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MATRIX CALCULUS
(brief revision)

Some of the slides are taken from the presentation "*Introduction to Matrix Algebra*" of **M. Rademeyer** given at the School on Fundamental Crystallography, Bloemfontein, South Africa, 2010

What is a matrix?

Definition:

- A rectangular array of numbers
- in m rows
- and n columns
- is called an $(m \times n)$ matrix $\boldsymbol{A}$

Use boldface italics upper case letters to indicate matrix, e.g. ***A*, *B*, *W***.

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix}.$$

An item in a matrix is called an entry or element

Square Matrix:

An $(n \times n)$ matrix

rows = # columns

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

Column Matrix:

An $(m \times 1)$ matrix

Row index changes

$$\begin{pmatrix} A_{11} \\ A_{21} \\ \vdots \\ A_{m1} \end{pmatrix}$$

Row Matrix:

A $(1 \times n)$ matrix

Column index changes

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \end{pmatrix}$$

Index 1 is often omitted for column and row matrices.

Transposed Matrix A^T

Let $\boldsymbol{A}$ be a (m x n) matrix

The (n x m) matrix obtained from $\boldsymbol{A} = (A_{ik})$ by exchanging rows and columns is called the **transposed matrix A^T**.

$$\boldsymbol{A} = \begin{pmatrix} 1 & 0 & \bar{1} \\ 2 & 4 & \bar{3} \end{pmatrix} \qquad \boldsymbol{A}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 \\ 0 & 4 \\ \bar{1} & \bar{3} \end{pmatrix}$$

Reminder: $\bar{z}$ means $-z$

Example 1: Transposed Matrix

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

determine $\boldsymbol{A}^{\mathrm{T}}$.

Symmetric Matrix

A square matrix is symmetric if $\boldsymbol{A^T} = \boldsymbol{A}$

i.e. if $A_{ik} = A_{ki}$ for any pair i,k.

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & \overline{5} \\ 3 & \overline{5} & 6 \end{pmatrix}$$

Symmetric with respect to main diagonal

- Top left to bottom right

SKEW-SYMMETRIC MATRIX

$\boldsymbol{A}^T = -\boldsymbol{A}$

0	0	-5
0	0	6
5	-6	0

If ***A*** is a skew-symmetric matrix, then

$A_{ii} = 0,\ i = 1,2,3$

as $A_{ik} = -A_{ki}$

EXERCISE 2.1.1

Problems

1. Construct the transposed matrix of the (3x1) row matrix:

$$\begin{pmatrix} 1 & 3 & 4 \end{pmatrix}$$

2. Determine which of the following matrices are symmetric and which are skew-symmetric:

$$\boldsymbol{A}=\begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix} \quad \boldsymbol{B}=\begin{pmatrix} 3 & 4 \\ -4 & 1 \end{pmatrix} \quad \boldsymbol{C}=\begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix} \quad \boldsymbol{D}=\begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} \quad \boldsymbol{E}=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\boldsymbol{F}= (3) \quad \boldsymbol{G}=\begin{pmatrix} 0 & 1 & -2 \\ -1 & 0 & 3 \\ 2 & -3 & 0 \end{pmatrix} \quad \boldsymbol{H}=\begin{pmatrix} 3 & 2 \\ 2 & 1 \\ 1 & 0 \end{pmatrix} \quad \boldsymbol{J}=\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Matrix Calculations

<u>Multiplication with a number (scalar product):</u>

An (m x n) matrix $\boldsymbol{A}$ is multiplied with a number λ by multiplying each element with λ:

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix} \longrightarrow \lambda \boldsymbol{A} = \begin{pmatrix} \lambda A_{11} & \lambda A_{12} & \dots & \lambda A_{1n} \\ \lambda A_{21} & \lambda A_{22} & \dots & \lambda A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda A_{m1} & \lambda A_{m2} & \dots & \lambda A_{mn} \end{pmatrix}$$

Example 2: Scalar product

Given that

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

determine $3\boldsymbol{A}$.

Matrix addition and subtraction:

Let A_{ik} and B_{ik} be general elements of matrices ***A*** and ***B***.

A and ***B*** must be of the same size (i.e. same number of rows and columns). Then the sum and the difference ***A*** ± ***B*** is:

$$\boldsymbol{C} = \boldsymbol{A} \pm \boldsymbol{B} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix} \pm \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1n} \\ B_{21} & B_{22} & \dots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{m1} & B_{m2} & \dots & B_{mn} \end{pmatrix} =$$

$$= \begin{pmatrix} A_{11} \pm B_{11} & A_{12} \pm B_{12} & \dots & A_{1n} \pm B_{1n} \\ A_{21} \pm B_{21} & A_{22} \pm B_{22} & \dots & A_{2n} \pm B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} \pm B_{m1} & A_{m2} \pm B_{m2} & \dots & A_{mn} \pm B_{mn} \end{pmatrix}$$

Element C_{ik} of ***C*** is equal to the sum or difference of the elements A_{ik} and B_{ik} of ***A*** and ***B*** for any pair i,k:

$C_{ik} = A_{ik} \pm B_{ik}$

EXERCISE 2.1.2

Problems

1. Find $3\boldsymbol{A}-2\boldsymbol{B}$, where

$$\boldsymbol{A}=\begin{bmatrix} 1 & 2 \\ 3 & 0 \end{bmatrix} \quad \boldsymbol{B}=\begin{bmatrix} 1 & 3 \\ 0 & -4 \end{bmatrix}$$

2. Show that the sum of any matrix and its transpose is a symmetric matrix, *i.e.*

$$(\boldsymbol{A}+\boldsymbol{A}^{\mathrm{T}})^{\mathrm{T}}=\boldsymbol{A}+\boldsymbol{A}^{\mathrm{T}}$$

3. Show that the difference of any matrix and its transpose is a skew-symmetric matrix, *i.e.*

$$(\boldsymbol{A}-\boldsymbol{A}^{\mathrm{T}})^{\mathrm{T}}=-(\boldsymbol{A}-\boldsymbol{A}^{\mathrm{T}})$$

Matrix multiplication

The multiplication of two matrices is only defined when:

- the number $n_{(lema)}$ of columns of the *le*ft *ma*trix is the same as
- the number of $m_{(rima)}$ of rows on the *ri*ght *ma*trix
- no restriction on $m_{(lema)}$ or rows of the *le*ft *ma*trix
- no restriction on $n_{(rima)}$ or rows of the *ri*ght *ma*trix

\# columns of left matrix = # rows of right matrix

Multiplication
Product of two matrices *A* and *B*:

The matrix product ***C*** = ***AB*** or

$$\begin{pmatrix} C_{11} & C_{12} & \dots & C_{1k} & \dots & C_{1n} \\ C_{21} & C_{22} & \dots & C_{2k} & \dots & C_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ C_{i1} & C_{i2} & \dots & C_{ik} & \dots & C_{in} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \dots & C_{mk} & \dots & C_{mn} \end{pmatrix} =$$

$$= \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1j} & \dots & A_{1r} \\ A_{21} & A_{22} & \dots & A_{2j} & \dots & A_{2r} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ A_{i1} & A_{i2} & \dots & A_{ij} & \dots & A_{ir} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mj} & \dots & A_{mr} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1k} & \dots & B_{1n} \\ B_{21} & B_{22} & \dots & B_{2k} & \dots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ B_{j1} & B_{j2} & \dots & B_{jk} & \dots & B_{jn} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ B_{r1} & B_{r2} & \dots & B_{rk} & \dots & B_{rn} \end{pmatrix}$$

is defined by $C_{ik} = A_{i\,1} B_{1k} + A_{i\,2} B_{2k} + \ldots + A_{i\,j} B_{jk} + \ldots + A_{i\,r} B_{rk}$

Examples: Matrix Multiplication

If $A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$,

then $C = A\,B = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$D = B\,A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$C \neq D$, *i. e.* matrix multiplication is *not always commutative.*
However, it is *associative*, *e. g.*, $(A\,B)\,D = A\,(B\,D)$
and *distributive*, *i. e.* $(A + B)\,C = A\,C + B\,C$

Example 5: Multiplication

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 1 & 0 \\ 2 & 2 & 2 \\ 3 & 2 & 1 \end{pmatrix}$$

and ***C*** = ***AB***.
Determine ***C***.

Determine ***D***=***BA***, check if ***C***=***D*** or not.

Multiplication
Product of matrix *A* with column *a*:

Example: How to get element d_1:

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_i \\ \vdots \\ d_m \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1k} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2k} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ A_{i1} & A_{i2} & \dots & A_{ik} & \dots & A_{in} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mk} & \dots & A_{mn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \\ \vdots \\ a_n \end{pmatrix}$$

$$d_1 = A_{11}\,a_1 + A_{12}\,a_2 + \dots\dots + A_{1k}\,a_k + \dots\dots + A_{1n}\,a_n$$

Example 3: Multiplication

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 3 \\ \bar{5} \\ 6 \end{pmatrix}$$

and $\boldsymbol{C} = \boldsymbol{AB}$.

Determine $\boldsymbol{C}$.

Multiplication
Product of matrix ***A*** with row a^T:

Example: How to get elements d_1 and d_2:

$$(d_1 \ d_2 \dots d_i \dots d_n) = (a_1 \, a_2 \dots a_k \dots a_m) \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1i} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2i} & \dots & A_{2n} \\ \vdots & \vdots & & \ddots \vdots & & \vdots \\ A_{k1} & A_{k2} & \dots & A_{ki} & \dots & A_{kn} \\ \vdots & \vdots & & \vdots & & \ddots \vdots \\ A_{m1} & A_{m2} & \dots & A_{mi} & \dots & A_{mn} \end{pmatrix}$$

$$d_1 = a_1 A_{11} + a_2 A_{21} + \dots\dots + a_k A_{k1} + \dots\dots + a_n A_{m1}$$

$$d_2 = a_1 A_{12} + a_2 A_{22} + \dots\dots + a_k A_{k2} + \dots\dots + a_n A_{m2}$$

Example 4: Multiplication

Given that

$$\boldsymbol{A} = \begin{pmatrix} \overline{5} & 2 & 4 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 1 & 0 \\ 2 & 2 & 2 \\ 3 & 2 & 1 \end{pmatrix}$$

and ***C*** = ***AB***.

Determine ***C***.

EXERCISE 2.1.3

Problems

1. Find the products ***AB*** and ***BA***, if they exist, where

A=

1	2
3	-4

B=

3	-2	2
1	0	-1

2. Find the matrix products ***AB*** and ***BA*** of the row vector ***A***=

1	2	3

, and the column vector ***B***=

-2
4
1

3. Prove that ***A***(***BC***)=(***AB***)***C*** where

A=

1	2
-1	3

B=

1	0	-1
2	1	0

C=

1	-1
3	2
2	1

Trace of a Matrix

The trace of a (n x n) square matrix $\boldsymbol{A}$ is the sum of the elements on the main diagonal.

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

$$tr(\boldsymbol{A}) = A_{11} + A_{22} + \dots + A_{nn}$$

Determinants

The determinant det(***A***) or |***A***| of ***A*** can be calculated for any (n x n) square matrix.

(2×2) matrix

$$\text{Let } \boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$\det(\boldsymbol{A}) = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix}$$

$$\det(\boldsymbol{A}) = A_{11}A_{22} - A_{12}A_{21}$$

Determinants

(3×3) matrix

$$\boldsymbol{B} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix}$$

$$\det(\boldsymbol{B}) = \begin{vmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{vmatrix}$$

$$\det(\boldsymbol{B}) = B_{11}\,B_{22}\,B_{33} + B_{12}\,B_{23}\,B_{31} + B_{13}\,B_{21}\,B_{32} - B_{11}\,B_{23}\,B_{32} - B_{12}\,B_{21}\,B_{33} - B_{13}\,B_{22}\,B_{31}$$

Example 6: Determinant

Given that

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

Determine det($\boldsymbol{A}$).

EXERCISE 2.1.4

Problems

1. Find the values of the traces and the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$ where

$$\boldsymbol{A}=\begin{bmatrix} 1 & 2 \\ -1 & 3 \end{bmatrix} \qquad \boldsymbol{B}=\begin{bmatrix} 0 & 4 & 2 \\ 4 & -2 & -1 \\ 5 & 1 & 3 \end{bmatrix}$$

2. Show that $\det(\boldsymbol{AB})=\det(\boldsymbol{A})\det(\boldsymbol{B})$ where

$$\boldsymbol{A}=\begin{bmatrix} 3 & 2 \\ 5 & 1 \end{bmatrix} \qquad \boldsymbol{B}=\begin{bmatrix} 1 & 6 \\ 2 & 9 \end{bmatrix}$$

3. Show that $\det(\boldsymbol{A})= \det(\boldsymbol{A}^T)$ where

$$\boldsymbol{A}=\begin{bmatrix} 1 & 1 & 3 \\ 2 & 2 & 2 \\ 3 & 2 & 3 \end{bmatrix}$$

Inverse of a Matrix

A matrix $\boldsymbol{C}$ which fulfills the condition $\boldsymbol{CA} = \boldsymbol{I}$ for a square matrix $\boldsymbol{A}$, is the inverse matrix $\boldsymbol{A}^{-1}$ of $\boldsymbol{A}$, i.e. $\boldsymbol{AA}^{-1} = \boldsymbol{I}$.

