1. Transformations and Symmetry

States of matter

There are three principal states of matter: gas, liquid, and solid. Gases and liquids are fluids. (They flow.)

gas:

-Isolated molecules with occasional collisions.

-No definite shape or volume (or density)

-Expand to occupy available space

liquid:

-Molecules in contact (approx.)

-Essentially incompressible (density ~ constant)

-No definite shape; conform to container

-Sufficient thermal energy to escape attraction of neighbors

solid:

-Crystalline materials with distinct atomic arrangements

-Definite shape and volume

-Insufficient thermal energy to change bonds among neighbors

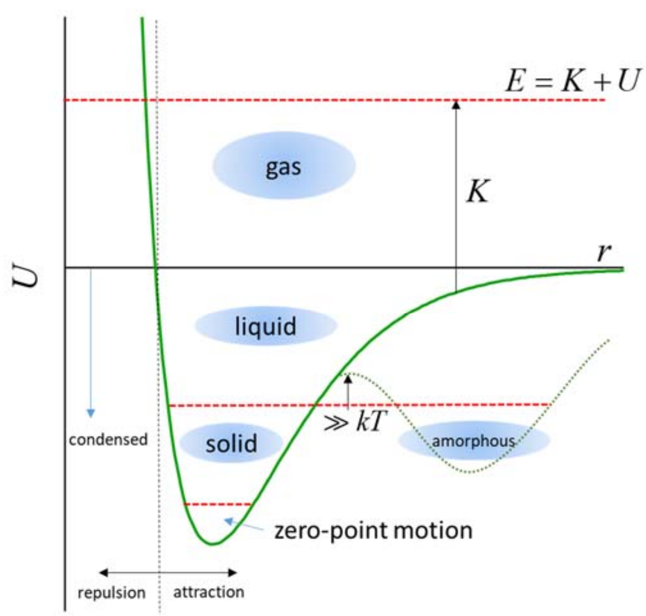
-Resists shear deformation

Microhomogeneity of crystals

The 3rd law of thermodynamics involves the entropy, which is defined by statistical mechanics as $S = k \cdot \ln W$, where k is the Boltzmann constant and W is the number of microstates that can be assumed by the constituent particles (atoms or molecules). The 3rd law is sometimes interpreted as *the entropy of a system tends towards zero as the temperature approaches absolute zero*. The Helmoltz free energy, expressed by $F = U - T \cdot S$, where U is the internal energy and T is the absolute temperature, is a minimum for a mechanically isolated system at constant T. At some finite temperature, the configuration that establishes this minimum depends on the coordinates and momenta of each of the particles. Thus, the state of a collection of particles at $T = 0$ K would be determined entirely by U, which depends only on the particle coordinates. If this configuration is unique (non-degenerate), only a single microstate would represent the ground state assumed at absolute zero, so that $W = 1$, in which case we would have $S = 0$. Whereas this would hold for an ensemble of featureless spherical particles without quantum-mechanical properties, in reality, there are other contributions to entropy, such as internal degrees of freedom, that will affect this conclusion. Nonetheless, it can be argues that a substance tends towards its ground state at low temperatures, and this state is likely to be small in number.

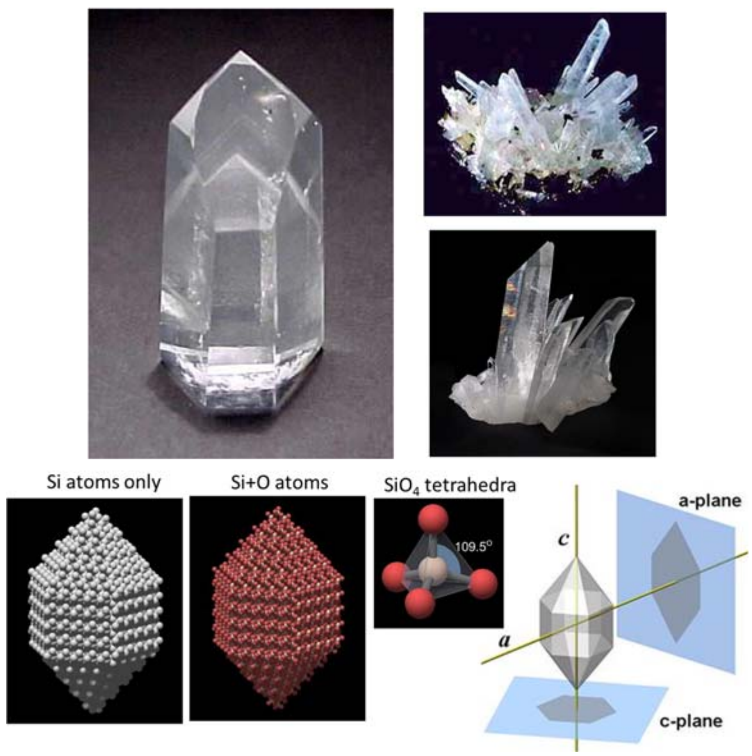
We do know that matter is discrete, meaning it is composed of atoms, rather than continuous. Though an atom may have spherical symmetry, its electronic structure changes with distance from the nucleus, so not all points are unique. Therefore, for a collection of atoms, some arrangement of the atoms must represent the minimum energy for the configuration, and any two matching collections of atoms must share the same ground-state configuration. If these collections represent subvolumes within a macroscopic system of condensed matter, then all other subvolumes selected from within this larger volume must share the same configuration. This requires the system to be translationally invariant, i.e., periodic. This property of "microhomogeneity" is used to argue that the minimum-energy (ground) state any material would be a crystalline solid. However, it may be difficult or impossible to reach that state for any given material at standard pressure, due to an inability to sufficiently cool the material. Increasing pressure has a similar effect to reducing temperature, so it sometimes possible to solidify ("freeze") materials (e.g., H) by increasing pressure.

