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Space groups on the quantum torus

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Abstract. Space groups in two dimension arise from the commutative translation group Z^2 and its automorphisms in GL(2, Z). From the free group F_2 and its automorphisms we construct 17 non-commutative groups and their homomorphisms to the 17 space groups with commutative translations.

1. Introduction

Any crystallographic space group G in 2D acts on the plane R^2 and admits a translation group with two commuting and independent generators. The translation group is isomorphic to Z^2 . The transversal (set of orbit representatives) of the action of the subgroup $Z^2 < G$ on R^2 is the unit cell R^2/Z^2 which, upon appropriate identification of the edges, becomes the torus. The two generators of Z^2 generate the homotopy group of the torus.

A non-commutative scheme is obtained if the translation group Z^2 is replaced by the free group F_2 with two generators $\langle x_1, x_2 \rangle$. In the context of non-commutative geometry with operator algebras proposed by Connes [1], the action and group algebra of F_2 have led to the notion of a 'quantized torus', cf Effros [2] and [1, p340-7]. Note that this differs from the concept of a quantum group which involves a deformation parameter.

In crystallographic terms, the group Z^2 associated with the torus is denoted by P1. We denote its non-commutative generalization associated with the quantum torus by $P1 = F_2$ and look for other non-commutative space groups. We construct groups which

(1) admit an at least two-generator subgroup of F_2 , and

(2) admit a homomorphism to one of the 17 space groups of 2D crystallography.

2. The automorphisms of the free group

We shall work with elements and subgroups of $\operatorname{Aut}(F_n)$ and its action on F_n . Nielsen [4] showed that $\operatorname{Aut}(F_n)$ is finitely generated. We shall use the involutive generators and the subgroup relations given in [5]. For general n, the group F_n is isomorphic to $\operatorname{Inn}(F_n)$. We denote by (T_1, T_2, \ldots) the images in $\operatorname{Aut}(F_n)$ of the generators (x_1, x_2, \ldots) under this isomorphism and interpret them as non-commutative translations. There are no finite-order elements in $\operatorname{Inn}(F_n)$, so we must look for them in the cosets. A method for finding the elements $g \in \operatorname{Aut}(F_n)$ of finite order is described by McCool [7]. For $H < \operatorname{Aut}(F_n)$ of finite order, we can construct the semidirect product subgroup ($\operatorname{Inn}(F_n) \times_s H$) $< \operatorname{Aut}(F_n)$ which we call a symmorphic NC space group. The relation to crystallographic space groups

is governed by the two homomorphisms

hom₁:
$$F_n \to Z^n$$

hom₂: Aut $(F_n) \to GL(n, Z)$.

Given an element of F_n , that is a word $w(x_1, x_2, ...)$, its image under the Abelianization hom₁ is found from the power sums $(n_1(w), n_2(w), ...)$ of the generators $x_1, x_2, ...$ in w. An automorphism $\phi \in \operatorname{Aut}(F_n)$ is specified by giving the images $y_1(x_1, x_2, ...), y_2(x_1, x_2, ...), \ldots$. We compose automorphisms according to Nielsen [4]. The image of ϕ under hom₂ is an $n \times n$ element from the matrix group GL(n, Z) whose entries are the power sums. In what follows we consider n = 2, 3.

3. 17 non-commutative space groups

The homomorphism hom₂ allows one to search for preimages of the space groups in the plane. A candidate for a non-commutative space group found in this way will be denoted by $\mathcal{G} < \operatorname{Aut}(F_2)$. The 17 space groups in the plane were described in terms of sets of generators and relations by Coxeter and Moser [8]. We construct a preimage \mathcal{G} for each space group G, with the same set of generators as Coxeter and Moser. The relators \mathcal{R} are checked within $\operatorname{Aut}(F_2)$ and fall into two classes: relators \mathcal{R}_1 equal to unity both in \mathcal{G} and in G, and relators \mathcal{R}_2 , equal to unity in G. The pairs of space groups are then $\mathcal{G} = \langle \ldots | \mathcal{R}_1, \mathcal{R}_2 \rangle$, respectively. The relators \mathcal{R}_2 determine in \mathcal{G} the kernel ker(hom) $\triangleleft \mathcal{G}$ of the specific homomorphism hom: $\mathcal{G} \to G$. We show that the relators \mathcal{R}_2 can always be reduced to the commutator $K((T_1)^{\pm 1}, (T_2)^{\pm 1})$, even if T_1, T_2 do not belong to the non-commutative translation group of \mathcal{G} . Any space group G is now a factor group

 $G = \mathcal{G} / \operatorname{ker}(\operatorname{hom})$.

