX & S_I \end{pmatrix}$$

are calculated for all generators of $\mathcal{S}$. The union of this set of generators, let us call it $Ge(\mathcal{N}_2)$, with the set of generators $Ge(\mathcal{N}_1)$ gives a complete set of generators for $\mathcal{N}$. In the case when X is not an integer matrix, one proceeds with step 5.

Step 5: The coset decomposition of $\mathcal{S}$ with respect to $\mathcal{S}'$, the subgroup of admissible pairs (S_E, S_I) to which an element of the normalizer $\mathcal{N}$ corresponds, is calculated. Then another application of Schreier's theorem gives a set of generators of $\mathcal{S}'$.

In order to obtain the coset decomposition $\mathcal{S} = \sum_j r_j \mathcal{S}'$, the following algorithm, which is based on the ρ matrices introduced above, can be used. Let $\{\tau_i\}$, $i = 1, \ldots, n_\tau$, be a basis of integer solutions of (23) and view them as nd-dimensional vectors. Add appropriate integer $d \times n$ matrices t_j, $j = 1, \ldots, nd - n_\tau$, such that they form together with the matrices τ_i a basis of the additive group of integer $d \times n$ matrices. Let τ_i^*, t_j^* be the matrices of the corresponding reciprocal basis (where we have identified the space of $d \times n$-dimensional matrices with $\mathbb{R}^{nd}$ with the usual inner product in the natural way). Then the ρ matrices $\rho(S_E, S_I) = X - S_I X S_E^{-1}$ can be expressed as linear combinations

$$\rho(S_E, S_I) = \sum_i a_i(S_E, S_I)\tau_i + \sum_j (S_E, S_I) b_j t_j$$

with $a_i(S_E, S_I) := \langle \tau_i^*, \rho(S_E, S_I) \rangle$ and $b_j(S_E, S_I) := \langle t_j^*, \rho(S_E, S_I) \rangle$, where $\langle \cdot, \cdot \rangle$ denotes the inner product. We now exploit the fact that there is a one-to-one correspondence of the cosets of $\mathcal{S}'$ in $\mathcal{S}$ and the vectors $([b_j(S_E, S_I)])$, where $[b_j]$ denotes the fractional part of b_j.

The set of coset representatives is now calculated recursively. The first coset representative is the unit element (I_n, I_d) with the corresponding vector $([b_j]) = \mathbf{0}$, where $\mathbf{0}$ denotes the $(nd - n_\tau)$-dimensional zero vector. Set $R_0 = \{(I_n, I_d)\}$ and $R'_0 = \{\mathbf{0} = ([b_j(I_n, I_d)])\}$. Let $\{(S_E^i, S_I^i), i = 1, \ldots, s\}$ be a complete set of generators of $\mathcal{S}$. The set R_{j+1} is calculated from the set R_j as follows: All elements of R_j are multiplied with all generators (S_E^i, S_I^i) and the corresponding vectors $([b_j])$ are calculated. The set of all $([b_j])$ that are not in one of the sets R_ℓ, $\ell \le j$, form the set R'_{j+1}. The corresponding pairs (S_E, S_I) constitute the set R_{j+1} {if there corresponds more than one pair (S_E, S_I) to a vector $([b_j])$, then only one of the corresponding pairs (S_E, S_I) is added to R_{j+1}}. The algorithm stops if $R'_{j+1} \sim R_{j+1}$ is the empty set. The set of coset representatives is now obtained by taking the union of all R_j.

Step 6: For each pair (S_E, S_I) of the set of generators of $\mathcal{S}'$ the corresponding matrix

$$S = \begin{pmatrix} S_E & 0 \\ \rho' S_E & S_I \end{pmatrix}$$

is calculated, where $\rho' = \sum_j b_j(S_E, S_I)t_j$, which is an integer matrix for $(S_E, S_I) \in \mathcal{S}'$. The union of these matrices with $Ge(\mathcal{N}_1)$ gives the desired set of generators of $\mathcal{N}$.

