

## Generators and subgroups for $\text{Aut}(F_3)$

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1995 J. Phys. A: Math. Gen. 28 379

(<http://iopscience.iop.org/0305-4470/28/2/014>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.68

The article was downloaded on 02/06/2010 at 00:51

Please note that [terms and conditions apply](#).

# Generators and subgroups for $Aut(F_3)$

Peter Kramer

Institut für Theoretische Physik der Universität, Tübingen, Germany

Received 19 September 1994, in final form 11 November 1994

**Abstract.** The automorphisms of the free group  $F_3$  with three generators form the group  $Aut(F_3)$ . New involutive generators and relations for  $Aut(F_3)$  are given which explain the relations given by Nielsen. Finite Coxeter groups and (normal) subgroups are derived which admit generalizations to  $n \geq 3$ .

## 1. Introduction

The free group  $F_n$  with  $n$  generators provides a description of non-commutative systems in physics. Therefore the group  $Aut(F_n)$  of its automorphisms, studied first by Nielsen [10], is of considerable interest for these systems. The groups  $F_n$  and  $Aut(F_n)$  have been used to formulate a non-commutative crystallography which encompasses aspects of quasicrystals, [1–3, 5–7]. In [8] a new system of involutive generators and relations for  $Aut(F_2)$  was introduced to derive the relations due to Nielsen. In what follows we present a similar analysis for  $Aut(F_3)$ . From Nielsen’s analysis,  $Aut(F_3)$  shows almost the full complexity of  $Aut(F_n)$ . Involutive generators and new relations are given and used to derive and explain the relations of Nielsen. Certain (normal) subgroups, among them the finite Coxeter groups  $A_3$  and  $B_3$ , are explicitly constructed, with counterparts for  $n \geq 3$ .

## 2. Nielsen generators and relations

Let  $F_n$  denote the free group with  $n$  generators, and denote by  $\Phi_n := Aut(F_n)$  its group of automorphism [10]. We present a set of four generators and relations  $R_i$  for  $\Phi_n$  due to Nielsen. The sign  $a \rightleftharpoons b$  indicates that  $a, b$  commute.

*Proposition 1 (Nielsen 1924) [10, 9].*  $Aut(F_n)$  is the group

$$\Phi_n := \langle P, Q, \sigma, U | R_1 \dots R_{18} \rangle \tag{1}$$

with relations

$$\begin{aligned} \sigma^2 &= P^2 = e && (R_1, R_2) \\ (P\sigma PU)^2 &= e && (R_3) \\ U^{-1} P U P \sigma U \sigma P \sigma &= e && (R_4) \\ U &\rightleftharpoons \sigma U \sigma && (R_5) \\ (QP)^{n-1} &= Q^n = e && (R_6, R_7) \\ P &\rightleftharpoons Q^{-i} P Q^i && i = 1 \dots [n/2] \quad (R_8) \\ \sigma &\rightleftharpoons Q^{-1} P Q && (R_9) \end{aligned} \tag{2a}$$

$$\begin{aligned}
 \sigma &= QP && (R_{10}) \\
 \sigma &= Q^{-1}\sigma Q && (R_{11}) \\
 (PQ^{-1}UQP)(Q^{-1}UQ) &= UQ^{-1}UQU^{-1} && (R_{12}) \\
 U &= Q^{-2}PQ^2 && (R_{13}) \\
 U &= QPQ^{-1}PQ && (R_{14}) \\
 U &= Q^{-2}\sigma Q^2 && (R_{15}) \\
 U &= Q^{-2}UQ^2 && (R_{16}) \\
 U &= PQ^{-1}\sigma U\sigma QP && (R_{17}) \\
 U &= PQ^{-1}PQPUPQ^{-1}PQP && (R_{18}).
 \end{aligned}
 \tag{2b}$$

The generators are defined as automorphisms of  $F_n = \langle x_1, \dots, x_n \rangle$  by

$$\begin{aligned}
 e &: x_1 & x_2 & x_3 & \dots & x_{n-1} & x_n \\
 P &: x_2 & x_1 & x_3 & \dots & x_{n-1} & x_n \\
 Q &: x_2 & x_3 & x_4 & \dots & x_n & x_1 \\
 \sigma &: (x_1)^{-1} & x_2 & x_3 & \dots & x_{n-1} & x_n \\
 U &: x_1x_2 & x_2 & x_3 & \dots & x_{n-1} & x_n.
 \end{aligned}
 \tag{3}$$

We now give the modifications of the relations for the case  $n = 3$ . From  $Q^3 = e$ ,  $R_7$ , one finds that relations  $R_9$  and  $R_{10}$  become equivalent and that  $R_{14}$  is trivial. With the help of (3) one finds that  $R_{13}$  and  $R_{16}$  are not valid and must be dropped for  $\Phi_3$ .