$\boldsymbol{A}^{-1}$ exists if and only if $\det(\boldsymbol{A}) \neq 0$.

Not all matrices have an inverse matrix.

Assume that $\boldsymbol{A}^{-1}$ exists. If $\boldsymbol{CA} = \boldsymbol{I}$ then $\boldsymbol{AC} = \boldsymbol{I}$ also holds.

A matrix is called orthogonal if $\boldsymbol{A}^{-1}=\boldsymbol{A}^{T}$, i.e. $\boldsymbol{AA}^{T}=\boldsymbol{A}^{T}\boldsymbol{A}=\boldsymbol{I}$

EXAMPLE

Inverse of a matrix $\boldsymbol{A}$:

$$(\boldsymbol{A}^{-1})_{ik} = (\det \boldsymbol{A})^{-1}(-1)^{i+k}\boldsymbol{B}_{ki}$$

Find the inverse, if it exists of $\boldsymbol{A}$, where $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 5 \\ 1 & 5 & 12 \end{pmatrix}$

(i) $\det \boldsymbol{A} = 3$, $\det \boldsymbol{A} \neq 0$

(ii) $(\boldsymbol{A}^{-1})_{11}$: $(1/3)(-1)^{1+1}\boldsymbol{B}_{11} = 11/3$

$$\boldsymbol{B}_{11} = \det \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 5 \\ 1 & 5 & 12 \end{pmatrix} = \det \begin{pmatrix} 3 & 5 \\ 5 & 12 \end{pmatrix} = 11$$

(iii) $(\boldsymbol{A}^{-1})_{12}$: $(1/3)(-1)^{1+2}\boldsymbol{B}_{21} = -9/3$

. . .

$$\boldsymbol{A}^{-1} = 1/3 \begin{pmatrix} 11 & -9 & 1 \\ -7 & 9 & -2 \\ 2 & -3 & 1 \end{pmatrix}$$

Is it correct?

EXERCISE 2.1.5

Problems

1. Determine the inverses of the following matrices:

$$\boldsymbol{A} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \boldsymbol{B} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \boldsymbol{C} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\boldsymbol{D} = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \boldsymbol{E} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \quad \boldsymbol{F} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

2. Given that $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ -1 & 0 & 3 \\ 2 & -1 & 0 \end{pmatrix}$, determine $\boldsymbol{A}^{-1}$.

EXERCISE 2.1.5

Problems

Given that $\boldsymbol{A} = \begin{bmatrix} 1 & 2 & 0 \\ -1 & 0 & 3 \\ 2 & -1 & 0 \end{bmatrix}$, determine $\boldsymbol{A}^{-1}$.

SOLUTION

$$\boldsymbol{A}^{-1} = \begin{bmatrix} 1/5 & 0 & 2/5 \\ 2/5 & 0 & -1/5 \\ 1/15 & 1/3 & 2/15 \end{bmatrix}$$

SYMMETRY OPERATIONS AND THEIR MATRIX-COLUMN PRESENTATION

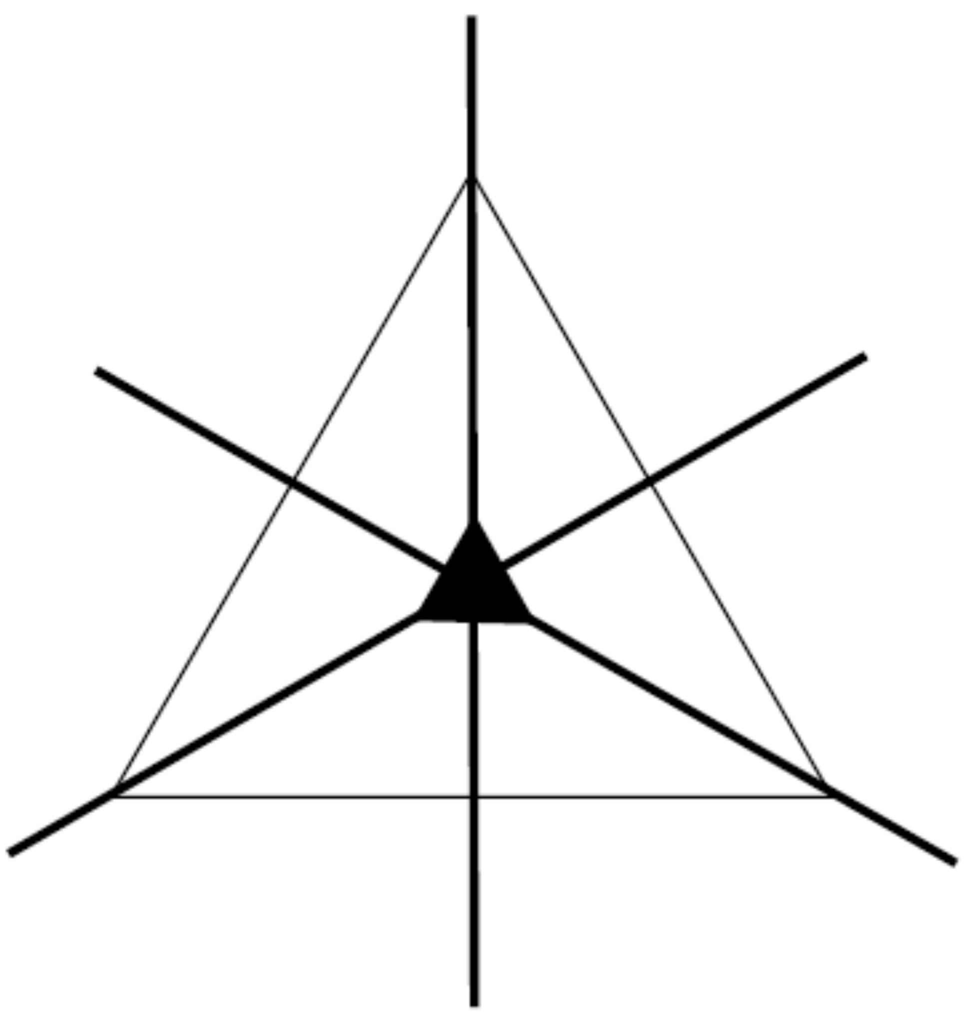
Crystallographic symmetry operations

Symmetry operations of an object

The isometries which map the object onto itself are called *symmetry operations of this object*. The *symmetry* of the object is the set of all its symmetry operations.

Crystallographic symmetry operations

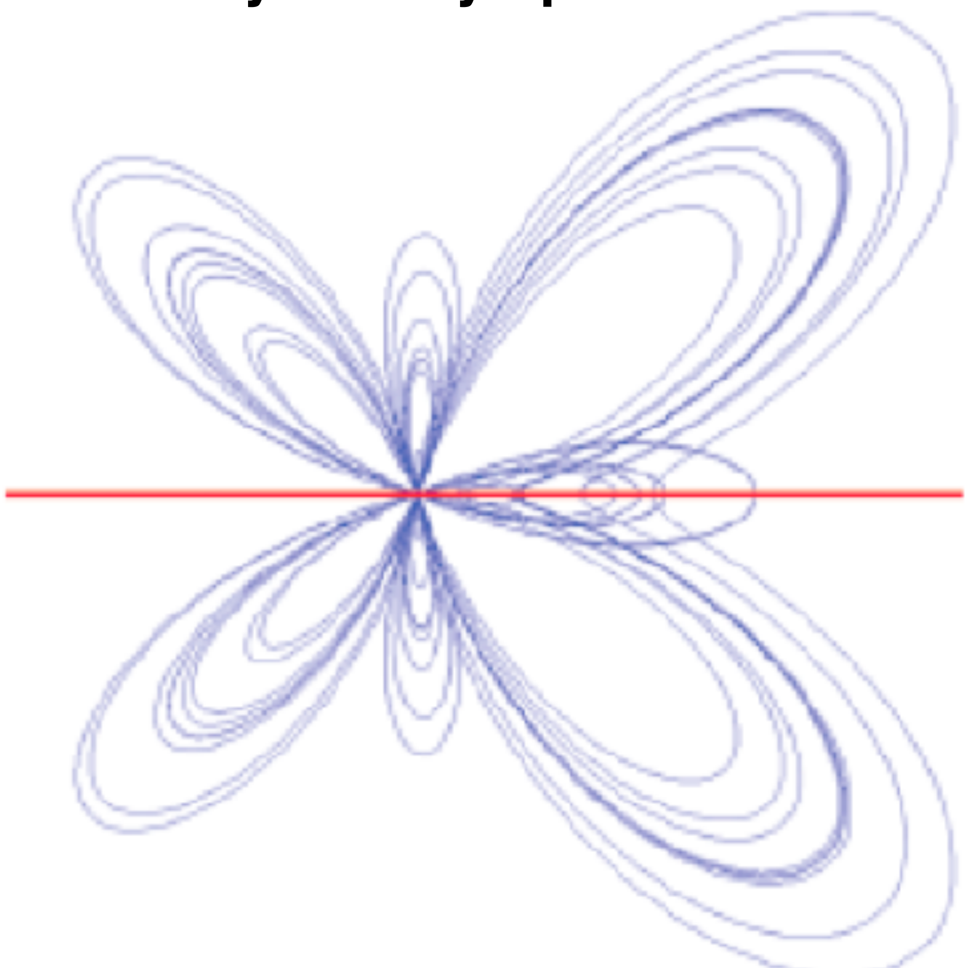
If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.



The equilateral triangle allows six symmetry operations: rotations by 120 and 240 around its centre, reflections through the three thick lines intersecting the centre, and the identity operation.

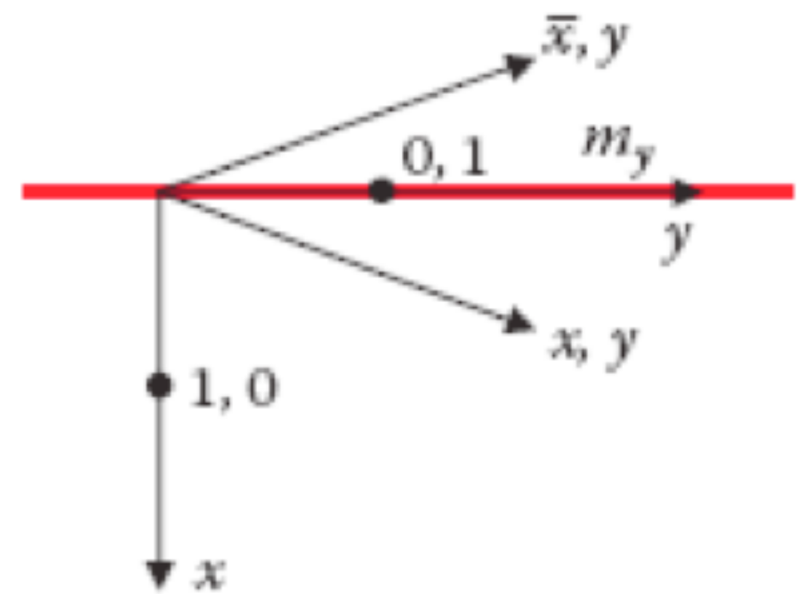
Example: Matrix presentation of symmetry operation

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Matrix representation

$$m_y \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix} = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\det \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ? \qquad \mathrm{tr} \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ?$$

Fixed points

$$m_y \begin{pmatrix} x_f \\ y_f \end{pmatrix} = \begin{pmatrix} x_f \\ y_f \end{pmatrix}$$

Description of isometries

coordinate system: $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$

isometry:

$\tilde{x} = F_1(x,y,z)$

$$\left|\begin{array}{rcl} \tilde{x} & = & W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} & = & W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} & = & W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3 \end{array}\right.$$

Matrix notation for system of linear equations

$$\begin{aligned}\tilde{x} &= W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1\\ \tilde{y} &= W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2\\ \tilde{z} &= W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3\end{aligned}$$

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix}W_{11} W_{12} W_{13}\\ W_{21} W_{22} W_{23}\\ W_{31} W_{32} W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix}$$

Matrix-column presentation of isometries

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$$

linear/matrix part

translation column part

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w}$$

$$\tilde{\boldsymbol{x}} = (\,\boldsymbol{W}, \boldsymbol{w}\,)\,\boldsymbol{x} \quad \text{or} \quad \tilde{\boldsymbol{x}} = \{\,\boldsymbol{W} \,|\, \boldsymbol{w}\,\}\,\boldsymbol{x}$$

matrix-column pair

Seitz symbol

EXERCISES

Problem 2.2.1

Referred to an 'orthorhombic' coordinated system ($a \neq b \neq c$; $\alpha=\beta=\gamma=90$) two symmetry operations are represented by the following matrix-column pairs:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} -1 & & & 0 \\ & 1 & & 0 \\ & & -1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the images X_i of a point X under the symmetry operations (W_i,w_i) where

$$X=\begin{pmatrix} 0,70 \\ 0,31 \\ 0,95 \end{pmatrix}$$

Can you guess what is the geometric 'nature' of (W_1,w_1)?

