Space groups - Exercises and solutions

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Exercise 1.
Prove that two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ commute (i.e. $\{g \mid t\} \cdot \{h \mid u\} = \{h \mid u\} \cdot \{g \mid t\}$) if and only if

(i) the linear parts g and h commute;

(ii) the translation parts fulfill $(g - id) \cdot u = (h - id) \cdot t$.

Conclude that an arbitrary affine mapping $\{g \mid t\}$ commutes with a translation $\{id \mid u\}$ if and only if u is fixed under the action of g.

Solution: Writing out the products gives

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid g \cdot u + t\} \text{ and } \{h \mid u\} \cdot \{g \mid t\} = \{hg \mid h \cdot t + u\}.$$

These two elements are equal if their linear parts and their translation parts coincide, i.e. if $gh = hg$ and $g \cdot u + t = h \cdot t + u$ which is the same as $g \cdot u - u = h \cdot t - t$.
If $h = id$, then $h \cdot t - t = 0$, hence $g \cdot u - u = 0$, i.e. $g \cdot u = u$.

Exercise 2.
Two space group elements are given by the following transformations:

$$\mathfrak{g} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} z + \frac{1}{2} \\ x + \frac{1}{2} \\ -y \end{pmatrix}, \quad \mathfrak{h} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -y \\ x + \frac{1}{2} \\ z + \frac{1}{2} \end{pmatrix}.$$

Determine the augmented matrices for $\mathfrak{g}$ and $\mathfrak{h}$ and compute the products $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$.

Solution: The augmented matrices are given by

$$\mathfrak{g} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & \frac{1}{2} \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} = \left(\begin{array}{ccc|c} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The products are

$$\mathfrak{g} \cdot \mathfrak{h} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & 1 \\ 0 & -1 & 0 & \frac{1}{2} \\ -1 & 0 & 0 & -\frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} \cdot \mathfrak{g} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & 1 \\ 0 & -1 & 0 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Exercise 3.
Prove the above corollary, i.e. show that if $g^{tr} F g = F$ for all $g \in P$ and $P' = \{X^{-1} \cdot g \cdot X \mid g \in P\}$, then $g'^{tr} X^{tr} F X g' = X^{tr} F X$ for all $g' \in P'$.

Solution: Let $g' = X^{-1} g X$, then $g = X g' X^{-1}$. We substitute the last expression for g in $g^{tr} F g = F$, this gives

$$X^{-tr} g'^{tr} X^{tr} F X g' X^{-1} = F.$$

Multiplying with X^{tr} from the left and with X from the right gives the claim.

Exercise 4.
The point group P (in the arithmetic class $\overline{3}$`m1P`) is generated by the matrices

$$g = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \; h = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(i) Check that P fixes the metric tensor $F = \begin{pmatrix} 2a & -a & 0 \\ -a & 2a & 0 \\ 0 & 0 & b \end{pmatrix}$. It thus acts on a hexagonal lattice.

(ii) P also acts on a rhombohedral lattice, which is obtained from the above hexagonal lattice by the basis transformation

$$X = \frac{1}{3} \begin{pmatrix} -1 & 2 & -1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \text{ with inverse transformation } X^{-1} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

Transform the metric tensor F of the hexagonal lattice to the metric tensor of the rhombohedral lattice (with the columns of X as lattice basis).

(iii) Transform P to the rhombohedral lattice (thus obtaining a point group P' in the arithmetic class $\overline{3}$`mR`) and check that the so obtained point group fixes the metric tensor computed in (ii).

Solution:

(i) Check by matrix multiplication that indeed $g^{tr} F g = F$ and $h^{tr} F h = F$.

(ii) Computing $F' = X^{tr} F X$ gives

$$F' = \frac{1}{9} \begin{pmatrix} 6a+b & -3a+b & -3a+b \\ -3a+b & 6a+b & -3a+b \\ -3a+b & -3a+b & 6a+b \end{pmatrix}.$$

(iii) Computing $g' = X^{-1} g X$ and $h' = X^{-1} h X$ gives

$$g' = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \; h' = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Now check that $g'^{tr} F' g' = F'$ and $h'^{tr} F' h' = F'$.

Exercise 5.

A space group G is generated by the elements

$$\mathfrak{g} = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{4} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{3}{2} \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

The point group P of G has 4 elements, the identity element and the linear parts of $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{g} \cdot \mathfrak{h}$.

(i) Determine the translation subgroup of G (which is not the standard lattice), transform G to a lattice basis of its translation lattice and write G in standard form. (Hint: $\mathfrak{g}^2$ and $\mathfrak{h}^2$ are translations.)

(ii) The elements $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$ have the same linear part. Check that their translation part only differs by a lattice vector of the translation lattice.