We have arranged the relations in an order such that the group  $\Phi_2 := \text{Aut}(F_2)$  which acts only on  $\langle x_1, x_2 \rangle$  is given by

$$\Phi_2 := \langle P, U, \sigma \mid R_1 \dots R_5 \rangle.
 \tag{4}$$

### 3. New generators and relations

In this section we define a group in terms of generators and relations, which in section 4 is shown to be isomorphic to the group  $\Phi_3 = \text{Aut}(F_3)$  of the free group  $F_3$ .

*Definition 2.* The group  $\Phi'_3$  is defined in terms of five generators and 20 relations  $Q_i$  as given below:

$$\Phi'_3 := \langle c_{12}, c_{23}, c_{34}, \sigma_1, c_2 \mid Q_1 \dots Q_{20} \rangle.
 \tag{5}$$

We shall arrange the relations  $Q_i$  into sets which determine certain subgroups of  $\Phi'_3$ .

The first set of relations determines a Coxeter group  $A_3$ :

$$\begin{aligned}
 A_3 &: \langle c_{12}, c_{23}, c_{34} \rangle \\
 (c_{ii+1})^2 &= e & i = 1, 2, 3 & (Q_1, Q_2, Q_3) \\
 (c_{12}c_{23})^3 &= e & (c_{23}c_{34})^3 &= e & (Q_4, Q_5) \\
 c_{12} &= c_{34} & (Q_6).
 \end{aligned}
 \tag{6}$$

In the standard notation for Coxeter groups [4], each generator carries a single index. Here we use the isomorphism  $A_n \sim S_{n+1}$  and interpret the generators of  $A_3$  as transpositions with respect to the pair of indices  $(i, i + 1)$ . Moreover we shall denote a general transposition of the pair of indices  $(i, j)$  by  $c_{ij} = c_{ji} \in A_3$ . The second set of relations determines a Coxeter group  $B_3$ :

$$\begin{aligned}
 B_3 &:= \langle c_{34}, c_{13}, \sigma_1 \rangle \\
 (c_{34})^2 &= (c_{13})^2 = e \\
 (\sigma_1)^2 &= e \quad (Q_7) \\
 (c_{34}c_{13})^3 &= e \quad (7) \\
 (c_{13}\sigma_1)^4 &= e \quad (Q_8) \\
 c_{34} &\equiv \sigma_1 \quad (Q_9) \\
 c_{13} &:= c_{12}c_{23}c_{12}.
 \end{aligned}$$

Note that  $A_3 \cap B_3 = A_2$  and that part of the equations arise already from  $Q_1 \dots Q_6$ .

The third set of relations is connected with subgroups of  $\Phi'_3$  described in definition 3 and in section 5.

$$\sigma_1 \equiv c_{23}(\sigma_1 c_{13})^2 c_{23} \quad (Q_{10}) \quad (8)$$

$$\sigma_1 \equiv c_{14}c_{23}\sigma_1 c_{23}c_{14} \quad (Q_{11}). \quad (9)$$

*Definition 3.* We define a subgroup  $\Psi_4 < \Psi'_3$  by

$$\Psi_4 := \langle c_{12}, c_{23}, c_{34}, \sigma_1 \mid Q_1 \dots Q_{11} \rangle. \quad (10)$$

This subgroup has only the first four generators of  $\Phi'_3$  and all the relations between them.

Now we turn to subgroups of  $\Phi'_3$  isomorphic to  $\Phi_2$ .

*Proposition 4.* The subgroup of  $\Phi'_3$  generated by  $\langle c_{23}, c_{13}, \sigma_1 \rangle$  fulfills the relations

$$\begin{aligned}
 (c_{23})^2 &= (c_{13})^2 = (\sigma_1)^2 = e \\
 (c_{23}c_{13})^3 &= e \\
 (c_{13}\sigma_1)^4 &= e \quad (Q_8) \\
 \sigma_1 &\equiv c_{23}(c_{13}\sigma_1)^2 c_{23} \quad (Q_{10}).
 \end{aligned} \quad (11)$$

and is a subgroup of  $\Psi_4$  isomorphic to  $\Phi_2$ .

*Proof.* The relations of (11) follow from  $Q_1 \dots Q_5, Q_7$ . It was shown in [8] that a group with three generators and the relations given in (11) is isomorphic to  $\Phi_2$ . Clearly the three generators  $\langle c_{23}, c_{13}, \sigma_1 \rangle$  generate a subgroup of  $\Psi_4$  given in definition 3.  $\square$

We turn to relations involving the generator  $c_2$ . It is an involution, hence we require

$$(c_2)^2 = e \quad (Q_{12}). \quad (12)$$

The next relations are given in terms of the elements

$$X_1 := c_2 c_3 c_{13} c_2 \quad X_2 := c_2 c_{23} \quad c_3 := c_{12} c_2 c_{12}. \quad (13)$$

For the two elements  $X_1, X_2$  we require as the fourth set of relations the following transformations under conjugation  $(g, X) \rightarrow X^g := gXg^{-1}$  with  $\langle c_2, c_3, \sigma_1 \rangle$ :

$$\begin{aligned}
 (X_1)^{c_2} &= X_1 X_2 & (X_2)^{c_2} &= (X_2)^{-1} & (Q_{13}, Q_{14}) \\
 (X_1)^{c_3} &= (X_2)^{-1} & (X_2)^{c_3} &= (X_1)^{-1} & (Q_{15}, Q_{16}) \\
 (X_1)^{\sigma_1} &= (X_1)^{-1} & (X_2)^{\sigma_1} &= X_2 & (Q_{17}, Q_{18}).
 \end{aligned} \quad (14)$$

The notation  $X_1, X_2$  will be explained later.