And of (W_2,w_2)?

Hint:

A drawing could be rather helpful

EXERCISES

Problem 2.2.1

Characterization of the symmetry operations:

$$\det\begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} = ?$$

$$\operatorname{tr}\begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} = ?$$

What are the fixed points of (W_1,w_1) and (W_2,w_2) ?

$$\left(\begin{matrix} -1 & & \\ & 1 & \\ & & -1 \end{matrix} \quad \begin{matrix} 1/2 \\ 0 \\ 1/2 \end{matrix}\right) \begin{pmatrix} x_f \\ y_f \\ z_f \end{pmatrix} = \begin{pmatrix} x_f \\ y_f \\ z_f \end{pmatrix}$$

Short-hand notation for the description of isometries

isometry:

$$X \bullet \xrightarrow{(W,w)} \bullet \tilde{X}$$

$$\left|\begin{array}{lcl} \tilde{x} & = & W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} & = & W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} & = & W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3 \end{array}\right.$$

notation rules:

-left-hand side: omitted

-coefficients 0, +1, -1

-different rows in one line

examples:

-1			1/2
	1		0
		-1	1/2

→ -x+1/2, y, -z+1/2

$\bar{x}$+1/2, y, $\bar{z}$+1/2

EXERCISES

Problem 2.2.2

Construct the matrix-column pair (W,w) of the following coordinate triplets:

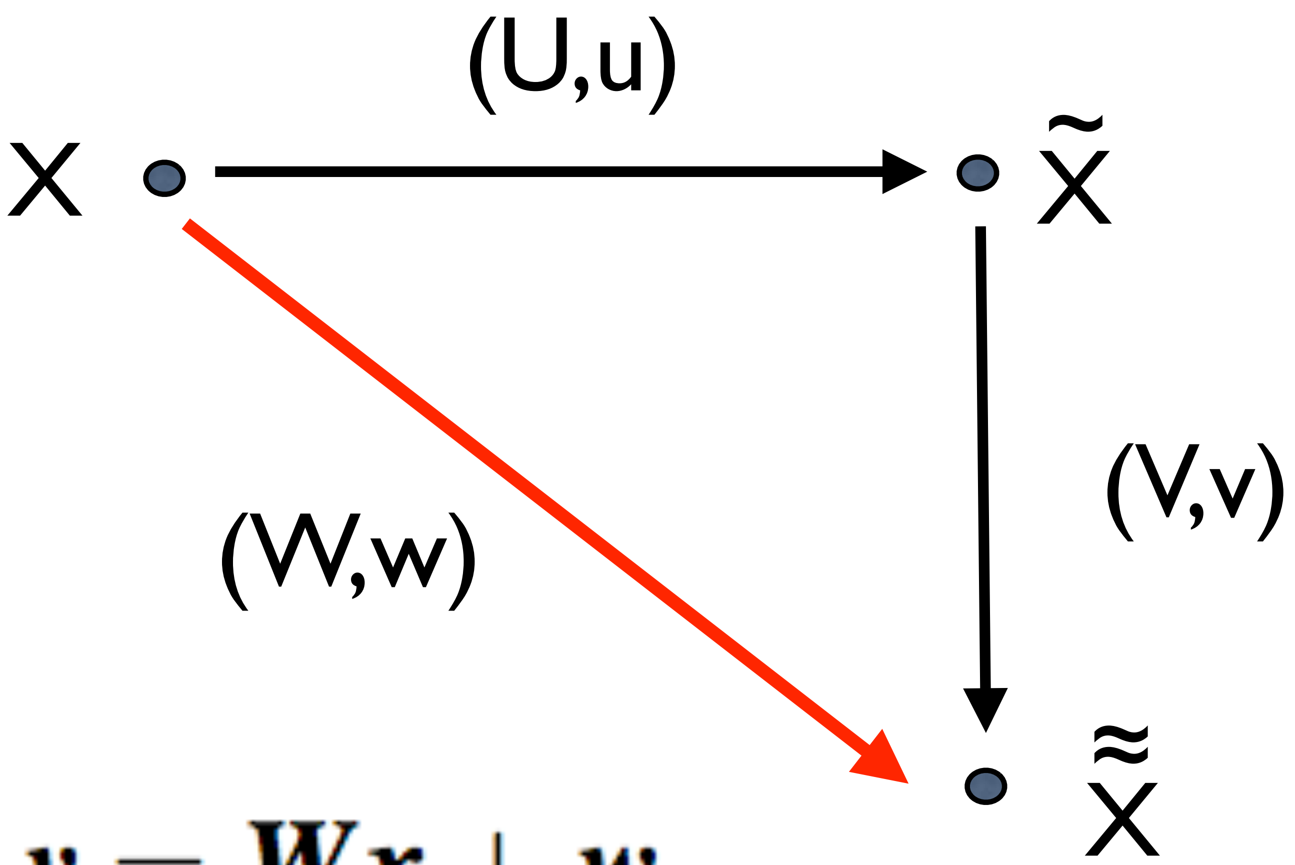
(1) x,y,z

(2) -x,y+1/2,-z+1/2

(3) -x,-y,-z

(4) x,-y+1/2, z+1/2

Combination of isometries



$$\tilde{\boldsymbol{x}} = \boldsymbol{U}\boldsymbol{x} + \boldsymbol{u};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\tilde{\boldsymbol{x}} + \boldsymbol{v};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}(\boldsymbol{U}\boldsymbol{x} + \boldsymbol{u}) + \boldsymbol{v};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\boldsymbol{U}\boldsymbol{x} + \boldsymbol{V}\boldsymbol{u} + \boldsymbol{v} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}.$$

$$\tilde{\tilde{\boldsymbol{x}}} = (\boldsymbol{V},\ \boldsymbol{v})\,\tilde{\boldsymbol{x}} = (\boldsymbol{V},\ \boldsymbol{v})(\boldsymbol{U},\ \boldsymbol{u})\boldsymbol{x} = (\boldsymbol{W},\ \boldsymbol{w})\boldsymbol{x}.$$

$$(\boldsymbol{W},\ \boldsymbol{w}) = (\boldsymbol{V},\ \boldsymbol{v})(\boldsymbol{U},\ \boldsymbol{u}) = (\boldsymbol{V}\boldsymbol{U},\ \boldsymbol{V}\,\boldsymbol{u} + \boldsymbol{v}).$$

EXERCISE 2.2.1

Problem

Consider the matrix-column pairs of the two symmetry operations:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & 1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine and compare the matrix-column pairs of the combined symmetry operations:

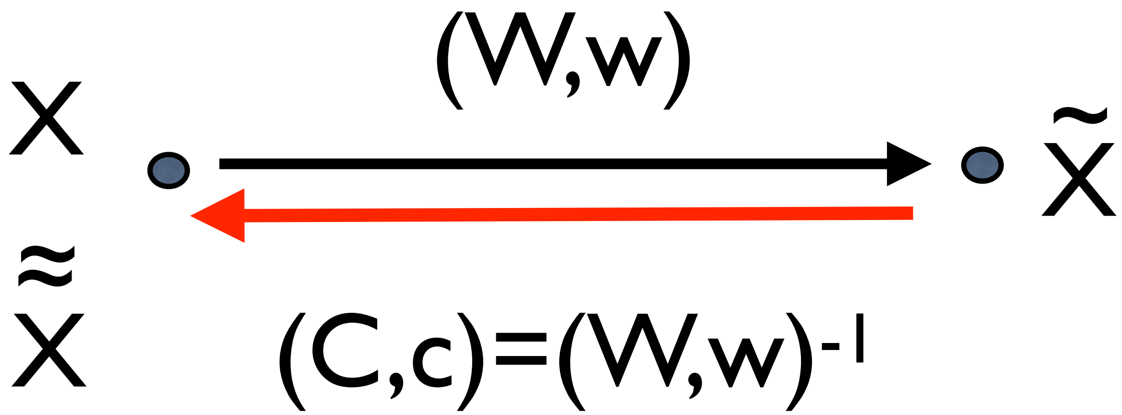
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

$$(W,w)'=(W_2,w_2)(W_1,w_1)$$

combination of isometries:

$$(V,v)(U,u)=(VU,Vu+v)$$

Inverse isometries



$\boldsymbol{I}$ = 3x3 identity matrix

$\boldsymbol{o}$ = zero translation column

$$(C,c)(W,w) = (\boldsymbol{I},\boldsymbol{o})$$

$$(C,c)(W,w) = (CW, Cw+c)$$

$CW=\boldsymbol{I}$ → $C=W^{-1}$

$Cw+c=\boldsymbol{o}$ → $c=-Cw=-W^{-1}w$

EXERCISES

Problem 2.2.1(cont)

Determine the inverse symmetry operations $(W_1,w_1)^{-1}$ and $(W_2,w_2)^{-1}$ where

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & 1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the inverse symmetry operation $(W,w)^{-1}$

$$(W,w)=(W_1,w_1)(W_2,w_2)$$

inverse of isometries:

$$(\boldsymbol{W},\,\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1},\,-\boldsymbol{W}^{-1}\,\boldsymbol{w})$$

EXERCISES

Problem 2.2.1(cont)

Consider the matrix-column pairs

$$(\boldsymbol{A},\boldsymbol{a}) = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,\bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \text{ and } (\boldsymbol{B},\boldsymbol{b}) = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(i) What is the matrix–column pair resulting from $(\boldsymbol{B},\,\boldsymbol{b})\,(\boldsymbol{A},\,\boldsymbol{a}) = (\boldsymbol{C},\boldsymbol{c})$, and $(\boldsymbol{A},\,\boldsymbol{a})\,(\boldsymbol{B},\,\boldsymbol{b}) = (\boldsymbol{D},\boldsymbol{d})$?

(ii) What is $(\boldsymbol{A},\boldsymbol{a})^{-1}$, $(\boldsymbol{B},\boldsymbol{b})^{-1}$, $(\boldsymbol{C},\boldsymbol{c})^{-1}$ and $(\boldsymbol{D},\boldsymbol{d})^{-1}$?

(iii) What is $(\boldsymbol{B},\boldsymbol{b})^{-1}\,(\boldsymbol{A},\,\boldsymbol{a})^{-1}$?

Matrix formalism: 4x4 matrices

$$\boldsymbol{x} \rightarrow \mathbb{x} = \begin{pmatrix} x \\ y \\ z \\ \hline 1 \end{pmatrix}; \; \tilde{\boldsymbol{x}} \rightarrow \tilde{\mathbb{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{pmatrix}$$

augmented matrices:

$$(\boldsymbol{W}, \boldsymbol{w}) \rightarrow \mathbb{W} = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

$\text{point } X \longrightarrow \text{point } \tilde{X}:$

$$\tilde{\mathbb{x}} = \mathbb{W}\,\mathbb{x} \qquad \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{pmatrix} = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} x \\ y \\ z \\ \hline 1 \end{pmatrix}$$

4x4 matrices: general formulae

point $X \longrightarrow$ point $\tilde{X}$:

$$\tilde{\mathbb{x}} = \mathbb{W}\,\mathbb{x}$$

$$\left(\begin{array}{c}\tilde{x}\\ \tilde{y}\\ \tilde{z}\\ \hline 1\end{array}\right) = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1\end{array}\right)\left(\begin{array}{c}x\\ y\\ z\\ \hline 1\end{array}\right)$$

combination and inverse of isometries:

$$(\mathbb{W})^{-1} = (\mathbb{W}^{-1})$$

$$\mathbb{W}^{-1} = \left(\begin{array}{ccc|c} & \boldsymbol{W}^{-1} & & -\boldsymbol{W}^{-1}\boldsymbol{w} \\ \hline 0 & 0 & 0 & 1\end{array}\right)$$

$$\mathbb{W}_3 = \mathbb{W}_2\,\mathbb{W}_1$$

EXERCISES

Problem 2.2.2 (cont.)