Amorphous materials
A pair of oppositely charged ions clearly has a net electrostatic attraction. But even neutral atoms typically have a net attraction due to the covalent sharing of electrons that overcomes the electrostatic repulsion of the positive nuclei. For both ionic and covalent bonding, some equilibrium separation is established.



A material may be trapped in a metastable, disordered or nanocrystalline state when, for example it is synthesized under non-equilibrium conditions, which may involve quenching from a high temperature. The physical properties of these materials may resemble those of solids, but they do not have long-range translation symmetry. They can be considered "overcooled" solids.

Glass and pitch are two common examples of amorphous materials. Disordered glass can be referred to as a-SiO_2. Its crystalline counterpart is crystal quartz, referred to as c-SiO_2. These have the same chemical formula (although glass often contains impurities to affect its properties) and are both optically transparent. However, glass fractures in an irregular manner, whereas quartz cleaves on distinct crystal faces. The small fragments of broken quartz exhibit many of the same facets as large pieces of quartz. Glass is composed of long changes of randomly arranged SiO_2 molecules. Quartz contains a periodic, 3-D repetition of SiO_2 molecules, which are arranged into SiO_4 tectrahedra. Glass has no definite melting temperature; it exhibits increasing fluidity as the temperature is increased. Essentially, the constituent atoms have insufficient mobility to crystallize in a measurable time. Quartz melts at near 1700 °C.



Transformations, congruence, and symmetry
Isometric transformations are movements that keep distances between particular points on an object unchanged.

Objects are *congruent* if there is a one-to-one correspondence between related points on the objects, such that the distance between two points on one of the objects is equal to that between the related points on the other object.

Congruence may be *direct* or *opposite*.

Objects with direct congruence may be brought into coincidence by direct *movement*. A direct movement of an object is one in which the object behaves like a rigid body. We can envision the undistorted object at all intermediate steps. Direct movements are also called motions, proper motions, direct motions, or motions of the fist kind. Only one of the following three kinds of direct movement are required, in general, to bring congruent objects into coincidence.

1) translation

2) rotation

3) rototranslation

Objects with opposite congruence are called *enantiomers* (enantiomeric). They are isometric, but not superposable on each other. Objects with opposite congruence may be brought into coincidence by opposite movement. An opposite movement of an object cannot be pictured as a continuous transformations of a rigid body. Opposite movements are also called improper motions, opposite motions, or motions of the second kind. Objects with opposite congruence may be brought into coincidence by the following improper motions:

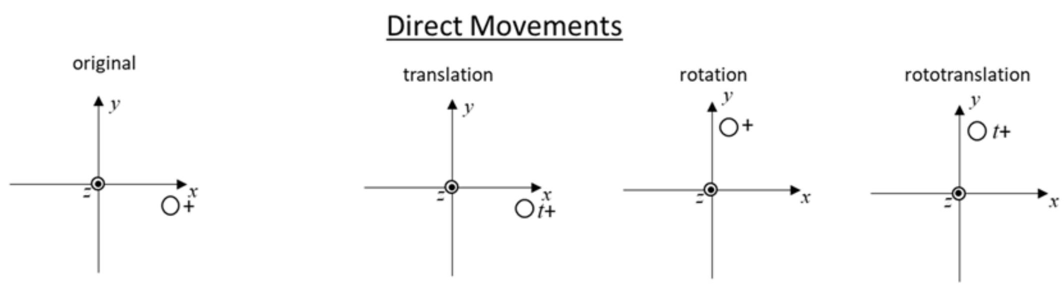
1) inversion (w.r.t. a point)