4. Examples

In order to illustrate this algorithm, we apply it to several examples. All examples deal with the case $n = 3$, $d = 2$ which corresponds to the physical situation of a three-dimensional physical space and a two-dimensional incommensurate modulation. As a first example, we consider the group generated by the matrix

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}, \qquad (25)$$

This group describes the symmetry of a system with a hexagonal basis structure and incommensurate modulation with wave vectors perpendicular to the sixfold axis. The modulation also exhibits a hexagonal symmetry. Examples of such structures can be found in TaS_2 (see *e.g.* Yamamoto, 1983) or quartz (see *e.g.* Dolino *et al.*, 1984; Berge *et al.*, 1986).

The first step consists in calculating the integer matrices τ_i that satisfy the equations

$$\tau\Gamma_E - \Gamma_I\tau = 0 \qquad (26)$$

for all matrices Γ. In fact, these equations are automatically satisfied if they hold true for all generators Γ. Thus it is sufficient to solve

$$\tau\begin{pmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}\tau. \qquad (27)$$

All its solutions can be written as an integer linear combination of the matrices

$$\tau_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & -1 & 0 \end{pmatrix}, \qquad (28)$$

which readily gives two generators of the normalizer:

$$s_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix}, \quad s_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{pmatrix}. \qquad (29)$$

Next we have to calculate the normalizers of the groups G_E and G_I, which are generated by

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix},$$

respectively. A set of generators for $\mathcal{N}_E(G_E)$ is given by

$$\gamma_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$
$$\gamma_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (30)$$

Similarly, $\mathcal{N}_I(G_I)$ is generated by

$$\delta_1 = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}, \quad \delta_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \qquad (31)$$

These sets of generators were calculated by *CARAT* and simplified afterwards. The next step consists in finding a set of generators for the group $\mathcal{S}$ of admissible pairs. First note that the direct product $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ is generated by the pairs

$$(\gamma_i, e_2), \quad (e_3, \delta_j), \quad i = 1, \ldots, 3, \quad j = 1, 2, \qquad (32)$$

where e_2 and e_3 are the two- and three-dimensional unit matrices, respectively. The coset decomposition of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ with respect to $\mathcal{S}$ reads

$$\mathcal{S} + (\gamma_3, e_2)\mathcal{S}, \qquad (33)$$

which is obtained by using the one-to-one correspondence between the cosets $r_j\mathcal{S}$ and the conjugated groups $r_jGr_j^{-1}$. By applying Schreier's theorem, we get a set of generators for $\mathcal{S}$, namely

$$(\gamma_1, e_2), (\gamma_2, e_2), (e_3, \delta_1), (\gamma_3, \delta_2). \qquad (34)$$

Since $X = 0$ in this example, we immediately get the following set of generators for the normalizer $\mathcal{N}$:

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, s_1, s_2, \qquad (35)$$

where s_1, s_2 are the two generators we have calculated in the beginning, see (29). Note that the normalizers $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$ are finite owing to the high symmetry of this example. However, the normalizer $\mathcal{N}$ is infinite owing to the generators s_1 and s_2, which are both of infinite order. Owing to the finiteness of $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$, several steps of the normalizer algorithm are trivially finite. Nevertheless, the algorithm is finite also in the case of infinite $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$.

In order to discuss an example with infinite normalizers $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$, we choose a subgroup of the previous example, namely the subgroup generated by

$$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \tag{36}$$

which can be interpreted as the symmetry reduction owing to a phase transition from a hexagonal phase to a monoclinic one.

As a first step in the determination of the normalizer, we calculate again the matrices τ that in this example have to satisfy

$$\tau \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tau. \tag{37}$$

A basis of solutions reads

$$\tau_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{38}$$

$$\tau_3 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \tau_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{39}$$

from which we obtain the first four generators of the normalizer $\mathcal{N}$:

$$s_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad s_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$s_3 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad s_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix}. \tag{40}$$

In the second step, we calculate sets of generators for $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$. They read

$$\gamma_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$
$$\gamma_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{41}$$

and

$$\delta_1 = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}, \quad \delta_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \delta_3 = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \tag{42}$$

respectively. Note that both $\mathcal{N}_E(G_E)$ and $\mathcal{N}_I(G_I)$ are infinite, which is due to the matrices γ_4 and δ_3, which are of infinite order.