Construct the (4x4) matrix-presentation of the following coordinate triplets:

(1) x,y,z

(2) -x,y+1/2,-z+1/2

(3) -x,-y,-z

(4) x,-y+1/2, z+1/2

CRYSTALLOGRAPHIC SYMMETRY OPERATIONS

Crystallographic symmetry operations

characteristics: fixed points of isometries $(W,w)X_f=X_f$
geometric elements

Types of isometries preserve handedness

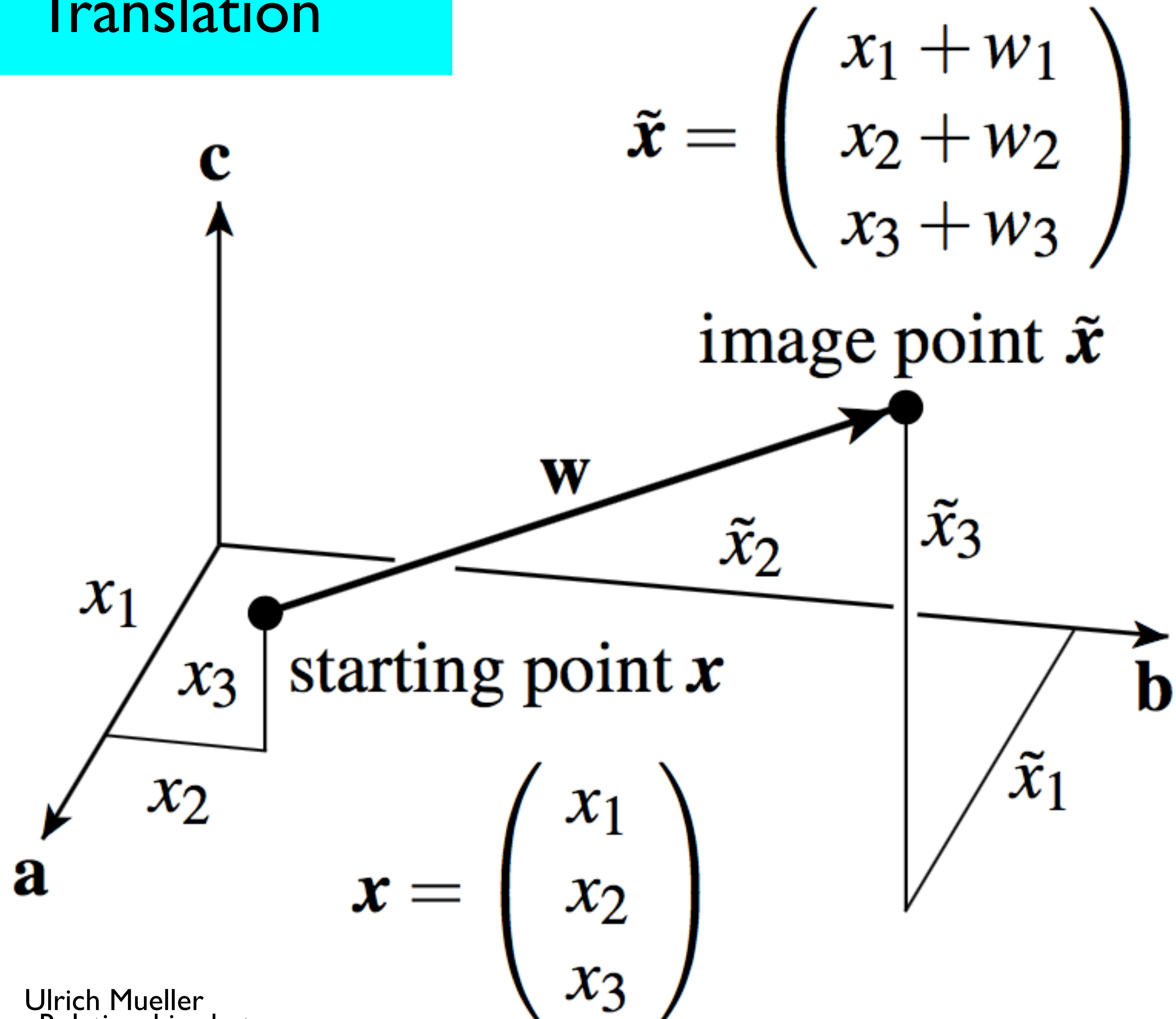
identity: the whole space fixed

translation t: no fixed point $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{t}$

rotation: one line fixed
rotation axis $\phi = k \times 360^\circ/N$

screw rotation: no fixed point
screw axis screw vector

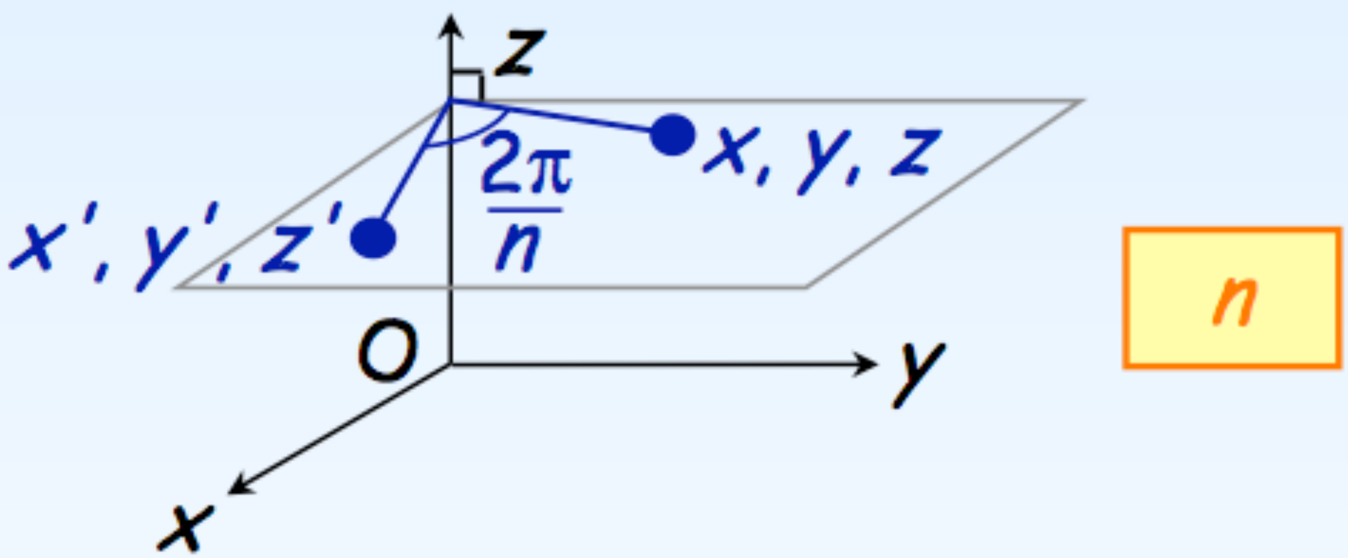
Translation



Crystallographic symmetry operations

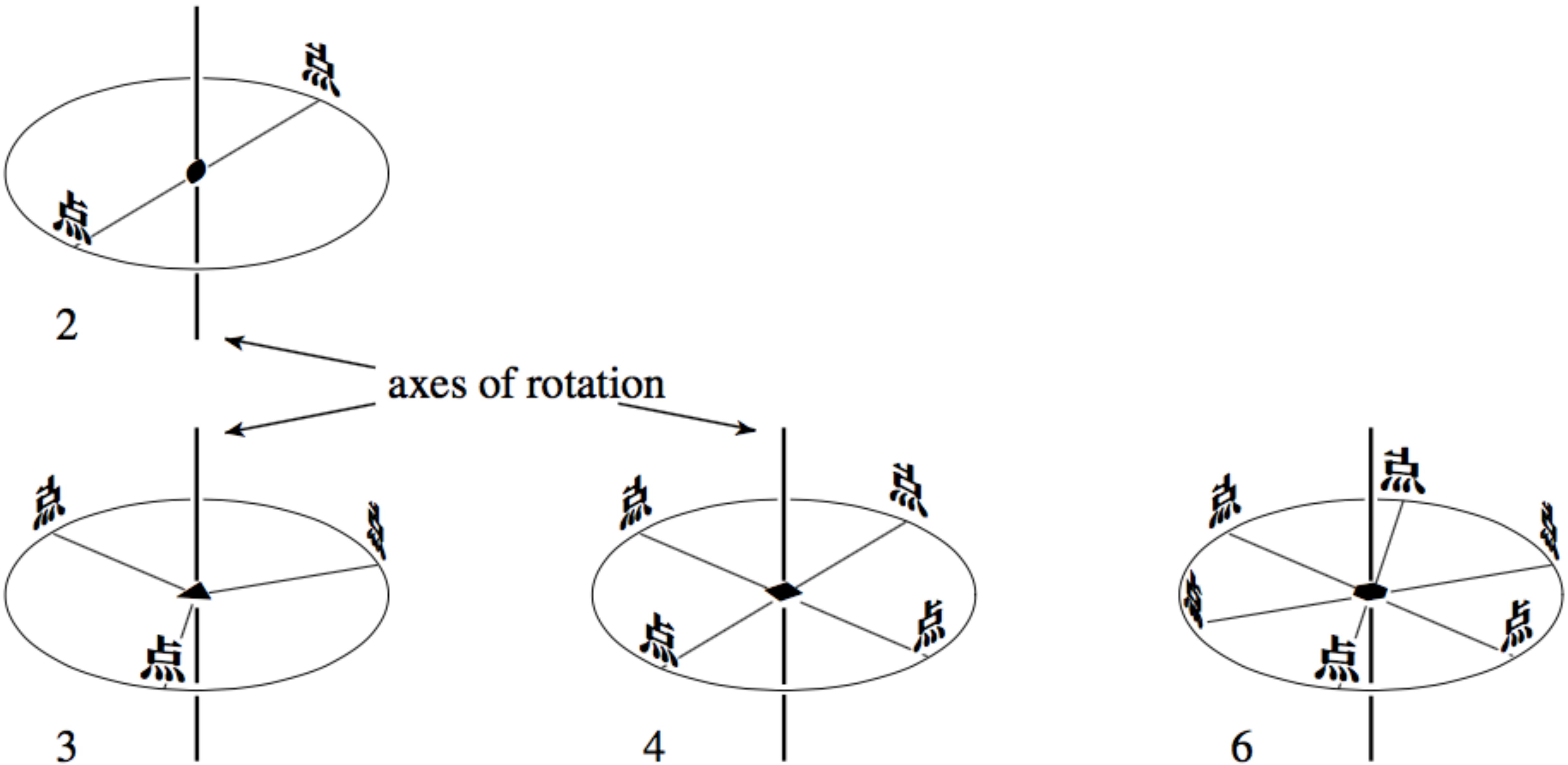
Rotation (around an axis)