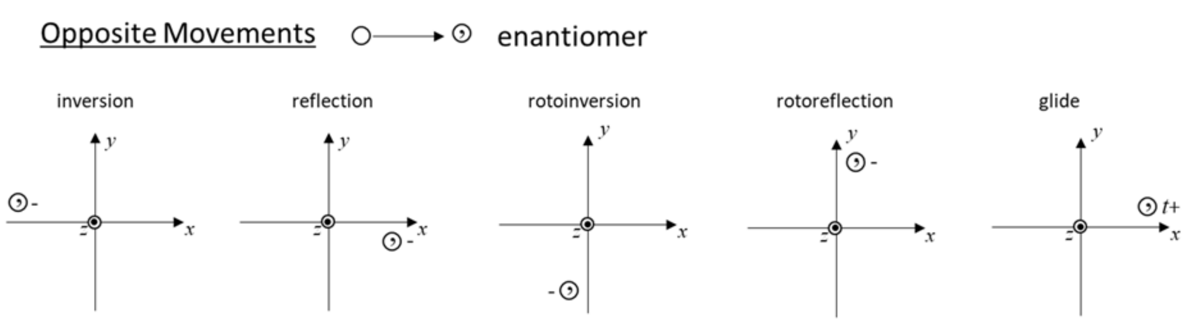
2) reflection (w.r.t. a plane)

3) rotoinversion (w.r.t. an axis and a point on the axis, in either order)

4) glide

5) rotoreflection





Symmetry operations and elements
A symmetry operation is an isometric transformation of an entire space that leaves all properties of the space unchanged.

A symmetry element is a point, line, or plane w.r.t. which symmetry operations are performed. Points on the symmetry element often remain unaffected by the transformation, except, for example, when a translation is involved.

Transformations

An affine transformation maps points to points, lines to lines, and planes to planes, but it does not necessarily preserve angles. These transformations can always be written in the general form

$$\mathbf{r}' = M \cdot \mathbf{r} + \mathbf{t}$$

where M is a matrix. We can specify a vector in cartesian coordinates as $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$. This can be factored into the product of a matrix with a column vector

$$\mathbf{r} = (\hat{\mathbf{x}} \quad \hat{\mathbf{y}} \quad \hat{\mathbf{z}}) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

For the moment, let's call the matrix A^T. We will study its properties later. In unit cartesian coordinates, it is simply identity. That is, the basis itself is same unit vectors referred to themselves

$$\mathrm{A}^T = (\hat{\mathbf{x}} \quad \hat{\mathbf{y}} \quad \hat{\mathbf{z}}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I$$

So we can pass between two forms to write a vector.

$$\mathbf{r} = X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Our affine transformation can be written

$$X' = M \cdot X + T$$

Types of isometric transformations

Consider a vector connecting two points 1 and 2: $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. After an affine transformation of all points in space, the vector is $\mathbf{r}' = \mathbf{r}_2' - \mathbf{r}_1'$, where $\mathbf{r}_1' = M \cdot \mathbf{r}_1 + \mathbf{t}$ and $\mathbf{r}_2' = M \cdot \mathbf{r}_2 + \mathbf{t}$. So $\mathbf{r}' = M \cdot \mathbf{r}$. If the transformation is isometric, then $|\mathbf{r}'| = |\mathbf{r}|$. We can use

$$|\mathbf{r}|^2 = \mathbf{r} \cdot \mathbf{r} = X^T \cdot X$$

and

$$|\mathbf{r}'|^2 = \mathbf{r}' \cdot \mathbf{r}' = X'^T \cdot X' = (MX)^T \cdot MX$$

So

$$X^T \cdot X = (MX)^T \cdot MX .$$

The transpose of a produce is the product of the transposes:

$$X^T \cdot X = \left(X^T \cdot M^T\right) \cdot M \cdot X = X^T \cdot \left(M^T \cdot M\right) \cdot X$$