We give the 17 space groups in the order and notation of the International tables [9]. For each group we first give alternative sets of generators $\langle a \rangle, \langle b \rangle, \ldots$, as in [8], with some changes of notation to avoid symbols used for $\operatorname{Aut}(F_2)$. We use alternative sets of generators to display representative elements for each space group. Under $(\hom)^{-1}$ we give in the next row a preimage in $\operatorname{Aut}(F_2)$ for each generator, compare also section 4. Under \mathcal{R} we give the relators $\mathcal{R} = (\mathcal{R}_1, \mathcal{R}_2)$. In the row that follows we give under ker for the relators \mathcal{R}_2 their expressions in $\operatorname{Aut}(F_2)$. They determine elements of infinite order in \mathcal{G} .

(a) (hom) ⁻¹ \mathcal{R} ker	$X = T_1 = XYX^{-1}Y^{-1} = K(T_1, T_2^{-1})$	$\begin{array}{c} Y\\ T_2^{-1} \end{array}$			(1)
$\mathcal{P}2$ (<i>a</i>) (hom) ⁻¹ \mathcal{R} ker	$\begin{array}{ccc} X & Y \\ T_1 & T_2^{-1} \\ T^2 & T X T \end{array}$	T $\sigma_1 \sigma_2$ $X TYT$	Y XYX K(T ₁	$(-1\gamma^{-1})^{-1}$	(2)
$\langle b angle$ (hom) ⁻¹ \mathcal{R} ker	$U_1 = YT$ S_3 $(U_1)^2$	$U_2 = T$ S_2 $(U_2)^2$	$U_3 = XU_2$ S_1 $(U_3)^2$	$(U_1U_2U_3)^2$ $K(T_2^{-1}, T_1)$	

$$Cm
(a) P Q R
(hom)^{-1} T_{1}c_{13} c_{13}T_{1} c_{13}
\mathcal{R} R^{2} RPRQ^{-1} P^{2}Q^{-2}
ker K(T_{1}, T_{2}^{-1})
(b) R S = PR
(hom)^{-1} c_{13} T_{1}
\mathcal{R} R^{2} (SR)^{2}(RS)^{-2}
ker K(T_{1}, T_{2}^{-1})$$
(5)

6408	P Kramer	
P2mg (a) (hom) ⁻¹ R ker	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	(7)
(b) (hom) ⁻¹ R ker	$V_{1} = PR \qquad V_{2} = QR \qquad R \\ T_{1}c_{13}m'' \qquad c_{13}T_{1}m'' \qquad m'' \\ (V_{1})^{2} \qquad (V_{2})^{2} \qquad R^{2} \qquad (V_{2}RV_{2})^{-1}(V_{1}RV_{1}) \\ \qquad $	
$\mathcal{P}2gg$ (a) (hom) ⁻¹ \mathcal{R} ker (b) (hom) ⁻¹ \mathcal{R} ker	$P \qquad Q \qquad T \\T_{1}c_{13} \qquad c_{13}T_{1} \qquad c_{13}m'' \\T^{2} \qquad TPTQ \qquad P^{2}Q^{-2} \\K(T_{1}, T_{2}^{-1}) \\P \qquad O = PT \\T_{1}c_{13} \qquad T_{1}m'' \\(PO)^{2} \qquad (P^{-1}O)^{2} \\K(T_{1}, T_{2}^{-1}) \\\end{cases}$	(8)