Rotation of order n = rotation by $\varphi = \frac{2\pi}{n}$

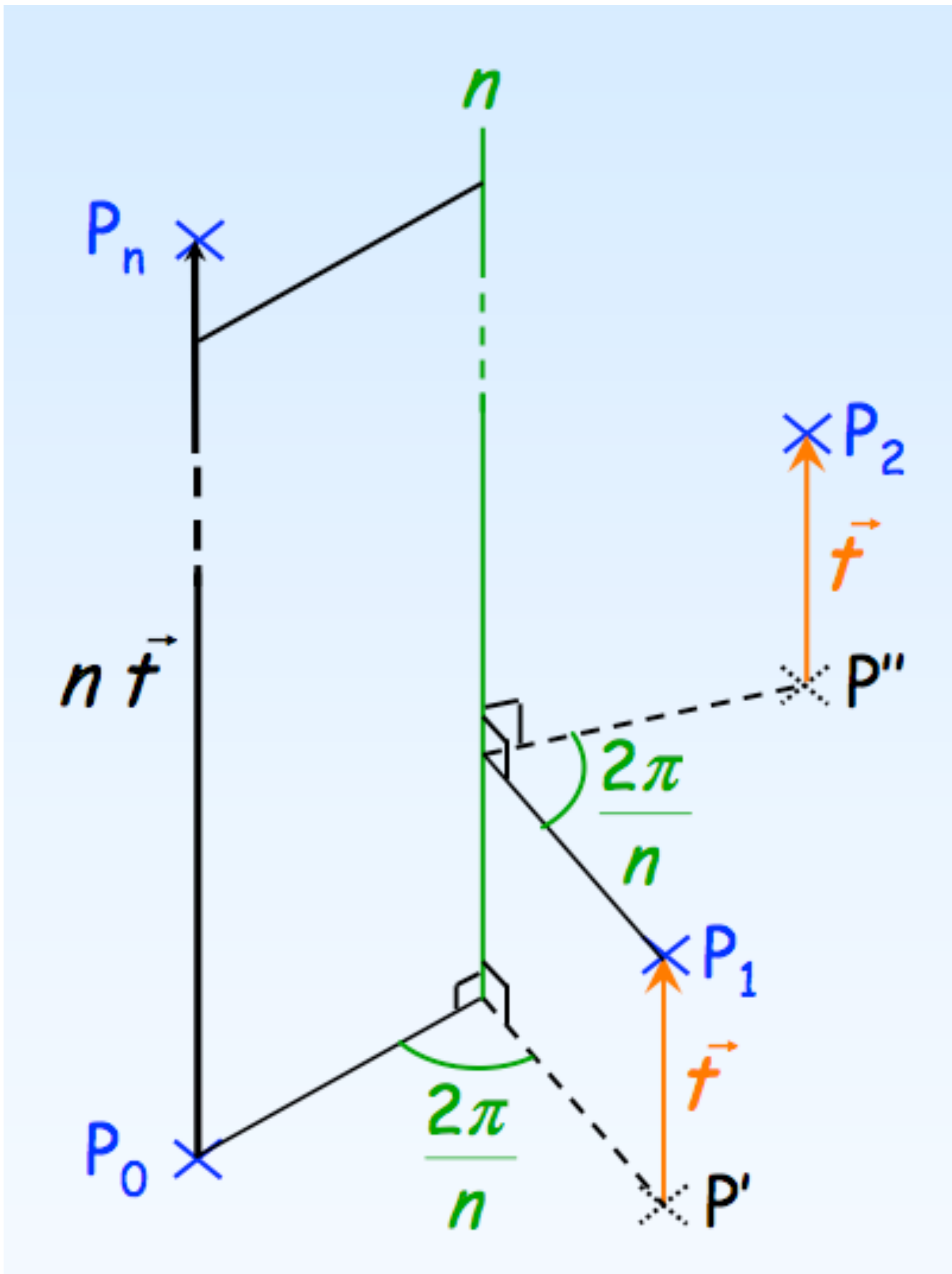


$$\alpha(n) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{Det} = +1$$

Rotations



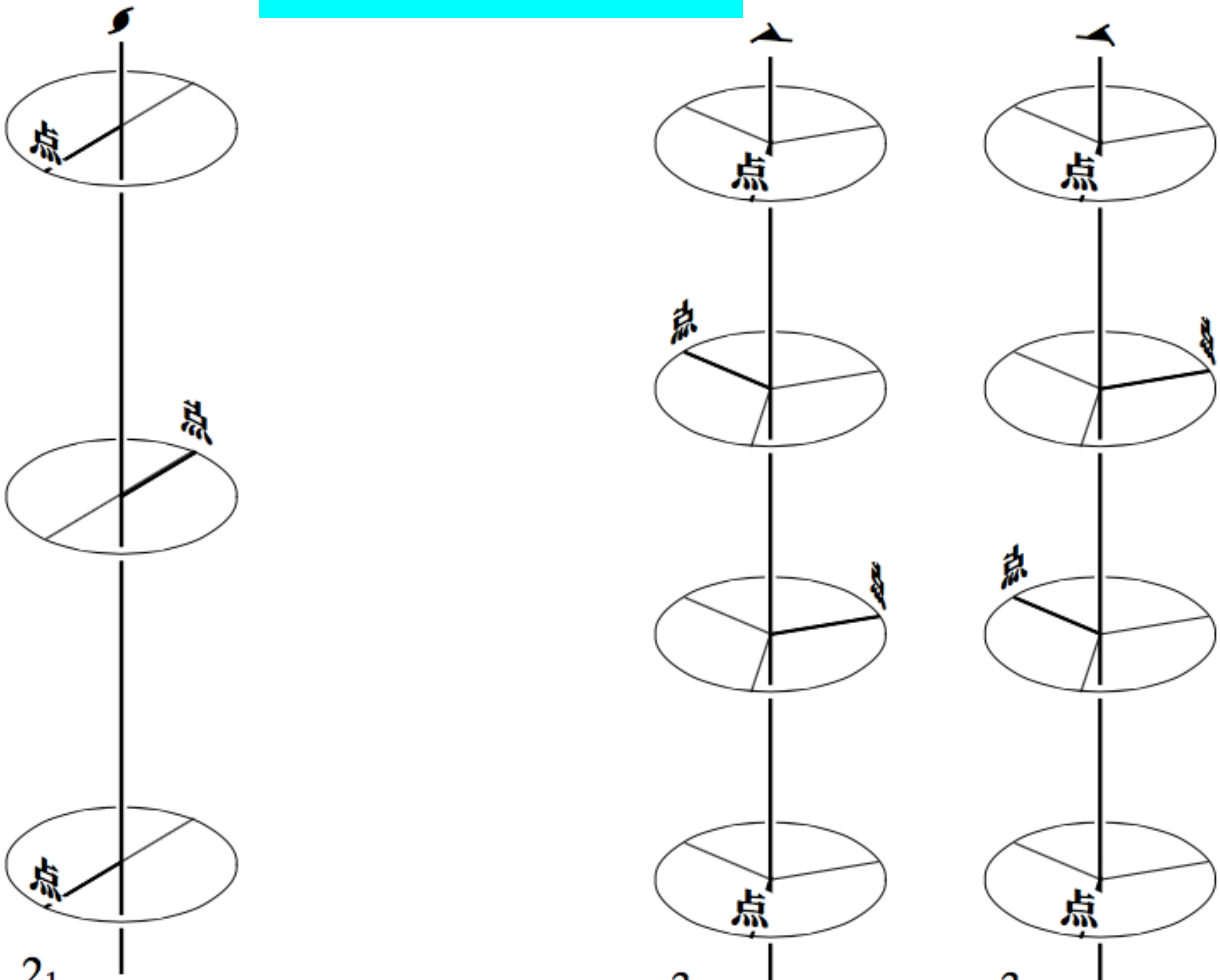
Screw rotation



n-fold rotation followed by a fractional translation $\frac{p}{n}\mathbf{t}$ parallel to the rotation axis

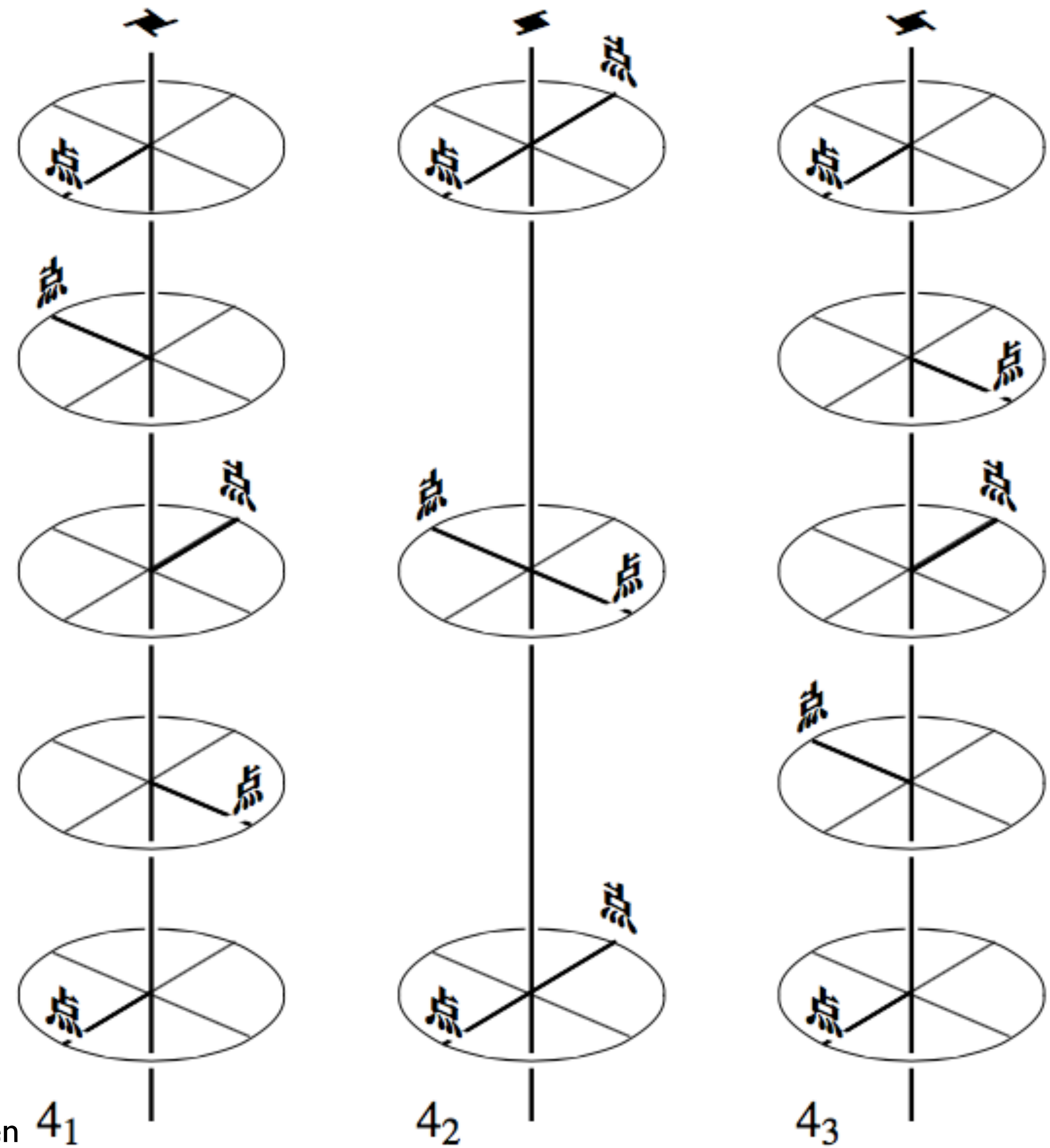
Its application *n* times results in a translation parallel to the rotation axis

Screw rotations



2_1 3_1 3_2

Screw rotations



The various rotation and screw axes and their symbol

printed symbol	symmetry axis	graphic symbol	nature of the screw translation
1	Identity	none	none
$\bar{1}$	Inversion	○	none
2	Rotation diad or twofold rotation axis	 (⊥ paper)  (// paper)	none
2_1	Screw diad or twofold screw axis	 (⊥ paper)  (// paper)	$c/2$ $a/2$ or $b/2$
3	Rotation triad	⊥ paper 	none
3_1 3_2	Screw triad		$c/3$ $2c/3$
$\bar{3}$	Inverse triad		none

printed symbol	symmetry axis	graphic symbol	nature of the screw translation
4	Rotation tetrad		none
4_1 4_2 4_3	Screw tetrads		$c/4$ $2c/4$ $3c/4$
$\bar{4}$	Inverse tetrad		none
6	Rotation hexad		none
6_1 6_2 6_3 6_4 6_5	Screw hexads		$c/6$ $2c/6$ $3c/6$ $4c/6$ $5c/6$
$\bar{6}$	Inverse hexad		none

Types of isometries do not preserve handedness

roto-inversion: centre of roto-inversion fixed
roto-inversion axis

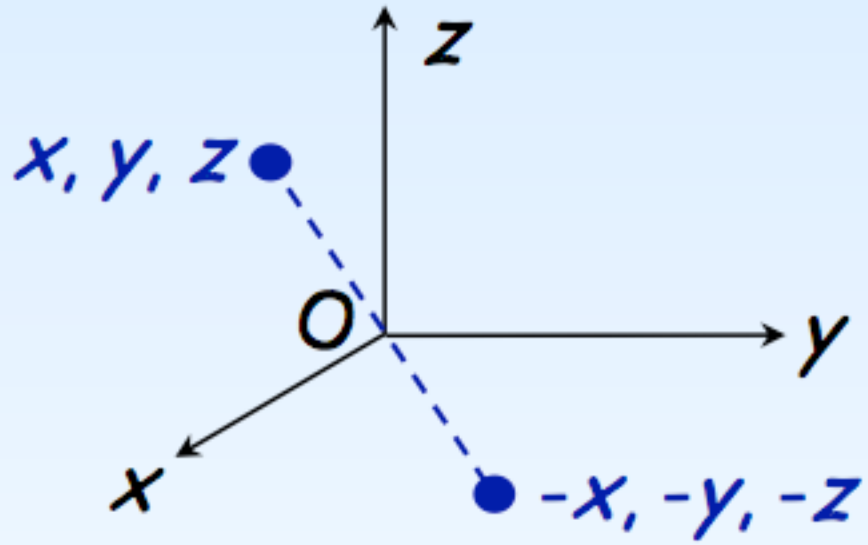
inversion: centre of inversion fixed

reflection: plane fixed
reflection/mirror plane

glide reflection: no fixed point
glide plane
glide vector

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\bar{1}$

a crystal which has the inversion symmetry is called centrosymmetrical.