Apparently $M^T \cdot M = I$, so $M^T = M^{-1}$. Since $\det(I) = 1$, we know that $\det\left(M^T \cdot M\right) = 1$. The determinant of a product is the product of the determinants (if the determinants exist), i.e., $\det(A \cdot B) = \det(A) \cdot \det(B)$. So $1 = \det\left(M^T\right) \cdot \det(M)$. But $\det\left(M^T\right) = \det(M)$, so $\det^2(M) = 1$. This means that $\det(M) = \pm 1$. We have two types of isometric transformations:

$$\det(M) = \begin{cases} +1, & \text{proper} \\ -1, & \text{improper} \end{cases}$$

In 2-D, we can write M in the generic form

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

Clearly

$$M^T \cdot M = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a^2 + c^2 & ab + cd \\ ab + cd & b^2 + d^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

So we know three things

i) $1 = a^2 + c^2 = b^2 + d^2$

ii) $0 = ab + cd$

iii) $\pm 1 = ad - bc$

From i), we can define two angles: $a = \cos\theta_1$, $b = -\sin\theta_2$ $c = \sin\theta_1$, and $d = \cos\theta_2$. From iii), we have

$$\pm 1 = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 = \cos(\theta_2 - \theta_1)$$

From ii), we know that $c/a = -b/d$, so $\tan\theta_1 = \tan\theta_2$. Then $\theta_2 - \theta_1 = n\pi$, where $n \in \mathbb{Z}$, where proper transformations have n even and improper have n odd. Let's rename $\theta_2 \to \theta$. We have

$$M = \begin{pmatrix} \cos(\theta - n\pi) & -\sin\theta \\ \sin(\theta - n\pi) & \cos\theta \end{pmatrix}$$

The proper transformations (*n* even) give

$$M = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

and the improper transformations (*n* odd) give

$$M = \begin{pmatrix} -\cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

Rotations

A point *P* can be located by the vector $\mathbf{r}$ pointing from the origin *O* to *P*. In 2-D cartesian coordinates:

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} = r \cdot \cos\phi\hat{\mathbf{x}} + r \cdot \sin\phi\hat{\mathbf{y}}$$

where r is the length of $\mathbf{r}$ and ϕ is the angle from the x axis.

Rotating *P* about the origin by an angle θ onto P', located by the vector $\mathbf{r}'$, gives

$$\mathbf{r}' = x'\hat{\mathbf{x}} + y'\hat{\mathbf{y}} = r \cdot \cos(\phi + \theta)\,\hat{\mathbf{x}} + r \cdot \sin(\phi + \theta)\,\hat{\mathbf{y}}$$

where the distance from the origin is unchanged. Using trig identities:

$$x' = r \cdot \cos(\phi + \theta) = r \cdot \cos\phi \cdot \cos\theta - r \cdot \sin\phi \cdot \sin\theta$$
$$y' = r \cdot \sin(\phi + \theta) = r \cdot \cos\phi \cdot \sin\theta + r \cdot \sin\phi \cdot \cos\theta$$

So

$$x' = \cos\theta \cdot x - \sin\theta \cdot y$$
$$y' = \sin\theta \cdot x + \cos\theta \cdot y$$

The coefficients can be represent by a matrix

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix}$$

or $\mathbf{r}' = R_\theta \cdot \mathbf{r}$. The matrix is the same as our 2-D proper transformation, so the angle in M for proper transformations can be identified as the angle of rotation.

Reflections

Consider the improper transformation with $\theta = 0$.

$$M = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Applying this to a point located by vector r gives

$$\mathbf{r}' = M \cdot \mathbf{r} = \begin{pmatrix} -x \\ y \end{pmatrix}$$

This is a reflection in x (across the y axis). So we can label this particular matrix

$$m_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Another case to consider is $\theta = 180°$:

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Now

$$\mathbf{r}' = M \cdot \mathbf{r} = \begin{pmatrix} x \\ -y \end{pmatrix}$$

so this is a reflection in y (across the x axis).

$$m_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

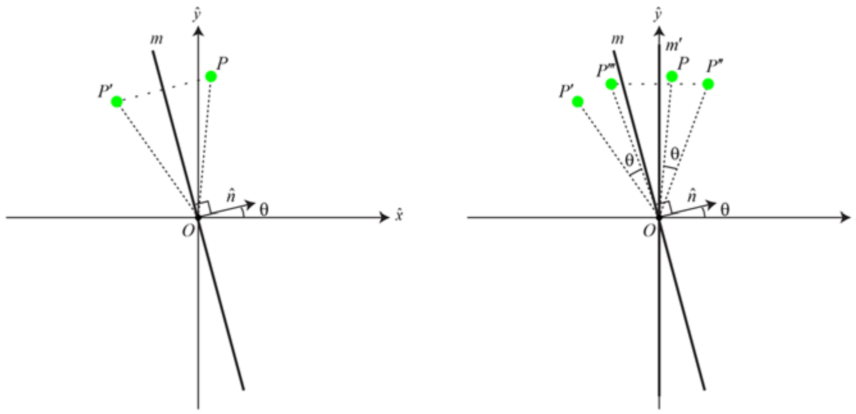
But x and y axes are 90° apart, so how do we interpret the angle θ?