*Proposition 5.* The subgroup of  $\Phi'_3$  generated by  $\langle c_2, c_3, \sigma_1 \rangle$ , with relations obtained from (11) by the replacement

$$c_{23} \rightarrow c_2 \quad c_{13} \rightarrow c_3 \quad \sigma_1 \rightarrow \sigma_1 \tag{15}$$

is isomorphic to  $\Phi_2$ .

*Proof.* The proof involves a transformation from the generators given in proposition 4 and uses the relations of (14). From (13) we find

$$c_{23} = c_2 X_2 \quad c_{13} = c_3 X_1 X_2. \tag{16}$$

Inserting these expressions into the relations of (11) and using the conjugation properties (14) of  $X_1, X_2$  in each case, one finds that all these relations are valid under the replacement (15). As an example we consider

$$\begin{aligned} e &= (c_{23}c_{13})^3 \\ &= (c_2 X_2 c_3 X_1 X_2)^3 \\ &= (c_2 c_3 X_2)^3 \\ &= (c_2 c_3)^3 (c_2 c_3)^{-2} X_2 (c_2 c_3)^2 (c_2 c_3)^{-1} X_2 (c_2 c_3) X_2 \\ &= (c_2 c_3)^3 (X_2^{-1} X_1^{-1}) X_1 X_2 \\ &= (c_2 c_3)^3. \end{aligned} \tag{17}$$

All the relations together determine a group  $\Phi_2$ . □

The two subgroups of propositions 4, 5 are isomorphic but not conjugate to one another. For the conjugation of the generator  $\sigma_1$  with elements from  $A_3$  we introduce the notation  $\sigma_{212} := \sigma_1$ . In view of the stability (equation (7))  $Q_9$  of  $\sigma_{212}$  under  $c_{34}$ , there are altogether 12 conjugates of  $\sigma_1$  under  $A_3$  which we denote by

$$i \neq j : \sigma_{ij} := (\sigma_{212})^{c_i c_j}. \tag{18}$$

Finally we require two more relations between  $c_2$  and generators not in  $\Phi_2$ :

$$\begin{aligned} c_2 &\equiv \sigma_{343} = (\sigma_1)^{c_4 c_3} & (Q_{19}) \\ c_{23} &= c_2 \sigma_2 q & (Q_{20}) \\ q &:= c_{23} c_{14} c_2 c_{14} c_{23} \\ \sigma_2 &:= c_3 \sigma_1 c_3. \end{aligned} \tag{19}$$

#### 4. Isomorphism with $Aut(F_3)$

In this section we relate  $\Phi'_3$  to  $\Phi_3 = Aut(F_3)$ . First we relate the sets of generators, then we derive the Nielsen relations of section 2 from the relations  $Q_1 \dots Q_{20}$  and thus prove the isomorphism of  $\Phi'_3$  with  $Aut(F_3)$ . The proofs are independent of the action of  $Aut(F_3)$  on  $F_3$ .

The group  $\Phi'_3$  contains two distinct subgroups isomorphic to  $\Phi_2$  (compare proposition 4, 5). Nielsen's  $\Phi_2$  is identified by

*Lemma 6.* Upon setting

$$\sigma = \sigma_1 \quad P = \sigma_1 c_3 \sigma_1 \quad U = c_3 \sigma_1 c_3 c_2 \quad c_3 := c_2 c_{12} c_2 \tag{20}$$

and using the relations  $Q_1 \dots Q_{18}$ , the Nielsen relations  $R_1 \dots R_5$  are fulfilled, and the subgroup  $\Phi_2 = \langle c_2, c_3, \sigma_1 \rangle$  is generated.

*Proof.* The lemma is obtained from proposition 5 derived from  $Q_{13} \dots Q_{18}$  and from the transformations (20). The Nielsen relations then follow as given in [8], proposition 1.  $\square$

*Lemma 7.* Define the Coxeter group conjugate to  $B_3$  with generators

$$P_{23} := (c_{34})^{c_2 c_{23} \sigma_1} \quad P_{12} := (c_{13})^{c_2 c_{23} \sigma_1} \quad \sigma_1 = (\sigma_1)^{c_2 c_{23} \sigma_1}. \quad (21)$$

Then with the transformations

$$P := P_{12} \quad Q := P_{23} P_{12} \quad \sigma = \sigma_1 \quad (22)$$

the Nielsen relations  $R_1, R_2, R_6 \dots R_{11}$  are fulfilled.