$$\alpha(\bar{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

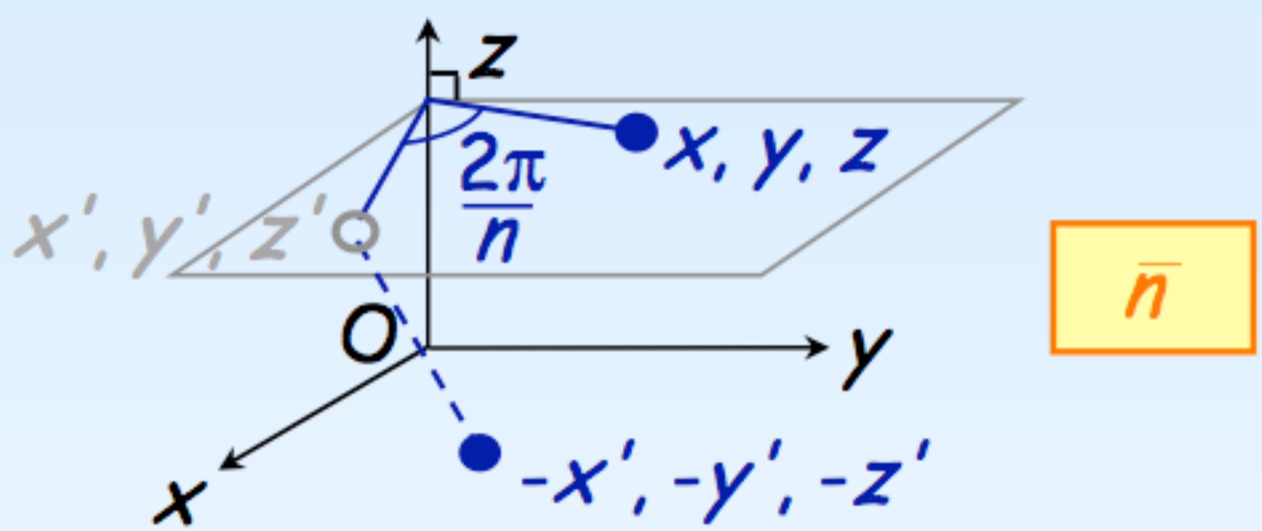
Det = -1

Symmetry operations in 3D
Rotoinvertions

Roto-inversion

(around an axis and through a point)

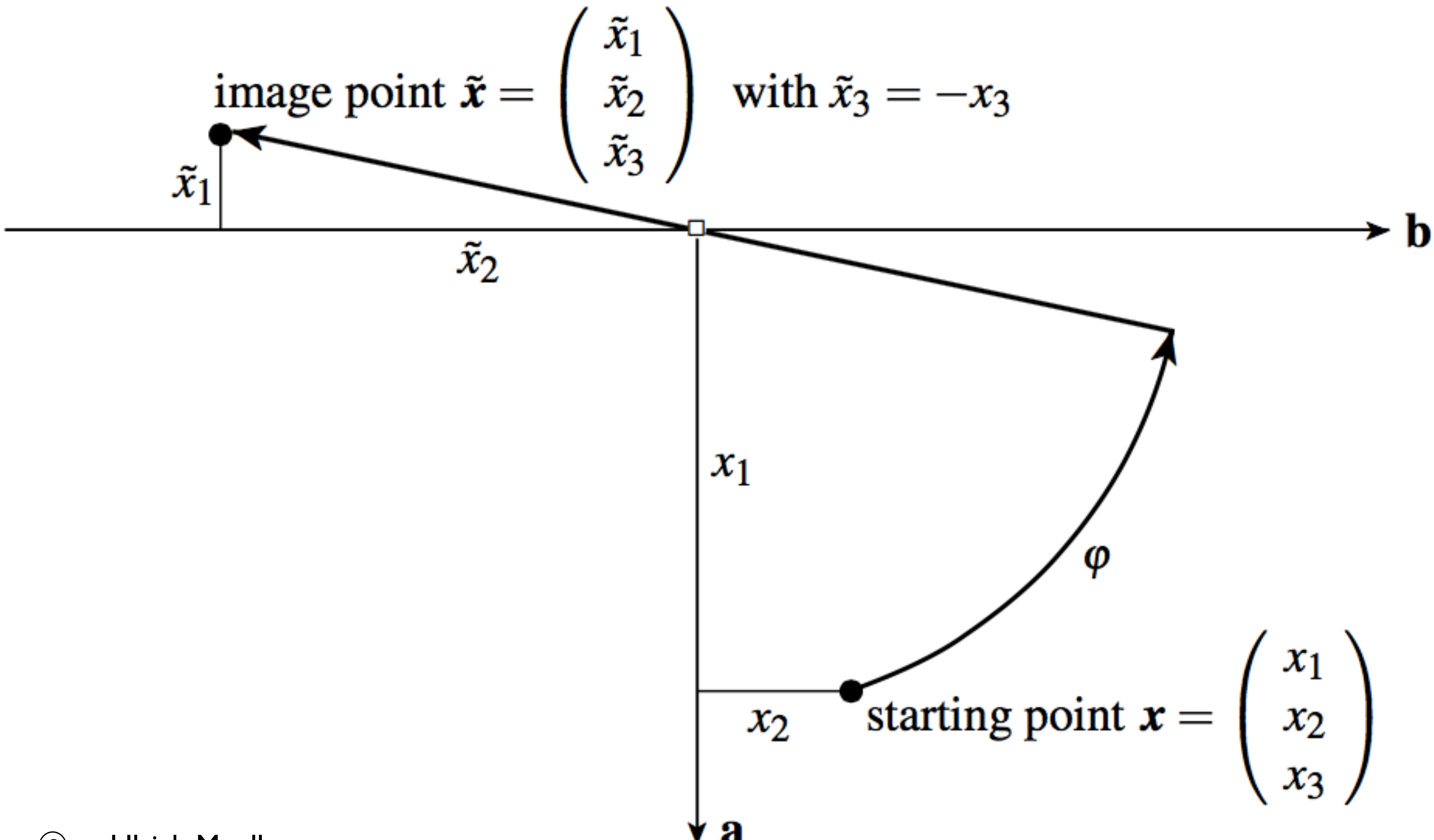
Rotation followed by an inversion



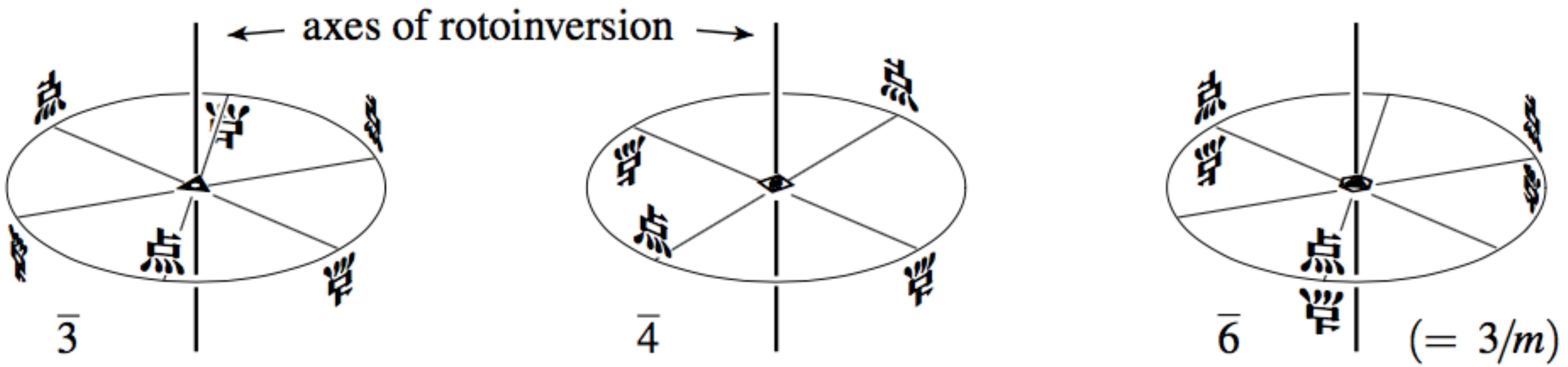
$$\alpha(\bar{n}) = \begin{pmatrix} -\cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

Rotoinversion

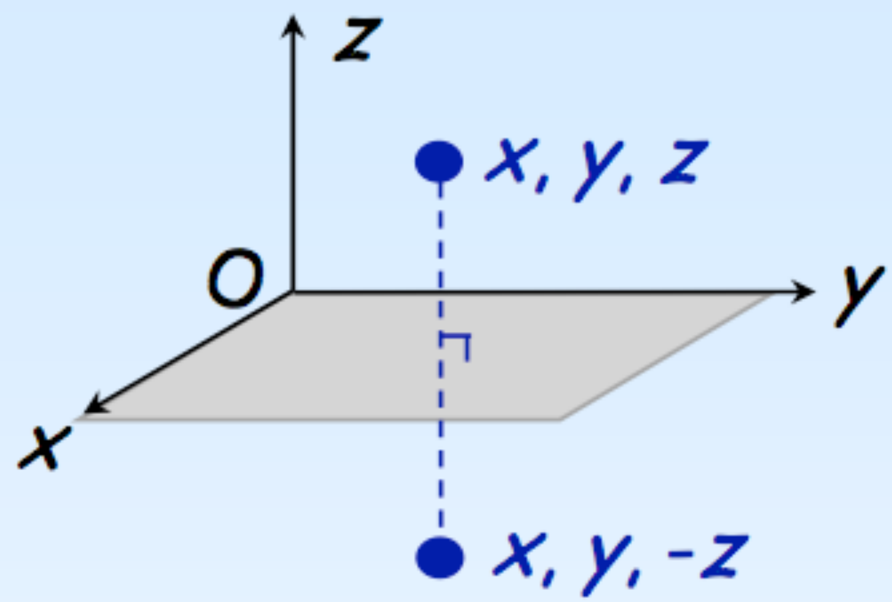


Rotoinversion



Symmetry operations in 3D
Reflection

Reflection (through a mirror plane)



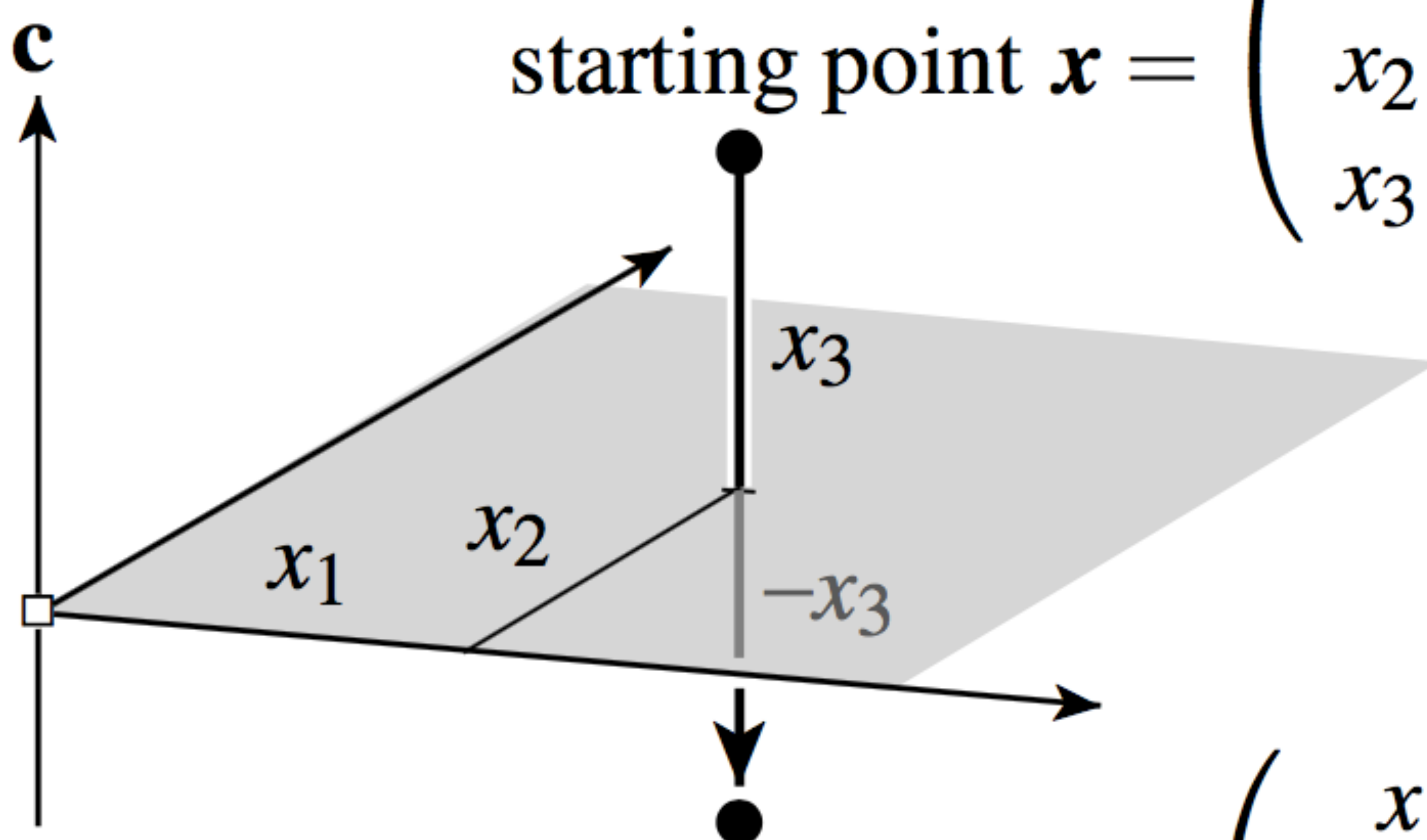
m

Note that: $m = \bar{2}$!