Let's reflect across a line with its normal at angle θ from the x axis. We can do this with the following steps: 1) rotate CW by θ; 2) reflect across x; 3) rotate CCW by θ. We will call the combined operation m_θ.

$$\mathbf{r}' = R_\theta \cdot m_x \cdot R_{-\theta} \cdot \mathbf{r} = m_\theta \cdot \mathbf{r}$$

where

$$m_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} -\cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{pmatrix}$$



So we need to use this form to reflect across a line with its normal at angle θ from the x axis. Now we can say $m_x = m_{0^\circ}$ and $m_y = m_{90^\circ}$.

Invariant points

The only matrices we need for isometric transformations in 2-D describe rotations (proper) are:

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

or reflections (improper)

$$m_\theta = \begin{pmatrix} -\cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{pmatrix}$$

We often associate the transformation with the locust of points that are unchanged by the transformation; that is, those with coordinates X satisfying $M \cdot X = X$. For a rotation in 2-D, the only invariant point, which must satisfy $R_\theta \cdot X = X$, is the origin O, i.e.

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

We recognize the transformation to be a CW rotation by θ about the origin.

Points that are invariant under reflection must satisfy $m_\theta \cdot X = X$. Some algebra gives the equation $\cos\theta \cdot x + \sin\theta \cdot y = 0$. We could write the locust of invariant points as

$$\begin{pmatrix} x \\ y \end{pmatrix} = s \cdot \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$$

where s is a free variable. We can see that this set of points crosses the origin when $s = 0$.

Consider the set of all points along the y axis, which is, by definition, a line

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ s \end{pmatrix}$$

We could rotate all points on the line by applying R_θ

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} 0 \\ s \end{pmatrix} = s \cdot \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$$

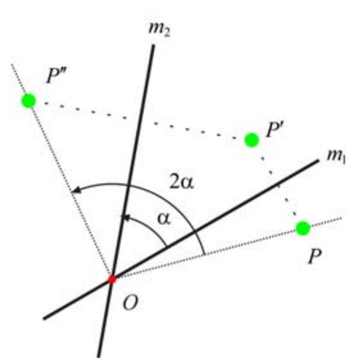
So we can see that the set of invariant points under reflection m_θ are this along a line rotated CW by an angle θ from the y axis. When we continue to 3-D transformations, we will see that is more practical to describe a reflection by the direction normal to the locust of invariant points. This normal direction is $90°$ from the line of reflection, corresponding to a CW rotation of θ from the x-direction.

Double reflection-intersecting lines

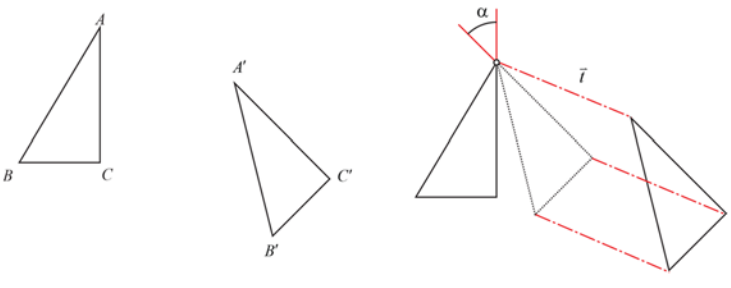
Now consider the sequential reflection in 2-D across two lines m_1 and m_2 at an angle α from each other. Let's assume the lines intersect at O. Their normals are at θ_1 and θ_2 from the x-axis. Reflecting first across m_1 , then across m_2 :

$$\mathbf{r}' = m_{\theta_2} \cdot m_{\theta_1} \cdot \mathbf{r}$$
$$= \begin{pmatrix} -\cos(2\theta_2) & -\sin(2\theta_2) \\ -\sin(2\theta_2) & \cos(2\theta_2) \end{pmatrix} \cdot \begin{pmatrix} -\cos(2\theta_1) & -\sin(2\theta_1) \\ -\sin(2\theta_1) & \cos(2\theta_1) \end{pmatrix} \cdot \mathbf{r}$$
$$\mathbf{r}' = \begin{pmatrix} \cos[2(\theta_2 - \theta_1)] & -\sin[2(\theta_2 - \theta_1)] \\ \sin[2(\theta_2 - \theta_1)] & \cos[2(\theta_2 - \theta_1)] \end{pmatrix} \cdot \mathbf{r} = R_{2(\theta_2 - \theta_1)} \cdot \mathbf{r}$$

The net effect is the rotation $R_{2\alpha}$, which is twice the angle between the lines.