$C2mm \langle a \rangle (hom)^{-1} \mathcal{R} ker \mathcal{R} ker ker$	R_1 $S_1m''S_1$ $(R_1)^2$ $(R_1R_2)^2$ $K(T_1, T_2^{-1})$	$R_2 c_{13} (R_2)^2 (R_2 R_3)^2$	R ₃ m" (R ₃) ² (R ₃ R K(T ₂	$(4)^2$	$R_4 S_1 c_{13} S_1 (R_4)^2 (R_4 R_1)^2$	$T S_1 T^2 TR_1 TR_3$	TR_2TR_4	(9)
$\langle b \rangle$ (hom) ⁻¹ \mathcal{R} ker	$ \begin{array}{cccc} R_1 & R_2 \\ S_1 m'' S_1 & c_1 \\ (R_1)^2 & (R_1)^2 \end{array} $	$ \begin{array}{ccc} 2 & T \\ 3 & S_1 \\ 3_2)^2 & T^2 \end{array} $	(R_1R_2) K(T_1,	$(T_2^{-1})^2$	(R_1TR_2)	<i>T</i>) ²		
$\mathcal{P}4$ $\langle a \rangle$ $(\text{hom})^{-1}$ \mathcal{R} ker \mathcal{R}	$U_1 \\ S_3 \\ (U_1)^2 \\ S^4$	$U_{2} \\ S_{2}S_{1}S_{2} \\ (U_{2})^{2} \\ S^{-i}U_{4}S^{i}U_{i}^{-i}$	-1	U_3 $S_2S_3S_2$ $(U_3)^2$ U_1U_2U	2 /3U4	$U_4 S_1 (U_4)^2$	S c ₁₃ σ ₁	(10)
ker (b) (hom) ⁻¹ R ker	S c ₁₃ σ ₁ S ⁴	$ \begin{array}{c} TU_4 \\ S_1 \\ T^2 \\ K \end{array} $	ST) ⁴ ((T ₂ , T	$K(T_2^{-1})$	', <i>T</i> ₁)			

$\mathcal{P}4mm$								
$\langle a \rangle$	R_1		R_2		R ₃	R_4	R	
(hom) ⁻¹	$\sigma_2 T_2$		σ_1		σ_2	$T_1\sigma_1$	c_{13}	
\mathcal{R}	$(R_1)^2$		$(R_2)^2$		$(R_3)^2$	$(R_4)^2$	R^2	
ker	,		/					(11)
R	$(R_1 R_2)$	2	$(R_2 R_3)^2$		$(R_2 R_4)^2$	$(R_{A}R_{1})^{2}$		()
ker	(12)		(25)		()4/	$K(T, T^{-1})$		
\mathcal{D}	DD.D	P .	PD. PP.			(11, 12)		
A. Iran	AAIAI	•4	AA2AA3					
Ker								
$\langle b \rangle$	R	R_1	R_2					
$(hom)^{-1}$	C13	$\sigma_2 T_2$	σ_1			-		
\mathcal{R}	R ²	$(R_1)^2$	$(R_2$)2	$(R_1 R_2)^2$	$(R_2 R)^4$	$(RR_{1})^{4}$	
ker		· ··	· -			. 2 /	$K(T, T^{-1})$	
NV1							M (1 , 1 , 1)	
D 4					-			
P4gm	ס	,	n		D	n	G	
$\langle a \rangle$	K_1	1	χ ₂		κ_3	K_4	2	
(hom)	$\sigma_2 I_2$	C .	$r_1 I_1$		$I_2\sigma_2$	$T_1\sigma_1$	$c_{13}\sigma_1$	
R	$(R_1)^2$	($(K_2)^2$		$(R_3)^2$	$(R_4)^2$	5+	
ker					•			
\mathcal{R}	$S^{-i}R_4S^iF$	R_{i}^{-1} ($(R_1R_2)^2$		$(R_2R_3)^2$	$(R_3R_4)^2$	$(R_4R_1)^2$	(12)
ker		1	$\mathcal{K}(T_2^{-1}, T_1$	⁻¹)	$K(T_1^{-1}, T_2)$	$K(T_2, T_1)$	$K(T_1, T_2^{-1})$	
$\langle \boldsymbol{b} \rangle$	$R = R_4$	S						
$(hom)^{-1}$	$T_1\sigma_1$	cura.						
D .	D2	¢[30] ¢4	$(\mathbf{p}\mathbf{s}^{-1})$	D C12				
No.	Λ	5		π-1∖	-			
Ker			<u>`</u> К (1],	$I_2^{(1)}$				
.								
P3	_ 11							
$\langle a \rangle$	U_1	U_2		U_3				
(hom) ⁻¹	C12C23	c_{12}	$c_{23}T_1$	T_1^-	$c_{12}c_{23}$	<u>،</u>	-	
\mathcal{R}	$(U_1)^3$	(U_i)	₂) ³	$(U_3$	i) ³	$U_{1}U_{2}U_{3}$		
ker			-	K(T_1^{-1}, T_2^{-1}			(13)
<i>(b</i>)	Π.	Ua						\ ,
$(bom)^{-1}$	CiaCan	C-0	$c_{\alpha\alpha}T_{\alpha}$					
\mathcal{D}	(12, 3)	(12	-3	aı.	11-13			
10	(01)	(0)	2)		r = 1 $r = 1$			
Ker				Λ(.	I_2, I_1)			
P3m1			~					-
$\langle a \rangle$	$U_1 = l$	J_2	R					
(hom) ⁻¹	$c_{12}c_{23}$ $c_{12}c_{23}$	$c_{12}c_{23}T_1$	c_{13}	_				
\mathcal{R}	$(U_1)^3$ ($(U_2)^3$	(U_1U_2)	$(2)^{3}$	$R^2 R$	$U_1 R U_1 = R U$	$V_2 R U_2$	
ker			$K(T_2)$	$^{-1}, T_{1}$	⁻¹)			
<i>(b)</i>	$R_1 = R I L$,	$R_2 = U \cdot K$	رح	$R_1 = R$	-		(14)
$(hom)^{-1}$	$r_1 = RO_2$ $r_2 T_1$	<u> </u>		. 1	· · · · ·	-	-	<u>\- · /</u>
τ	$(\mathbf{p}_1)^2$	4	-23 (P-)2		13 D-12			
/C Iron	(AD-	•	(K2) ⁻	(N3) ⁻			
Ker D	(ההא		in n 3	,	D D \3			
к. •	$(K_1K_2)^{-1}$	_1	$(\kappa_2 \kappa_3)^{*}$	($\kappa_3\kappa_1$			
ker	$K(T_1^{-1}, T_2)$	2 ⁻ ')						