*Proof.* Clearly a conjugation transformation preserves the commutator properties of the group  $B_3$ . Next we note that the expressions for  $P$  given in (20) and (22) agree by use of  $Q_{18}$ . The Nielsen relations  $R_1, R_2, R_6 \dots R_{11}$  involve only the generators  $P, Q, \sigma$ . It is easy to see that they arise from the Coxeter group  $B_3$ , hence from  $Q_1 \dots Q_{11}$  and equations (21), (22), and yield this group in Nielsen form.  $\square$

The two-index notation for  $B_3$  introduced in lemma 7 anticipates the action of this group on the generators of  $F_3$ , but it has no simple relation with the two-index notation for  $A_3$  introduced in (6). For later use we note that from (13), (14),  $Q_{18}$  we have

$$c_2 c_{23} \sigma_1 = \sigma_1 c_2 c_{23} \quad (23)$$

which allows us to rewrite equation (21) in the form

$$P_{23} = (c_{24})^{\sigma_1 c_2} \quad P_{12} = (c_{12})^{\sigma_1 c_2} \quad \sigma_1 = (\sigma_{313})^{\sigma_1 c_2}. \quad (24)$$

Taking the group  $B_3$  in Nielsen form and using equations (19), (23) one finds

$$\sigma_2 = P_{12} \sigma_1 P_{12} \quad \sigma_3 := P_{23} \sigma_2 P_{23}. \quad (25)$$

The elements  $\sigma_i$  are easily shown to commute with one another. They are permuted under conjugation with the permutations of  $B_3$ .

With the expressions of lemmas 6 and 7, the Nielsen generators are given as functions of the generators (5) of  $\Phi'_3$ . We turn now to the inverse transformations.

*Proposition 8.* The generators of  $\Phi'_3$  can be expressed as functions of the Nielsen generators.

*Proof.* From the subgroup  $\Phi_2$  of lemma 6 one finds (cf [8]) the expressions

$$\sigma_1 = \sigma \quad c_2 = \sigma P \sigma P \sigma U \quad c_3 = \sigma P \sigma. \quad (26)$$

We obtain by conjugation from (24)

$$c_{12} = c_2 \sigma P_{12} \sigma c_2 \quad c_{24} = c_2 \sigma P_{23} \sigma c_2. \quad (27)$$

With  $P_{12} = P, P_{23} = QP$  and (26), the right-hand sides of (27) become functions of the Nielsen generators. With  $c_{14} = c_{12} c_{24} c_{12}$  we get this transposition as a function of Nielsen generators. From  $Q_{20}$ , (A1) and (29) one may now write the generator  $c_{23}$  as a function of the Nielsen generators. Since  $c_{34} = c_{23} c_{14} c_{23}$ , we can then express the five generators of  $\Phi'_3$  as functions of the Nielsen generators.  $\square$

*Proposition 9.* The generators of  $\Phi'_3$  act on the free group  $F_3$  according to

$$\begin{aligned}
 e &: x_1 & x_2 & x_3 \\
 c_{12} &: (x_1)^{-1} & x_1x_2 & x_3 \\
 c_{23} &: x_1x_2 & (x_2)^{-1} & x_2x_3 \\
 c_{34} &: x_1 & x_2x_3 & (x_3)^{-1} \\
 \sigma_1 &: (x_1)^{-1} & x_2 & x_3 \\
 c_2 &: x_1x_2 & (x_2)^{-1} & x_3.
 \end{aligned} \tag{28}$$

*Proof.* We use proposition 8 to pass to the Nielsen generators and equation (3) to find the action on  $F_3$ .  $\square$

*Lemma 10.* The Nielsen relations (2),  $R_{12} \dots R_{18}$  follow by transforming with proposition 8 to the generators of  $\Phi'_3$  and use of the relations  $Q_1 \dots Q_{20}$ .

*Proof.* See appendix A.

*Proposition 11.* The groups

$$\begin{aligned}
 \Phi_3 &= \langle P, Q, \sigma, U \mid R_1 \dots R_{18} \rangle \\
 \Phi'_3 &= \langle c_{12}, c_{23}, c_{34}, \sigma_1, c_2 \mid Q_1 \dots Q_{20} \rangle
 \end{aligned} \tag{29}$$

are isomorphic.