2-D transformations
We can use an asymmetric right triangle as a "metric" in 2-D. Say we want to map congruent triangles onto each other. One way to map $A'B'C'$ onto ABC is to translate by the vector $\mathbf{t} = A - A'$, which bring A' into coincidence with A. Then we rotate to bring B' and C' into coincidence with B and C . We could have brought any corresponding points on the metric into coincidence, then used that point as the rotation center.



We can write out the 2-D transformation $X' = M \cdot X + T$ as follows:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} t_x \\ t_y \end{pmatrix} = \begin{pmatrix} m_{11}x + m_{12}y + t_x \\ m_{21}x + m_{22}y + t_y \end{pmatrix}$$

Let's define a new type of column vector with one extra row.

$$Y' = \begin{pmatrix} x' \\ y' \\ 1 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} & t_x \\ m_{21} & m_{22} & t_y \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ 1 \end{pmatrix} = N \cdot Y$$

We could write this new matrix as

$$N = \begin{pmatrix} (M) & \mathbf{t} \\ 0 & 1 \end{pmatrix}$$

Say we know three points of corresponding point pairs, i.e. $X_1 \to X_1'$, $X_2 \to X_2'$, $X_3 \to X_3'$. These can be sorted into matrices

$$Y = \begin{pmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ 1 & 1 & 1 \end{pmatrix} \text{ and } Y' = \begin{pmatrix} x_1' & x_2' & x_3' \\ y_1' & y_2' & y_3' \\ 1 & 1 & 1 \end{pmatrix}$$

If Y is invertible, we can now find N using $N = Y' \cdot Y^{-1}$.

Inverting a matrix
A general procedure for inverting a matrix M is described by the notation

$$M^{-1} = \frac{1}{\det(M)} \cdot adj(M)$$

where $\det(M)$ is the determinant and $adj(M)$ refers to the adjugate matrix $adj(M) = C^T$, where C contains the cofactors of M

$$C_{ij} = (-1)^{i+j} \cdot \det[M(i \mid j)]$$

Here, $M(i \mid j)$ is found from M with row i and column j removed. This can be used to write the determinant in a recursive form

$$\det(M) = \sum_j (-1)^j \cdot M_{1j} \cdot \det[M(1 \mid j)]$$

Transformations with translations

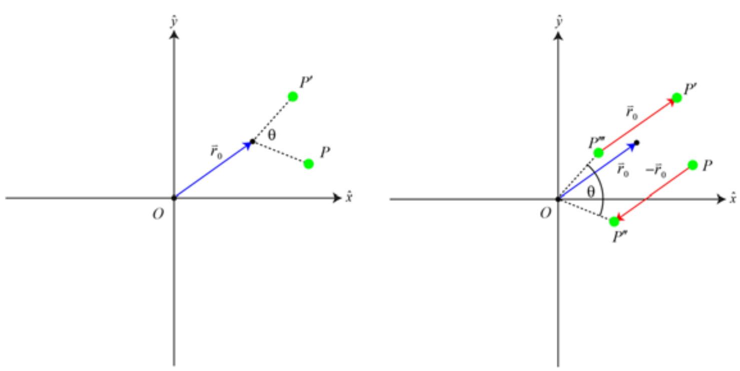
We will often want to group a transformation $\mathbf{r}' = M \cdot \mathbf{r} + \mathbf{t}$ differently to make the type of transformation more obvious, for example

$$\mathbf{r}' = M \cdot (\mathbf{r} - \mathbf{r}_0) + \mathbf{r}_0 + \mathbf{t}_0$$