$$\alpha(\bar{1}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

Reflection

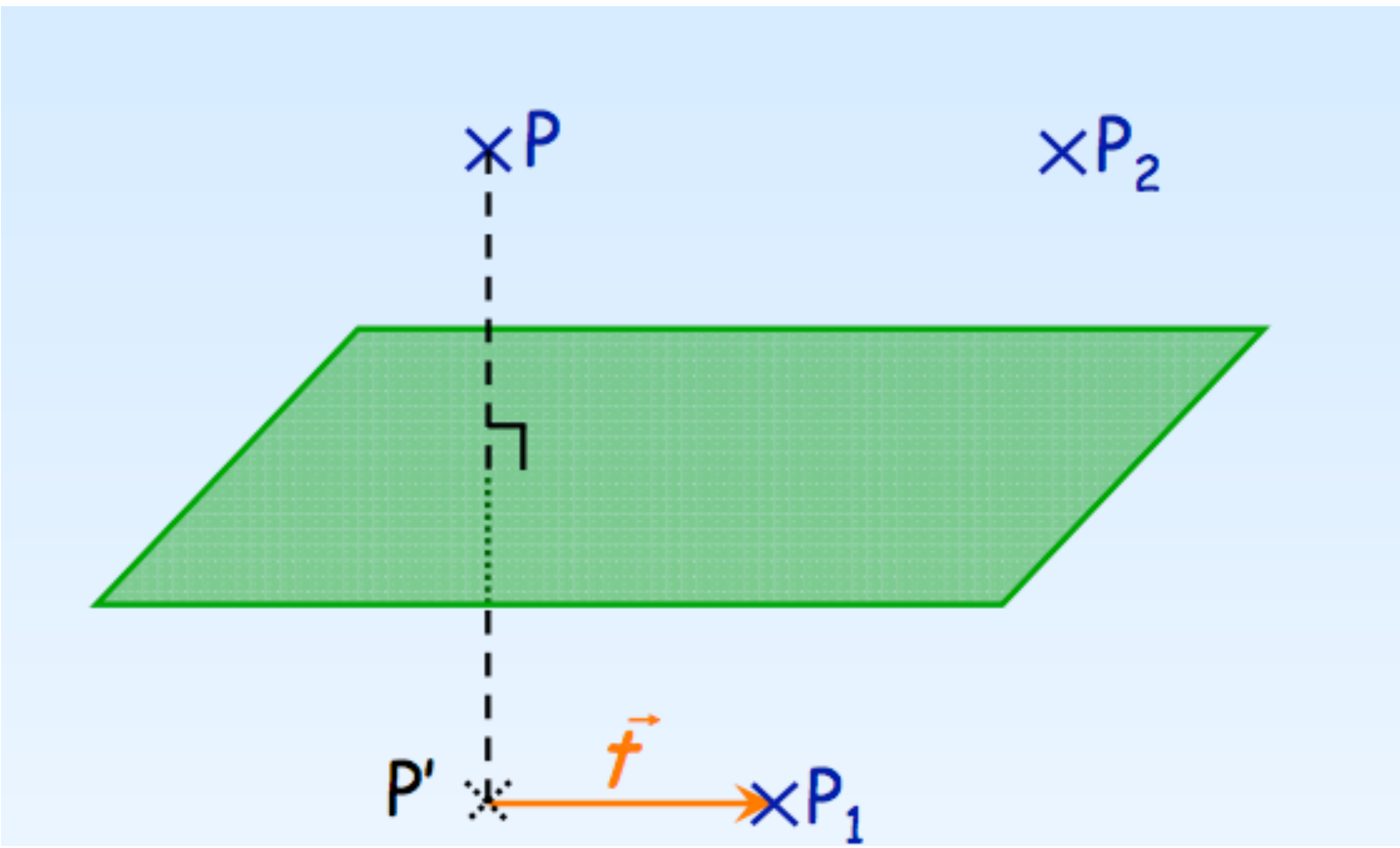


starting point $\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$

image point $\tilde{\boldsymbol{x}} = \begin{pmatrix} x_1 \\ x_2 \\ -x_3 \end{pmatrix}$

Crystallographic symmetry operations

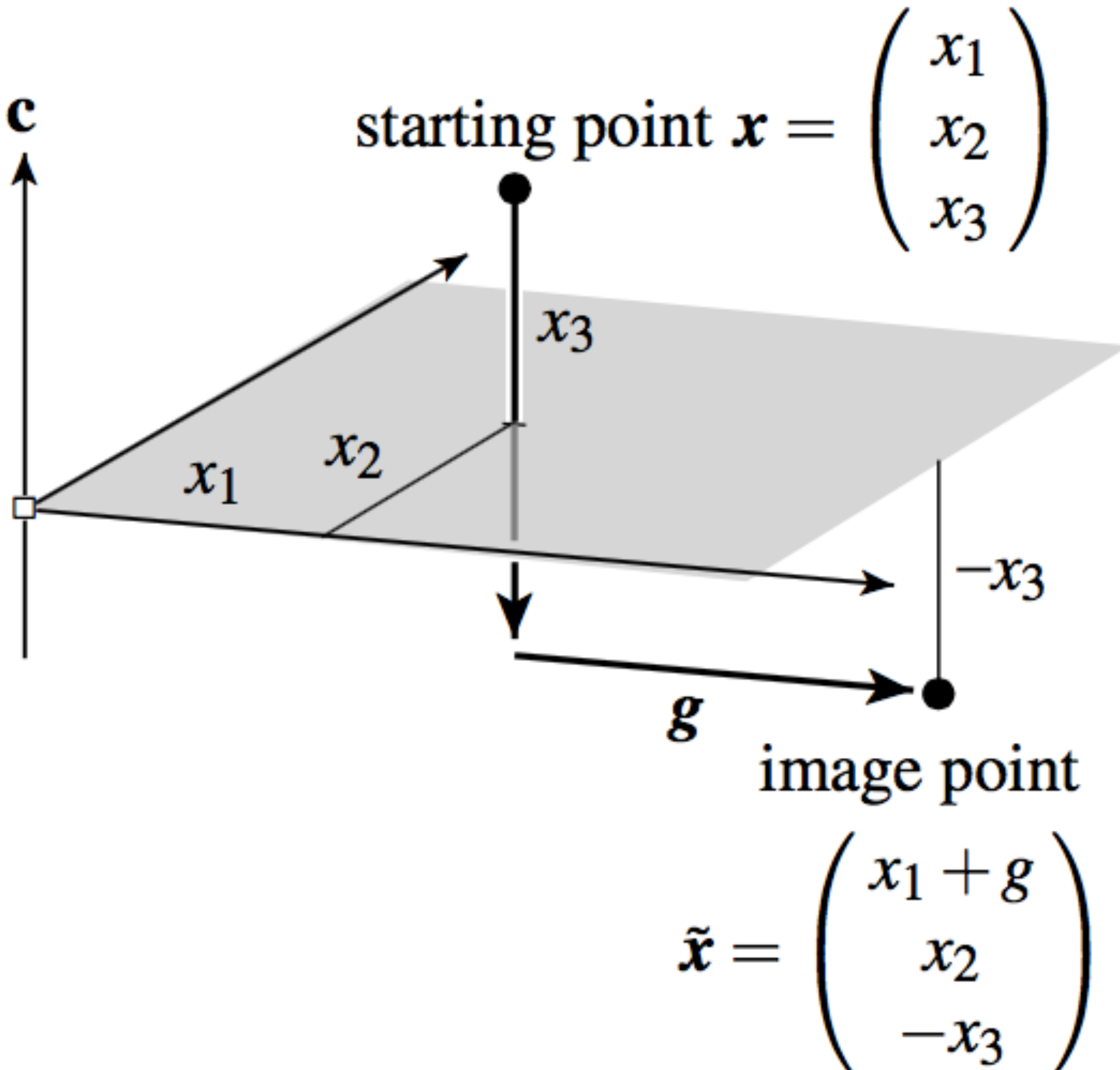
Glide plane



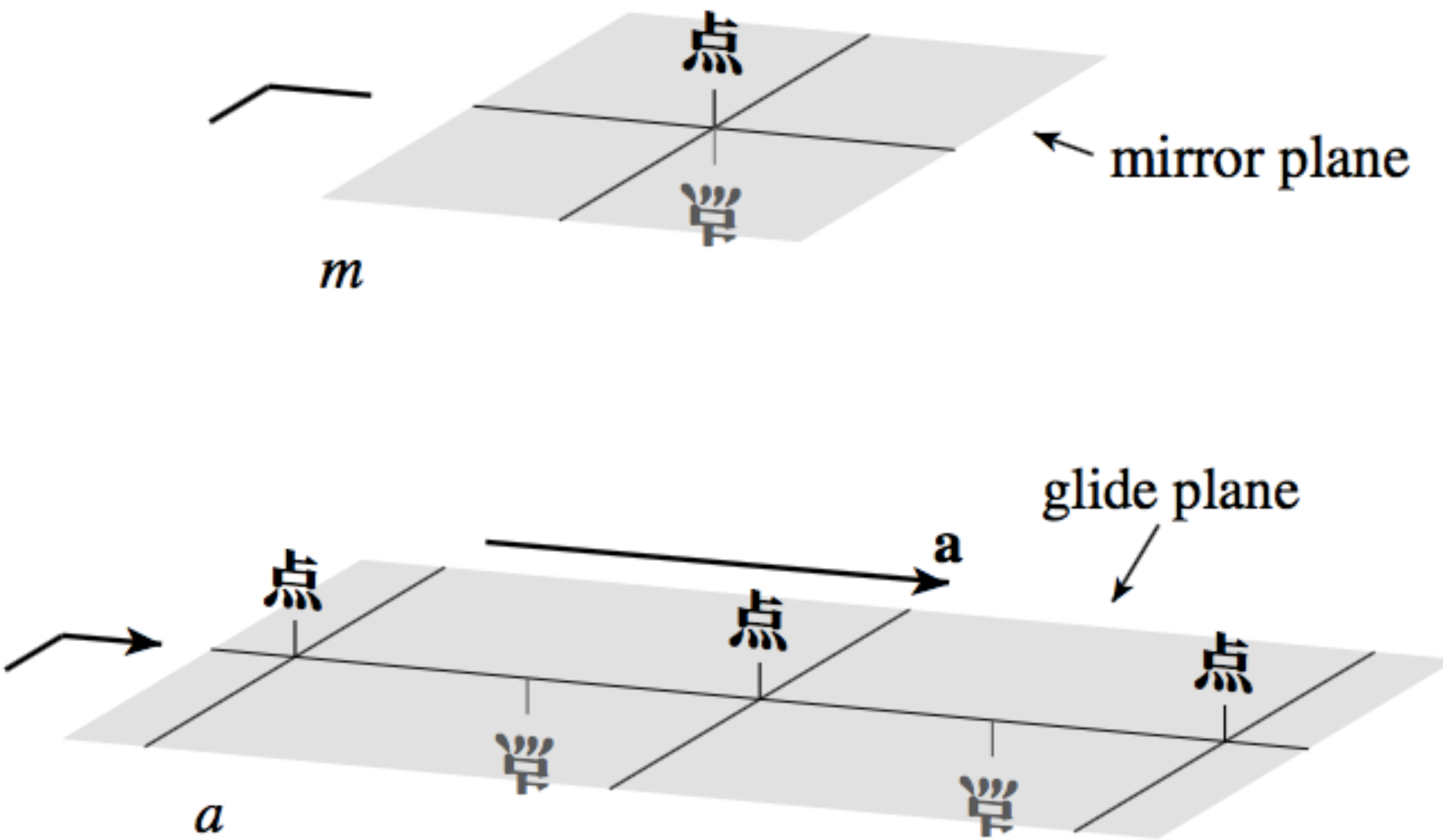
reflection followed by a fractional translation $\frac{1}{2}\mathbf{t}$ parallel to the plane

Its application 2 times results in a translation parallel to the plane

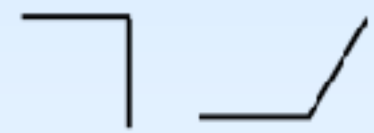
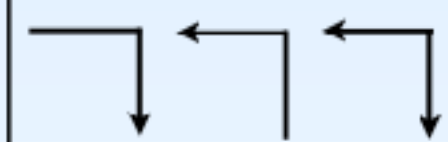
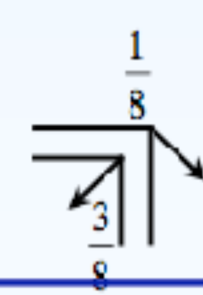
Glide reflection