*Proof.* From lemma 10, it follows that  $\Phi'_3 \leq \Phi_3$ . Through the expressions of proposition 9, it can be checked that relations  $Q_1 \dots Q_{20}$  of  $\Phi'_3$  hold true in terms of actions on  $F_3$ . It follows that  $\Phi'_3$  produces no relations beyond  $\Phi_3$ , hence  $\Phi'_3$  is isomorphic to  $\Phi_3$ .  $\square$

## 5. Subgroups of $Aut(F_3)$

The generators for  $\Phi_3$  given in section 3 were already adapted to the subgroups  $A_3$ ,  $B_3$  and  $\Phi_2$ . In the latter case we found two isomorphic but non-conjugate subgroups. Their relation may be interpreted by deriving the action of the group elements  $X_1, X_2$  from (13) and (28). One finds

$$\begin{aligned}
 e &: x_1 & x_2 & x_3 \\
 X_1 &: x_1 & x_2 & x_1x_3 \\
 X_2 &: x_1 & x_2 & x_2x_3.
 \end{aligned} \tag{30}$$

It is easy to see that these two elements of  $\Phi_3$  generate a subgroup isomorphic to  $F_2$ . Considering now the action of  $\Phi_2$  by conjugation on  $X_1, X_2$  given in (14), one finds that  $F_2 = \langle X_1, X_2 \rangle$  may be combined with  $\Phi_2 = \langle c_2, c_3, \sigma_1 \rangle$  into a semidirect product  $F_2 \rtimes \Phi_2$  in which the factor  $F_2$  is an invariant subgroup.

A different type of subgroup is found within  $\Psi_4$ :

*Proposition 12.* In the group  $\Psi_4$ , the elements

$$\begin{aligned}
 S_1 &:= \sigma_{121}\sigma_{131}\sigma_{141} & S_2 &:= \sigma_{212}\sigma_{232}\sigma_{242} \\
 S_3 &:= \sigma_{313}\sigma_{323}\sigma_{343} & S_4 &:= \sigma_{414}\sigma_{424}\sigma_{434}
 \end{aligned} \tag{31}$$

are involutive and generate a normal subgroup  $\mathcal{A}_4$ . The conjugation properties of the elements (31) under  $p \in A_3$  and  $\sigma_1$  are

$$(S_i)^p = S_{p(i)} \tag{32}$$

$$(S_1)^{\sigma_1} = S_2S_1S_2 \quad (S_2)^{\sigma_1} = S_2 \quad (S_3)^{\sigma_1} = S_3 \quad (S_4)^{\sigma_1} = S_4. \tag{33}$$

*Proof.* From  $Q_8$  one finds that  $(c_{13}\sigma_1)^2 = (\sigma_1c_{13})^2$  so that  $\sigma_{212} \rightleftharpoons \sigma_{232}$ . By conjugation with  $c_{34}$  and use of  $Q_9$ , one finds  $\sigma_{212} \rightleftharpoons \sigma_{242}$  and, by conjugation with  $c_{14}$ ,  $\sigma_{242} \rightleftharpoons \sigma_{232}$ . Hence  $S_2$  is a product of three commuting involutions so that  $(S_2)^2 = e$ . Since  $S_1, S_3, S_4$  can be obtained from  $S_2$  by conjugation, they are also involutions. To examine the normal property it suffices to conjugate the  $S_i$  with the four generators of  $\Psi_4$ . Under  $A_3$ , one easily finds that  $S_1, S_2, S_3, S_4$  are permuted as given in (35). Under  $\sigma_1$  one finds with the help of  $Q_{10}, Q_{11}$  and their conjugates the results of (36). Since the conjugates under all the generators of  $\Psi_4$  are expressed by  $S_1, S_2, S_3, S_4$ , the normal property follows.  $\square$

From this group we pass to the following proposition.

*Proposition 13.* The subgroup  $\mathcal{F}_3 = \langle T_1, T_2, T_3 \rangle$

$$T_1 = S_1S_2 \quad T_2 = S_2S_3 \quad T_3 = S_3S_4, \tag{34}$$

written in terms of the involutive generators of  $\mathcal{X}_4$ , is the normal subgroup  $Inn(F_3) \triangleleft Aut(F_3)$  of inner automorphisms in  $\Phi_3$  and is isomorphic to  $F_3$ . Under conjugation with the generators of  $Aut(F_3)$ , the transformation laws are

$$\begin{aligned} T_i &: T_1 & T_2 & T_3 \\ (T_i)^{c_{12}} &: (T_1)^{-1} & T_1T_2 & T_3 \\ (T_i)^{c_{23}} &: T_1T_2 & (T_2)^{-1} & T_2T_3 \\ (T_i)^{c_{34}} &: T_1 & T_2T_3 & (T_3)^{-1} \\ (T_i)^{\sigma_1} &: (T_1)^{-1} & T_2 & T_3 \\ (T_i)^{\sigma_2} &: T_1T_2 & (T_2)^{-1} & T_3 \end{aligned} \tag{35}$$

Moreover the generators  $\langle T_1, T_2, T_3 \rangle$  are the images of  $\langle x_1, x_2, x_3 \rangle$  under the isomorphism.

*Proof.* See appendix B.

Computation of the action of  $\langle T_1, T_2, T_3 \rangle$  on  $F_3$  shows that these automorphisms generate the inner automorphisms  $T_i : w \rightarrow (w)^{x_i^{-1}}$ ,  $i = 1, 2, 3$  respectively. For any free group,  $Inn(F_n)$  is isomorphic to  $F_n$ . Comparing the action (35) of the generators by conjugation on  $\langle T_1, T_2, T_3 \rangle$  with their action on  $\langle x_1, x_2, x_3 \rangle$  given in (28), one finds the correspondence  $T_i \sim x_i$  under this isomorphism.