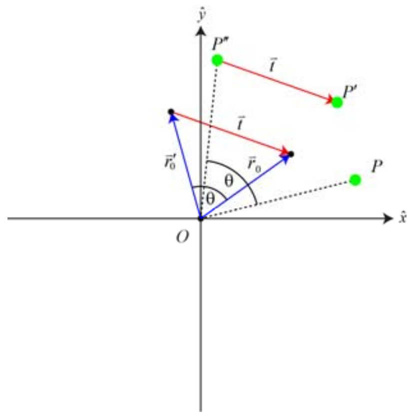
in which case $\mathbf{t} = (I - M) \cdot \mathbf{r}_0 + \mathbf{t}_0$. In the form above, $\mathbf{r}_0$ represents the plane, line, or point at which the reflection, rotation, or inversion, respectively, is performed, while $\mathbf{t}_0$ represents the translation component of the transformation. We first translate the point at $\mathbf{r}_0$ to the origin, apply M, translate back, then apply the pure translation by $\mathbf{t}_0$. This will be useful for the symmetry operations relevant to crystallography, because we are interested in those for which the multiplication by M commutes with the addition of $\mathbf{t}_0$. (This allows identification unique set of transformations that don't depend on how we decide to group terms.) Therefore, $M \cdot (\mathbf{r} - \mathbf{r}_0) + \mathbf{r}_0 + \mathbf{t}_0 = M \cdot (\mathbf{r} - \mathbf{r}_0 + \mathbf{t}_0) + \mathbf{r}_0$, which requires $M \cdot \mathbf{t}_0 = \mathbf{t}_0$.

Rotation about an arbitrary point

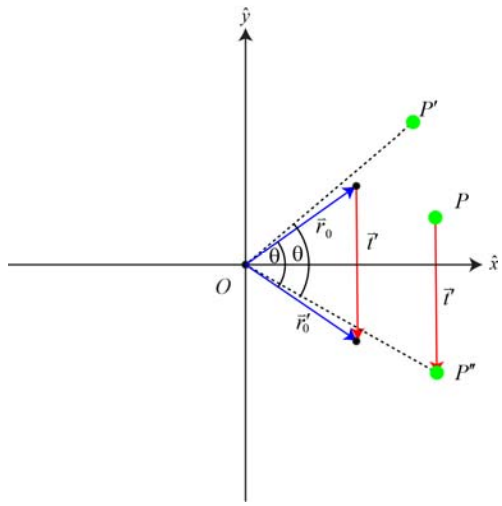
The rotation matrix R_θ rotates by θ about O. To rotate a space by θ about an arbitrary point at $\mathbf{r}_0$, we can first translate by $-\mathbf{r}_0$, then apply R_θ, then translate back by $\mathbf{r}_0$, so $\mathbf{r}' = R_\theta \cdot (\mathbf{r} - \mathbf{r}_0) + \mathbf{r}_0$.



Grouping things differently leads to other possibilities. For example, defining $\mathbf{t} = \mathbf{r}_0 - R_\theta \cdot \mathbf{r}_0$, we can write $\mathbf{r}' = R_\theta \cdot \mathbf{r} + \mathbf{t}$. This is a rotation about O, *followed* by a translation by $\mathbf{t}$.

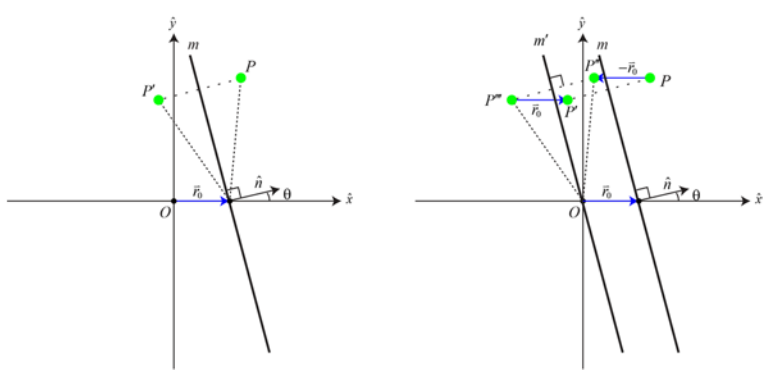


If we define $\mathbf{t}' = R_{-\theta} \cdot \mathbf{r}_0 - \mathbf{r}_0$, then the transformation is $\mathbf{r}' = R_\theta \cdot (\mathbf{r} + \mathbf{t}')$, which represents a rotation about O *after* a translation by $\mathbf{t}'$.