In this example all the generators

$$(\gamma_i, e_2), \quad (e_3, \delta_j), \quad i = 1, \ldots, 4, j = 1, \ldots, 3, \tag{43}$$

of $\mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$ are admissible pairs, so that we have $\mathcal{S} = \mathcal{N}_E(G_E) \otimes \mathcal{N}_I(G_I)$. Since again $X = 0$, we obtain immediately the following set of generators:

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, s_1, s_2, s_3, s_4. \tag{44}$$

In order to discuss an example where $X \neq 0$, we modify the previous example slightly and consider the group generated by

$$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}. \tag{45}$$

This symmetry group describes again a monoclinic phase whose modulation vectors are perpendicular to the twofold rotation axis. However, the transformation law of the modulation vectors is different now.

The first steps of this example are the same as in the previous examples, in particular the generators s_i, $i = 1, \ldots, 4$, and the group $\mathcal{S}$ are the same. However, in this case we have

$$X = \tfrac{1}{2} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

and we have to use the group $\mathcal{S}' \subseteq \mathcal{S}$ instead of $\mathcal{S}$ for calculating the normalizer elements. To this end, we have to calculate the coset decomposition of $\mathcal{S}$ with respect to $\mathcal{S}'$. Owing to the one-to-one correspondence of the cosets of $\mathcal{S}'$ and the corresponding equivalence classes of ρ matrices, we calculate the ρ matrices for all generators of $\mathcal{S}$ and their inverses:

$$\rho(\gamma_1, e_2) = \rho(\gamma_1^{-1}, e_2) = 0 \tag{46}$$

$$\rho(\gamma_2, e_2) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \simeq 0$$

$$\rho(\gamma_3, e_2) = 0$$

$$\rho(\gamma_4, e_2) = \rho(\gamma_4^{-1}, e_2) = 0$$

$$\rho(e_3, \delta_1) = \tfrac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix} \tag{47}$$

$$\rho(e_3, \delta_1^{-1}) = \tfrac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{48}$$

$$\rho(e_3, \delta_2) = \rho(e_3, \delta_1)$$

$$\rho(e_3, \delta_3) = \rho(e_3, \delta_3^{-1}) = 0.$$

Here, $\simeq$ denotes the equivalence modulo an integer matrix and a rational linear combination of the matrices τ_i, $i = 1, \ldots, 4$. From these equations, we see that there are three inequivalent ρ matrices. In fact, there could exist additional inequivalent ρ matrices. So we have to check whether products of two generators and their inverses give rise to new ρ matrices. However, it turns out that there are no new ρ matrices and hence the matrices 0, $\rho(e_3, \delta_2)$ and $\rho(e_3, \delta_2^{-1})$ are the only ones. Thus the coset decomposition reads

$$\mathcal{S} = \mathcal{S}' + (e_3, \delta_2)\mathcal{S}' + (e_3, \delta_2^{-1})\mathcal{S}'. \tag{49}$$

We can now apply Schreier's theorem to obtain generators for $\mathcal{S}'$. The standard procedure gives a long list of generators, some of which occur twice or are a product of other generators. A simplified but complete set of generators of $\mathcal{S}'$ is given by

$$(\gamma_1, e_2), (\gamma_2, e_2), (\gamma_3, e_2), (\gamma_4, e_2), (e_3, \delta_3), (e_3, \delta_1^3),$$
$$(e_3, \delta_2\delta_1), \left(e_3, \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\right). \tag{50}$$

Finally, we have to calculate for any generator (S_E, S_I) of $\mathcal{S}'$ the corresponding matrices

$$S = \begin{pmatrix} S_E & 0 \\ \rho' S_E & S_I \end{pmatrix} \tag{51}$$

with $\rho'(S_E, S_I) = \sum_j b_j(S_E, S_I)t_j$. In this example, we have always $\rho'(S_E, S_I) = \rho(S_E, S_I)$ and thus we obtain the following set of generators of $\mathcal{N}$:

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 2 & 1 \end{pmatrix}, \tag{52}$$

to which we have to add the four generators s_j.

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