### 6. Towards non-commutative crystallography

As one possible field of applications we indicate here the elements of non-commutative (NC) crystallography. The subgroups of  $Aut(F_3)$  given in the previous sections allow one to construct generalized notions for the translation, point and space groups of standard crystallography.

From proposition 13, an isomorphic image of the free group  $F_3$  appears in  $Aut(F_3)$  as the normal subgroup  $\mathcal{F}_3$ . We interpret this normal subgroup as an NC translation group  $\mathcal{T} := \mathcal{F}_3 = \langle T_1, T_2, T_3 \rangle$  with the following motivation:

- (i) By the homomorphism  $hom_1 : F_3 \rightarrow Z^3$  called abelianization,  $F_3$  and hence  $\mathcal{T}$  maps into the Abelian group  $Z^3$  with three generators, isomorphic to a translation group.
- (ii) By extending the affine representation given in [8] from  $Aut(F_2)$  to  $Aut(F_3)$ , it can be shown that the generators  $\langle T_1, T_2, T_3 \rangle$  admit a representation by discrete shifts on a 3D lattice. Any closed path formed from discrete shifts represents an element from the kernel  $ker(hom_1)$ .



There is a second homomorphism  $hom_2 : Aut(F_3) \rightarrow Gl(3, Z)$  [9] which links automorphisms to symmetry transformations on a lattice. Moreover the two Coxeter subgroups given in section 3 (6),(7) are isomorphic to crystallographic point groups,  $A_3 = T_d = \bar{4}3m$ ,  $B_3 = O_h = m\bar{3}m$ . They may then be taken as *finite point groups* in NC crystallography.

Clearly the generators of these groups must map by conjugation  $\mathcal{T} \rightarrow \mathcal{T}$ . It is not difficult to check that the subgroup  $\mathcal{T}$ , combined with each one of these point groups, fulfills the condition for a semidirect product in which the subgroup  $\mathcal{T}$  is normal. This allows one to introduce the two NC *symmorphic space groups*  $\mathcal{T} \times_s A_3$  and  $\mathcal{T} \times_s B_3$ .

We have then within  $Aut(F_3)$  all the elements of a NC crystallography in which the commutativity of the translation group is broken and the point symmetry can be preserved. Quasicrystals lack the periodicity of crystals and therefore display a type of order where this scheme may apply. To implement it one should explore within this scheme production rules that can describe quasicrystals (cf [2]).

### 7. Conclusion

We have given new involutive generators and relations for  $Aut(F_3)$ . The new generators for  $Aut(F_3)$  are adapted to some finite and infinite subgroups. In all cases we give the explicit generators of these subgroups. The new relations lead to an interpretation of the relations given by Nielsen: they are closely connected to the existence of certain (normal) subgroups of  $Aut(F_3)$ .

We indicate the generalization to  $n \geq 3$ : the finite Coxeter groups  $A_n$  and  $B_n$  appear in full analogy as subgroups of  $Aut(F_n)$ . This is shown in [1] for  $A_n$  and from Nielsen [9, 10] clearly for  $B_n$ . Both these subgroups together generate a subgroup  $\Psi_{n+1}$  which generalizes the group  $\Psi_4$  of definition 3. Their intersection is  $A_n \cap B_n = A_{n-1}$ .  $\Psi_{n+1}$  has a normal subgroup  $\mathcal{X}_{n+1}$  which generalizes  $\mathcal{X}_4$  of proposition 12, and  $\mathcal{X}_{n+1}$  has a subgroup normal in  $Aut(F_n)$  which is  $Inn(F_n)$  and isomorphic to  $F_n$ . In  $Aut(F_3)$ , the new generator  $c_2$  appeared which does not belong to  $\Psi_4$ . The case  $n = 2$  is special since then  $Aut(F_2) \sim \Psi_3$  (cf [8]).

### Appendix A. Derivation of the Nielsen relations and proof of lemma 10

Since  $R_1 \dots R_{11}$  have previously been treated, it suffices to consider the remaining relations  $R_{12} \dots R_{20}$ . Of these,  $R_{14}$  is trivial and  $R_{13}, R_{16}$  are not valid for  $n = 3$ . We turn to the remaining relations  $R_{12}, R_{15}, R_{17}$  and  $R_{18}$ .

$R_{12}$ :

To deal with  $R_{12}$  we need an important intermediate result from relation  $Q_{20}$ . We multiply from the right with  $c_{23}$  and obtain for  $c_{14}c_{23}$  the expression

$$\begin{aligned} c_{14}c_{23} &= \sigma_2 c_2 c_{14} c_2 \\ &= \sigma_2 \sigma_1 (c_{14})^{\sigma_1 c_2} \sigma_1 \\ &= (\sigma_1 \sigma_2 \sigma_3) P_{13}. \end{aligned} \tag{A1}$$

We used the relations of (24), (25) from  $B_3$  in Nielsen form in the last step. Expression (A1) is remarkable since the left-hand side is an element of  $A_3$ , while the right-hand side is an element of  $B_3$  in Nielsen form.