We check the condition (1) given in the introduction. In equation (18) we give for 13 space groups the construction of T_1, T_2 from its generators.

	$\mathcal{P}1$	$\mathcal{P}2$	$\mathcal{P}m$.	Cm	$\mathcal{P}2mm$	C2mm		
$T_1:$	X	•	X	PR	Y^{-1}	TR_2R_3		
$T_2:$	Y^{-1}	•	Y^{-1}	$(RP)^{-1}$	R'R	$R_3 T R_2$		(10)
	$\mathcal{P}4$	$\mathcal{P}4mm$	$\mathcal{P}3$	$\mathcal{P}3m1$	$\mathcal{P}31m$	$\mathcal{P}6$	P6m	(18)
$T_1:$	U_4S^2	R_4R_2	$(U_1)^{-1}U_2$	•	•	$(U_1)^{-1}U_2$	$R_3R_2R_3R_1$	
T_2 :	S^2U_1	R_3R_1	$U_2(U_1)^{-1}$	•		$U_2(U_1)^{-1}$	$R_3R_1R_3R_2.$	

It follows that the group $Inn(F_2)$ forms a subgroup of these 13 groups \mathcal{G} . The nonsymmorphic group $\mathcal{P}g$ is the first exception. Its generators P, Q are not in Inn(F_2) but yield the four elements $T_1^2 = PQ$, $T_1T_2 = PQ^{-1}$, $T_2T_1 = P^{-1}Q$, $T_2^2 = P^{-1}Q^{-1}$ of $Inn(F_2)$. These four elements generate the subgroup of words of even length in $Inn(F_2)$. Due to the presence of the generators P, Q, the same holds true for the groups $\mathcal{P}2mg$, $\mathcal{P}2gg$, $\mathcal{P}4gm$. Upon Abelianization we are of course left with two, not four translations. With this splitting into 13 + 4, all groups G match condition (1) given in the introduction.

4. The geometric representation

D 12

We pass to a geometric representation of the space groups. It is shown in [5] that the group $Aut(F_2)$ may be lifted into an isomorphic image in $Aut(F_3)$. Upon lifting an element of Aut(F_2) into Aut(F_3) and then applying hom₂, one obtains a 3 × 3 block triangular matrix representative for the space group element. In the columns of the following (19) we give for the generators $\langle c_{23}, c_{13}, \sigma_1 \rangle$ of the lifted group Aut (F_2) the images $\langle y_1, y_2, y_3 \rangle$ of $\langle x_1, x_2, x_3 \rangle$, each followed by the three power sums. The image under hom₂ is then the 3×3 matrix in GL(3, Z) formed from the three rows:

е	C23	hom_2		c_{13} hom ₂			σ_1	hom ₂					
x_1	$x_1 x_2$	1	1	0.	$(x_2)^{-1}$	0	-1	0	$(x_1)^{-1}$	-1	0	0	(10)
x_2	$(x_2)^{-1}$	0	-1	0	$(x_1)^{-1}$	-1	0	0	x_2	0	1	0	(19)
x_3	x_2x_3	0	1	1	$x_1 x_2 x_3$	1	1	1	x_3	0	0	1.	