Reflection and Glide reflection



The various symmetry planes and their symbol

printed symbol	symmetry plane	graphical symbol: normal to plane of projection	graphical symbol: parallel to plane of projection	nature of glide translation
m	reflection plane (mirror)	———————		none
a, *b*	axial glide plane	- - - - - -		*a*/2 or *b*/2
c	axial glide plane	··················	none	*c*/2
n	diagonal glide plane (*net*)	- · - · - · - · -		(*a*+*b*)/2, (*b*+*c*)/2 or (*c*+*a*)/2; OR (*a*+*b*+*c*)/2 for *t* and *c* systems
d	"diamond" glide plane			(*a*±*b*)/4, (*b*±*c*)/4 or (*c*±*a*)/4; OR (*a*±*b*±*c*)/4 for *t* and *c* systems

Matrix-column presentation of some symmetry operations

Rotation or rotoinversion around the origin:

$$\left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & 0 \\ W_{21} & W_{22} & W_{23} & 0 \\ W_{31} & W_{32} & W_{33} & 0 \end{array}\right) \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Translation:

$$\left(\begin{array}{ccc|c} 1 & & & w1 \\ & 1 & & w2 \\ & & 1 & w3 \end{array}\right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x+w1 \\ y+w2 \\ z+w3 \end{pmatrix}$$

Inversion through the origin:

$$\left(\begin{array}{ccc|c} -1 & & & 0 \\ & -1 & & 0 \\ & & -1 & 0 \end{array}\right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

GEOMETRIC INTERPRETATION OF THE MATRIX-COLUMN PRESENTATION OF THE SYMMETRY OPERATIONS

Geometric meaning of (W, w)

W information

(a) type of isometry

$\mathrm{tr}(\boldsymbol{W})$	$\det(\boldsymbol{W}) = +1$					$\det(\boldsymbol{W}) = -1$				
	3	2	1	0	−1	−3	−2	−1	0	1
type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
order	1	6	4	3	2	2	6	4	6	2

order: $\boldsymbol{W}^n = \boldsymbol{I}$

rotation angle $\cos\varphi = (\pm\mathrm{tr}(\boldsymbol{W}) - 1)/2$

EXERCISES

Problem 2.2.2 (cont.)

Determine the type and order of isometries that are represented by the following matrix-column pairs:

(1) x,y,z (2) -x,y+1/2,-z+1/2

(3) -x,-y,-z (4) x,-y+1/2, z+1/2

(a) type of isometry

	det(**W**) = +1					det(**W**) = −1				
tr(**W**)	3	2	1	0	−1	−3	−2	−1	0	1
type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
order	1	6	4	3	2	2	6	4	6	2

EXERCISES

Problem 2.2.1(cont.)

Consider the matrix-column pairs

$$(\boldsymbol{A}, \boldsymbol{a}) = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,\bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \text{ and } (\boldsymbol{B}, \boldsymbol{b}) = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(i) What is the matrix–column pair resulting from $(\boldsymbol{B}, \boldsymbol{b})(\boldsymbol{A}, \boldsymbol{a}) = (\boldsymbol{C}, \boldsymbol{c})$, and $(\boldsymbol{A}, \boldsymbol{a})(\boldsymbol{B}, \boldsymbol{b}) = (\boldsymbol{D}, \boldsymbol{d})$?

(ii) What is $(\boldsymbol{A}, \boldsymbol{a})^{-1}$, $(\boldsymbol{B}, \boldsymbol{b})^{-1}$, $(\boldsymbol{C}, \boldsymbol{c})^{-1}$ and $(\boldsymbol{D}, \boldsymbol{d})^{-1}$?

(iii) What is $(\boldsymbol{B}, \boldsymbol{b})^{-1}(\boldsymbol{A}, \boldsymbol{a})^{-1}$?

Determine the type and order of isometries that are represented by the matrices ***A***, ***B***, ***C*** and ***D***:

Geometric meaning of (W, w)
W information

(b) axis or normal direction $\boldsymbol{u}$: $\boldsymbol{W}\boldsymbol{u} = \pm\boldsymbol{u}$

(b1) rotations:

$$\boldsymbol{Y}(\boldsymbol{W}) = \boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I}$$

(b2) roto-inversions: $\boldsymbol{Y}(-\boldsymbol{W})$

reflections: $\boldsymbol{Y}(-\boldsymbol{W}) = -\boldsymbol{W} + \boldsymbol{I}$

Direction of rotation axis/normal

Example:

$$(W,w)=\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{array}\right)$$

det W=?

tr W=?

What is the type and order of the isometry?

Determine its rotation axis?

$$\boldsymbol{Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I}$$

$$Y(W)=\underbrace{\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{W^3}+\underbrace{\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{W^2}+\underbrace{\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{W}+\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{I}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

Problem 2.2.2 (cont)

Determine the rotation or rotoinversion axes (or normals in case of reflections) of the following symmetry operations

(2) -x,y+1/2,-z+1/2 (4) x,-y+1/2, z+1/2

rotations: $\boldsymbol{Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I}$

reflections: $\boldsymbol{Y(-W) = -W + I}$

Geometric meaning of (W, w)

W information

(c) sense of rotation:

for rotations or
rotoinversions with k>2

det(Z): $\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\,\boldsymbol{W}\boldsymbol{x}]$

$\boldsymbol{x}$ non-parallel to $\boldsymbol{u}$

Sense of rotation

Example:

$$(W,w)=\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{array}\right)$$

det W=1 tr W=1

$W=4_{001}$

What is its sense of rotation ?

$$\det(Z): \quad \boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}]$$

det Z=?

$$\mathbf{u}=\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \mathbf{x}=\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{Wx}=\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{Z}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

What is the sense of rotation of the operation

-y, x-y+1/2,-z+1/2

Fixed points of isometries

$(W,w)X_f = X_f$

solution:
point, line, plane or space

$$\left(\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix} \right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Fixed points?

NO solution:

$$\left(\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix} \right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

translation part **w**= $\begin{pmatrix} w1 \\ w2 \\ w3 \end{pmatrix}$

intrinsic
(screw, glide)

location

Fixed points of isometries

$$(W,w)X_f=X_f$$

Fixed points?

$$\left(\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}0\\0\\1/2\end{pmatrix}\right)\begin{pmatrix}x\\y\\z\end{pmatrix}=\begin{pmatrix}x\\y\\z\end{pmatrix}$$

solution:

point, line, plane or space

$$\left(\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}0\\1/2\\1/2\end{pmatrix}\right)\begin{pmatrix}x\\y\\z\end{pmatrix}=\begin{pmatrix}x\\y\\z\end{pmatrix}$$

NO solution:

translation part **w**= $\begin{pmatrix}w1\\w2\\w3\end{pmatrix}$

intrinsic (screw, glide)

location

Glide or **Screw** component (intrinsic translation part)

$$(\boldsymbol{W},\boldsymbol{w})^k = (\boldsymbol{W},\boldsymbol{w}).\,(\boldsymbol{W},\boldsymbol{w}).\,\ldots\,.(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{t})$$

$$(\boldsymbol{W},\boldsymbol{w})^k = (\boldsymbol{W}^k, (\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{t})$$

screw rotations : $\boldsymbol{t}/k = 1/k\;(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}$

glide reflections: $\boldsymbol{t}/k = \frac{1}{2}(\boldsymbol{W} + \boldsymbol{I})w$

EXERCISES

Problem 2.2.2 (cont.)

Determine the intrinsic translation parts (if relevant) of the following symmetry operations

(1) x,y,z　　(2) -x,y+1/2,-z+1/2

(3) -x,-y,-z　　(4) x,-y+1/2, z+1/2

screw rotations: $\boldsymbol{t}/k = 1/k\,(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}$

glide reflections: $$\boldsymbol{t}/k = \frac{1}{2}(\boldsymbol{W} + \boldsymbol{I})w$$

Fixed points of (W,w)

Location (fixed points x_F):

(B1) $t/k = 0$:

$$(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}_F = \boldsymbol{x}_F$$

(B2) $t/k \neq 0$:

$$(\boldsymbol{W}, \boldsymbol{w}_{lp})\boldsymbol{x}_F = \boldsymbol{x}_F$$

$$\boldsymbol{w}_{lp} = \boldsymbol{w} - \boldsymbol{t}/k$$

EXERCISES

Problem 2.2.2(cont.)

Determine the fixed points of the following symmetry operations:

(1) x,y,z (2) -x,y+1/2,-z+1/2

(3) -x,-y,-z (4) x,-y+1/2, z+1/2

fixed points: $(\boldsymbol{W}, \boldsymbol{w}_{lp})\boldsymbol{x}_F = \boldsymbol{x}_F$

Example **SOLUTION**

(i)

$$(W,w)(1)=\left(\begin{array}{ccc|c} 1 & & & 0 \\ & 1 & & 0 \\ & & 1 & 0 \end{array}\right)$$

$$(W,w)(2)=\left(\begin{array}{ccc|c} -1 & & & 0 \\ & 1 & & 1/2 \\ & & -1 & 1/2 \end{array}\right)$$

$$(W,w)(3)=\left(\begin{array}{ccc|c} -1 & & & 0 \\ & -1 & & 0 \\ & & -1 & 0 \end{array}\right)$$

$$(W,w)(4)=\left(\begin{array}{ccc|c} 1 & & & 0 \\ & -1 & & 1/2 \\ & & 1 & 1/2 \end{array}\right)$$

(ii) *ITA* description: under **Symmetry operations**

(1)	(2)	(3)	(4)
1	$2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$	$\bar{1}\ 0,0,0$	$c\ x,\frac{1}{4},z$

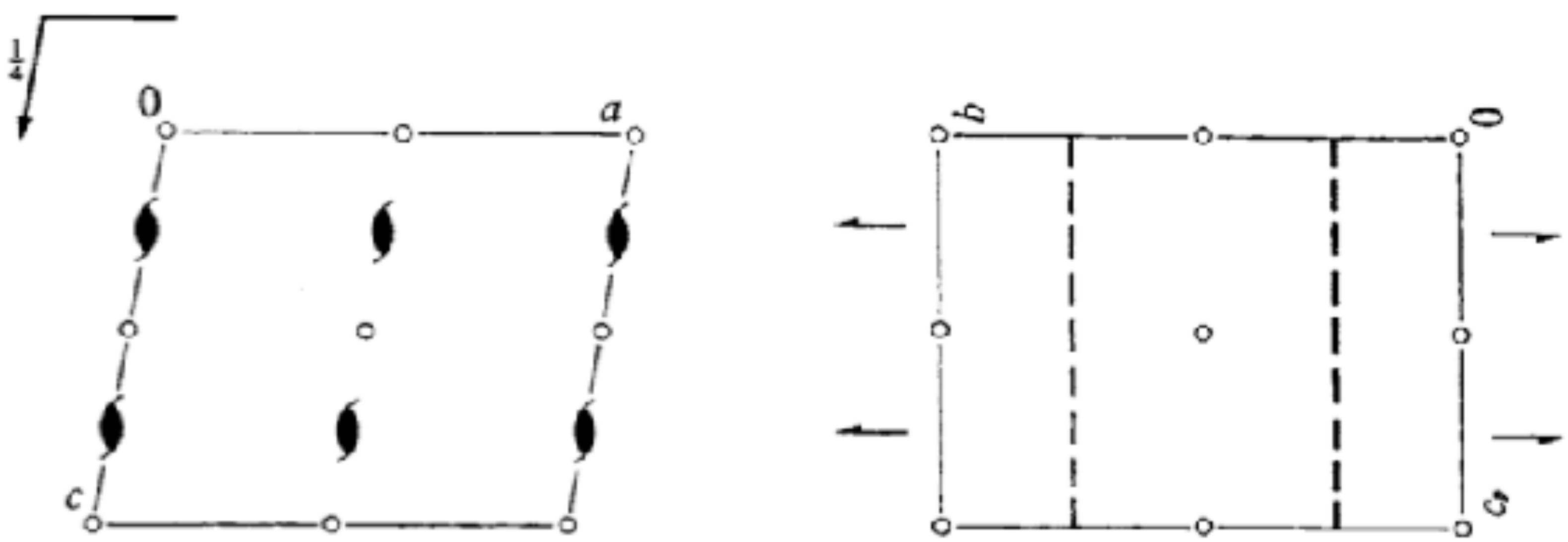
Space group $P2_1/c$ (No. 14)

$P2_1/c$ C_{2h}^5 $2/m$

No. 14 $P12_1/c1$ Patterson sy

UNIQUE AXIS *b*, CELL CHOICE 1

EXAMPLE



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Matrix-column presentation

4	*e*	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

Geometric interpretation

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$