To construct the left-hand side of  $R_{12}$  we start from  $c_{34} = c_{24}c_{23}c_{24}$  and obtain by use of the relations for  $B_3$  in Nielsen form and by those indicated to the right

$$\begin{aligned}
 (c_{34})^{\sigma_1 c_2} &= P_{23}(c_{23})^{\sigma_1 c_2} P_{23} \\
 &= P_{23} \sigma_1 c_2 (c_{14} c_{23} c_2 c_{23} c_{14} \sigma_2 c_2) c_2 \sigma_1 P_{23} \quad (Q_{20}) \\
 &= P_{23} (\sigma_1 \sigma_2 \sigma_3) (\sigma_2 c_2) P_{13} \sigma_2 c_2 P_{13} (\sigma_1 \sigma_2 \sigma_3) \sigma_2 \sigma_1 P_{23} \quad (Q_{19}) \quad (A2) \\
 &= (\sigma_1 \sigma_2 \sigma_3) (P_{23} (\sigma_2 c_2) P_{23}) (P_{23} P_{13} \sigma_2 c_2 P_{13} P_{23}) (\sigma_1 \sigma_2) \\
 &= (\sigma_1 \sigma_2 \sigma_3) (P Q^{-1} U Q P) (Q^{-1} U Q) (\sigma_1 \sigma_2).
 \end{aligned}$$

In the last steps we used the expression  $U = c_3 \sigma_1 c_3 c_2 = \sigma_2 c_2$  and equation (22).

To construct the right-hand side of  $R_{12}$  we use  $c_{34} = c_{14} c_{23} c_{12} c_{23} c_{14}$  and derive from (20) and  $\Phi_2$ , lemma 6,

$$c_{12} = c_3 c_2 c_3 = \sigma_2 P_{12} \sigma_2 c_2 P_{12} \sigma_1 \sigma_2. \quad (A3)$$

Inserting this expression and using (A1) we find

$$\begin{aligned}
 (c_{34})^{\sigma_1 c_2} &= \sigma_1 c_2 (\sigma_1 \sigma_2 \sigma_3) P_{13} (\sigma_2 P_{12} \sigma_2 c_2 P_{12} \sigma_1) P_{13} (\sigma_1 \sigma_2 \sigma_3) c_2 \sigma_1 \\
 &= (\sigma_1 \sigma_2 \sigma_3) \sigma_2 c_2 P_{13} P_{12} \sigma_2 c_2 P_{12} P_{13} c_2 \sigma_2 (\sigma_1 \sigma_2) \quad (Q_{19}) \quad (A4) \\
 &= (\sigma_1 \sigma_2 \sigma_3) (U Q^{-1} U Q U^{-1}) (\sigma_1 \sigma_2).
 \end{aligned}$$

By equating the final expressions (A2) and (A4), and taking out the same factors on the left and on the right, we obtain relation  $R_{12}$ .

$R_{15}$ :

This relation may be rewritten with (25) and  $\sigma_2$  from (19) in the form

$$\sigma_2 c_2 \rightleftharpoons \sigma_3. \quad (A5)$$

Since from (25)  $\sigma_2 \rightleftharpoons \sigma_1$ ,  $\sigma_{343} = \sigma_3 \rightleftharpoons \sigma_1$ ,  $R_{15}$  reduces to  $c_2 \rightleftharpoons \sigma_{343}$ , which is  $Q_{19}$ .

$R_{17}$ :

To prove  $R_{17}$  we rewrite the left-hand side using (A1), by the steps

$$\begin{aligned}
 Q(\sigma_3 c_{34}) Q^{-1} &= P_{12} P_{13} (\sigma_3 c_{34}) P_{13} P_{12} \\
 &= (\sigma_1 \sigma_2 \sigma_3) P_{12} c_{14} c_{23} (\sigma_3 c_{34}) c_{23} c_{14} P_{12} (\sigma_1 \sigma_2 \sigma_3) \quad (A6) \\
 &= \sigma_2 c_2 = U
 \end{aligned}$$

where commutators from  $\Phi_2$ , lemma 6 were used in the last step. The right-hand side is transformed with lemma 6 as

$$P_{23} \sigma U \sigma P_{23} = Q(c_{12} \sigma_1) Q^{-1} \quad (A7)$$

so that  $R_{17}$  is equivalent to

$$R_{17} : \sigma_3 c_{34} \rightleftharpoons c_{12} \sigma_1. \quad (A8)$$

This relation can be shown from relations in  $B_3$  (7) and their conjugates, and from relations in  $A_3$  (6).