In the expressions for the space group elements we use the following short-hand symbols, part of which appear in relation to subgroups of $Aut(F_3)$ [5]. We express these automorphisms as functions of the generators as follows:

$$c_{12} := c_{23}c_{13}c_{23} \qquad \sigma_2 := c_{13}\sigma_1c_{13} \qquad m'' := \sigma_1c_{13}\sigma_1$$

$$S_2 := (c_{13}\sigma_1)^2 \qquad S_3 := c_{23}S_2c_{23} \qquad S_1 := c_{12}S_2c_{12} \qquad (20)$$

$$T_1 := S_1S_2 \qquad T_2 := S_2S_3.$$

The action on $\langle x_1, x_2, x_3 \rangle$ and the image under hom₂ can be computed by group multiplication from these expressions and from (19). For convenience we give some results of this computation:

е	S_2	hom_2			T_1	hom ₂			T_2	hom_2			
x_1	$(x_1)^{-1}$	-1	0	0	x_1	1	0	0	$(x_2)^{-1}x_1x_2$	1	0	0	(21)
x_2	$(x_2)^{-1}$	0	-1	0	$(x_1)^{-1}x_2x_1$	0	1	0	<i>x</i> ₂	0	1	0	(21)
<i>x</i> 3	$x_{2}^{2}x_{3}$	0	2	1	$x_1^{-1}x_2^{-1}x_1^{-1}x_2x_3$	-2	0	1	$x_2^{-2}x_3$	0	-2	1.	

By applying a matrix from Gl(3, Z) from the left to a column formed by three vectors (x_1, x_2, x_3) , which geometrically represent the algebraic generators of F_3 , one obtains a linear action of the space group element on the plane spanned by (x_1, x_2) . The third vector can then be suppressed. The automorphisms T_1 , T_2 under hom₂ are seen to map into translations by twice the length of the vectors which represent (x_1, x_2) . In the following figures, the two vectors have been adapted so that the torus or unit cell corresponds to the setting of [9]. The rotation axes, and the generators of mirror and glide lines (full and broken lines) for each of the 17 space groups, are shown on the right, with symbols





Figure 5. Cm and Cm.



Figure 6. P2mm and P2mm.



Figure 7. P2mg and P2mg.



Figure 11. P4mm and P4mm.

which represent typical generators and combinations from [8] and appear in the algebraic expressions of section 3. The left-hand side of each figure gives in the same geometry the two vectors $\langle x_1, x_2 \rangle$, where x_1 starts at the end point of x_2 . Symbols ∞ mark the preimages of infinite order in \mathcal{G} for finite-order elements in G.



Figure 12. P4gm and P4gm.





Figure 13. P3 and P3.



Figure 14. $\mathcal{P}3m1$ and P3m1.





Figure 15. P31m and P31m.





Figure 16. P6 and P6.



Figure 17. P6m and P6m.

5. Conclusion

We give some comments on the results. The distribution of infinite-order preimages for the rotation axes can be seen from the figures. We omit a corresponding discussion of mirror and glide lines. The group $\mathcal{P}2$ is the universal Coxeter group with three generators. In the groups $\mathcal{P}4gm$, P4gm we mark one representative glide line. In $\mathcal{P}3m1$ compared to the Coxeter group P3m1, the product R_1R_2 gets infinite order. There is no element of order 6 in Aut(F_2) and so the corresponding preimages in $\mathcal{P}6$, $\mathcal{P}6m$ have order ∞ .

If the transversals under the action of the 17 space groups on the plane are connected at corresponding edges, one obtains the 17 orbifolds described by Montesinos [3], p 80–2. For P1 we again find a torus, and any other orbifold admits an unfolding into an appropriate torus. The orbifold for the example Pg is Klein's bottle. If we extend the notion of the quantized torus mentioned in the introduction, each of the 17 groups \mathcal{G} provides a quantum version of the corresponding orbifold.

One field of application for non-commutative crystallography are quasicrystals [6]. Other applications, among them to the theory of dislocations, are under study.

Acknowledgments

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