Solution:

(i) We have

$$\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 2 \\ \hline 0 & 0 & 1 \end{array}\right)$$

and $(\mathfrak{g} \cdot \mathfrak{h})^2$ is the identity element of G. A basis of the translation lattice is thus

$$\left(\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right)$$

and with respect to this basis the four given generators become

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} -1 & 0 & 3 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

In standard form, the group becomes the space group `p2mg` given by the generators

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

(ii) With respect to the original basis we have

$$\mathfrak{g} \cdot \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{7}{4} \\ 0 & -1 & -1 \\ \hline 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} \cdot \mathfrak{g} = \left(\begin{array}{cc|c} -1 & 0 & \frac{5}{4} \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right),$$

the linear parts thus differ by

$$\begin{pmatrix} \frac{7}{4} \\ -1 \end{pmatrix} - \begin{pmatrix} \frac{5}{4} \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -2 \end{pmatrix}$$

which is a lattice vector according to (i).

Exercise 6.

Show that an inner derivation $\{t_g = (g - id) \cdot v \mid g \in P\}$ fulfills the product condition $t_{gh} \equiv g \cdot t_h + t_g \bmod T$ by showing that even the equality $t_{gh} = g \cdot t_h + t_g$ holds.

Solution: We have $t_g = g \cdot v - v$, $t_h = h \cdot v - v$ and $t_{gh} = gh \cdot v - v$, thus

$$g \cdot t_h + t_g = gh \cdot v - g \cdot v + g \cdot v - v = gh \cdot v - v = t_{gh}.$$

Exercise 7.

Compute the inner derivations and the solutions of the Frobenius congruences modulo the inner derivations for the following point groups P:

(1) P is generated by

$$g = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ h = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

(2) P is generated by

$$g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^4, y^2, (xy)^2 \rangle$.

Solution:

(1) Computing the inner derivation for $v = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ gives the inner derivation

$$\left(t_g = \begin{pmatrix} -1 \\ 1 \end{pmatrix},\ t_h = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \right),$$

computing the inner derivation for $v' = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ gives the inner derivation

$$\left(t'_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix},\ t'_h = \begin{pmatrix} -2 \\ -2 \end{pmatrix} \right).$$

This shows that modulo inner derivations the first coordinate of t_g and the first coordinate of t_h can be chosen as 0.

We therefore insert the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & a \\ \hline 0 & 0 & 1 \end{array} \right),\ \mathfrak{h} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ -1 & 0 & b \\ \hline 0 & 0 & 1 \end{array} \right),$$

into the relators, which yields

$$\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & a \\ 0 & 1 & a \\ \hline 0 & 0 & 1 \end{array} \right),\ \mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & -b \\ 0 & 1 & b \\ \hline 0 & 0 & 1 \end{array} \right).$$

This implies $a = b = 0$, hence the only solutions to the Frobenius congruences are the inner derivations.

(2) The matrix $g - id$ is invertible, hence $(g - id) \cdot v$ runs over all vectors of $\mathbb{R}^2$ and we can thus assume that the SNoT element t_g of g is $t_g = 0$. We insert the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array} \right),\ \mathfrak{h} = \left(\begin{array}{cc|c} 1 & 0 & a \\ 0 & -1 & b \\ \hline 0 & 0 & 1 \end{array} \right),$$

into the relators, which yields

$$\mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & 2a \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right),\ (\mathfrak{g}\mathfrak{h})^2 = \left(\begin{array}{cc|c} 1 & 0 & a-b \\ 0 & 1 & a-b \\ \hline 0 & 0 & 1 \end{array} \right).$$

The solutions of the Frobenius congruences modulo the inner derivations are thus $a = b = 0$ and $a = b = \frac{1}{2}$.

Exercise 8.

A certain point group P (known as $\mathtt{m\overline{3}}$) is generated by

$$g = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \; h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^6, y^2, (xy)^3, (x^3y)^2 \rangle$.
Since $g - id$ is invertible, $(g - id) \cdot v$ runs over all vectors in $\mathbb{R}^3$, hence by a shift of origin the translation part of g may be assumed to be 0.
The integral normalizer of P contains the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ which interchanges the second and third basis vector.
Determine the solutions of the Frobenius congruences for P (assuming that $t_g = 0$) and check which of the resulting SNoTs lie in one orbit under the integral normalizer of P.

Solution: We insert the matrices

$$\mathfrak{g} = \left(\begin{array}{ccc|c} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \; \mathfrak{h} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & a \\ 0 & 1 & 0 & b \\ 0 & 0 & 1 & c \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

into the relators, this gives

$$\mathfrak{h}^2 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2b \\ 0 & 0 & 1 & 2c \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \; (\mathfrak{g}\mathfrak{h})^3 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & a-b-c \\ 0 & 1 & 0 & -a+b+c \\ 0 & 0 & 1 & a-b-c \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

$$(\mathfrak{g}^3\mathfrak{h})^2 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & -2a \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

The solutions to the Frobenius congruences are thus $a = b = c = 0$ and $a, b, c \in \{0, \frac{1}{2}\}$ with $a + b + c = 1$. and give rise to the four SNoTs

$$t_h^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \; t_h^{(2)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, \; t_h^{(3)} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}, \; t_h^{(4)} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

Conjugation of h with the normalizer element $a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ gives $a^{-1}ha = h$, thus only the action of a on the SNoT vectors t_h has to be considered. One sees that $t_h^{(1)}$ and $t_h^{(4)}$ are fixed under the action of a, but that $t_h^{(2)}$ and $t_h^{(3)}$ are interchanged and give thus rise to the same space group.