$R_{18}$ :

This relation in  $\Phi_3$  becomes

$$R_{18} : U \rightleftharpoons P_{13}UP_{13}. \tag{A9}$$

With the help of (A1), the right-hand side can be rewritten as

$$P_{13}\sigma_2c_2P_{13} = \sigma_3q\sigma_2\sigma_3. \tag{A10}$$

With  $Q_{19}$  we get the equivalent form

$$R_{18} : \sigma_2c_2 \rightleftharpoons q\sigma_2 (Q_{19}, Q_{20}). \tag{A11}$$

In this form, the relation can be derived from  $Q_{20}$ , rewritten as

$$c_{23} = c_2\sigma_2q = q\sigma_2c_2. \tag{A12}$$

□

Note that relations  $Q_{19}, Q_{20}$ , not related to one of the subgroups  $\Phi_2, A_3, B_3$ , are needed in the proof and hence are implicit in the Nielsen relations.

### Appendix B. The normal subgroup $\langle T_1, T_2, T_3 \rangle$ ; proof of proposition 13

The conjugation with the first four generators of  $Aut(F_3)$  follows from proposition 12 and (34). It suffices to conjugate the three group elements with the remaining generator  $c_2$ . For this purpose we factorize the elements  $S_i, i = 1, 2, 3$  into a first factor from the group  $\Phi_2 = \langle c_2, c_3, \sigma_1 \rangle$  of lemma 6 and a second factor with simple conjugation properties under  $\Phi_2$ . These factorizations become

$$\begin{aligned} S_1 &= v_1(X_1X_2)^2\sigma_{141} & v_1 &= c_1\sigma_1\sigma_2c_1 & \sigma_{141} &= (X_1X_2)^{-1}\sigma_{343}(X_1X_2) \\ S_2 &= v_2(X_2)^2\sigma_{242} & v_2 &= \sigma_1\sigma_2 & \sigma_{242} &= (X_2)^{-1}\sigma_{343}X_2. \\ S_3 &= v_3\sigma_{343} & v_3 &= c_2\sigma_1\sigma_2c_2 \end{aligned} \tag{B1}$$

Note that  $\sigma_{343}$  from relations  $Q_9, Q_{11}, Q_{19}$  commutes with all elements of  $\Phi_2$ . Under conjugation with  $c_2$  we get

$$(S_i)^{c_2} : \quad \begin{matrix} S_1 & S_2 & S_3 \\ v_1X_1\sigma_{343}X_1 & v_3(X_2)^{-1}\sigma_{343}(X_2)^{-1} & v_2\sigma_{343}. \end{matrix} \tag{B2}$$

Next we derive for the automorphisms  $X_1, X_2$  defined in (16) the relations

$$\sigma_{343}X_i\sigma_{343} \rightleftharpoons X_j \quad ij = 11, 22, 12, 21. \tag{B3}$$

For  $i = j$ , equation (B3) follows from relation  $Q_{10}$ , written in terms of the generators of  $\Phi_2$ , and for  $ij = 21$  from conjugates of (A8). Using equations (B1)–(B3) and conjugations under  $\Phi_2$  one finds

$$\begin{aligned} (S_1S_2)^{c_2} &= S_1S_3 = (S_1S_2)(S_2S_3) \\ (S_2S_3)^{c_2} &= S_3S_2. \end{aligned} \tag{B4}$$

To conjugate  $S_3S_4$  we make use of

$$S_3S_4 = c_{14}c_{23}S_2S_1c_{23}c_{14} \quad c_2 = c_{14}c_{23}q c_{23}c_{14} \quad q = \sigma_2c_2c_{23} \tag{B5}$$

to derive

$$(S_2S_1)^q = (S_2S_1) \leftrightarrow (S_3S_4)^{c_2} = S_3S_4. \tag{B6}$$

Equations (B4), (56) together with (34) yield the last row of (35) for  $\langle T_1, T_2, T_3 \rangle$  and lead to the normal property of the subgroup generated by them. □

## References

- [1] Garcia-Escudero J and Kramer P 1993 *Anales de Fisica, Monografias* **1**, vol 1 (Madrid) pp 339–42
- [2] Garcia-Escudero J and Kramer P 1993 *J. Phys. A: Math. Gen.* **26** L1029–35
- [3] Garcia-Escudero J and Kramer P 1993 *Proc. Int. Wigner Symposium* (Oxford)
- [4] E J Humphreys 1990 *Reflection Groups and Coxeter Groups* (Cambridge: Cambridge University Press)
- [5] Kramer P 1993 *Anales de Fisica, Monografias* **1**, vol 2 (Madrid) pp 370–3
- [6] Kramer P 1993 *J. Phys. A: Math. Gen.* **26** 213–28
- [7] Kramer P 1993 *J. Phys. A: Math. Gen.* **26** L245–50
- [8] Kramer P 1994 *J. Phys. A: Math. Gen.* **27** 2011–22
- [9] Magnus W, Karras A and Solitar D 1976 *Combinatorial Group Theory* (New York: Dover)
- [10] Nielsen J 1924 *Math. Ann.* **91** 169–209