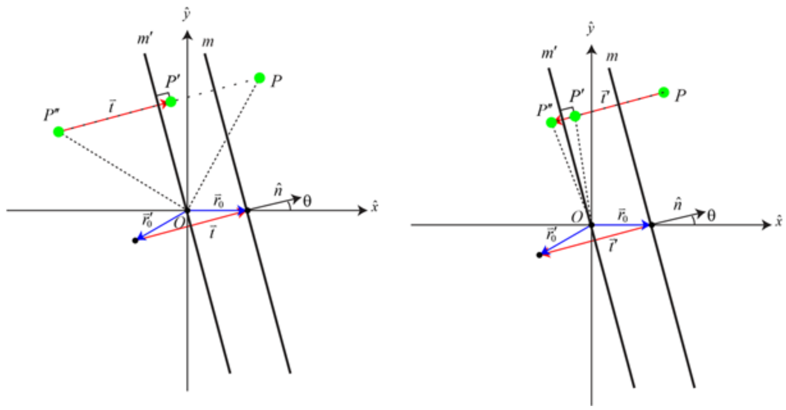


Reflection across an arbitrary line

Now let's reflect across a rotated line that does not pass through O. We can locate the line by a vector $\mathbf{r}_0$ that points from O to any point on the line (so it is not unique). Translate by $-\mathbf{r}_0$, apply m_θ, then translate back by $\mathbf{r}_0$: $\mathbf{r}' = m_\theta \cdot (\mathbf{r} - \mathbf{r}_0) + \mathbf{r}_0$.



Again, we can group things in different ways. Defining $\mathbf{t} = \mathbf{r}_0 - m_\theta \cdot \mathbf{r}_0$, we have $\mathbf{r}' = m_\theta \cdot \mathbf{r} + \mathbf{t}$, which represents a reflection, followed by a translation. Alternatively, using $\mathbf{t}' = m_\theta \cdot \mathbf{r}_0 - \mathbf{r}_0$, we can write $\mathbf{r}' = m_\theta \cdot (\mathbf{r} + \mathbf{t}')$, which describes a translation, followed by a reflection.



How can we interpret the form $\mathbf{r}' = m_\theta \cdot \mathbf{r} + \mathbf{t}$, where $\mathbf{t} = (I - m_\theta) \cdot \mathbf{r}_0$? The difference matrix is:

$\mathbf{t} = (I - m_\theta) \cdot \mathbf{r}_0$. Notice

$$I - m_\theta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} -\cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{pmatrix} = 2 \cdot \begin{pmatrix} \cos^2\theta & \sin\theta \cdot \cos\theta \\ \sin\theta \cdot \cos\theta & \sin^2\theta \end{pmatrix}$$

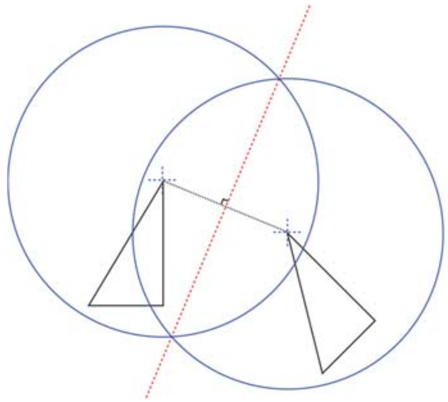
We can write this as

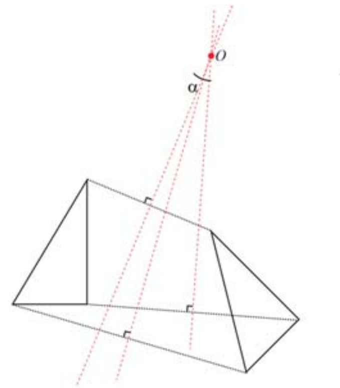
$$I - m_\theta = 2 \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \cdot (\cos\theta \quad \sin\theta) = 2N \cdot N^T$$

This notation refers to a column vector N that contains the components of a unit vector $\hat{\mathbf{n}}$ oriented normal to the reflecting plane. Writing the components of $\mathbf{t}$ and $\mathbf{r}_0$ as T and X_0, respectively, this gives $T = 2N \cdot (N^T \cdot X_0)$,. We can identify the normal component of $\mathbf{r}_0$ as $r_0^{(\perp)} = \hat{\mathbf{n}} \cdot \mathbf{r}_0$. Thus $\mathbf{t} = 2r_0^{(\perp)}\hat{\mathbf{n}}$, indicating that we can affect the reflection across the offset line by first reflecting across a parallel line through the origin, then translating by twice the normal component of the position vector.

Chasles center

In 2-D, it is always possible to perform the transformation by rotation only, where the rotation center is a unique point, called the *Chasles center*. It can be found by construction: find the line segment connecting any two corresponding points. Then find the line normal to the connecting line that passes through the midpoint. The Chasles center is somewhere on this second line. Now repeat for another pair of corresponding points. This second bisecting line will intersect the first at the Chasles center.





Translation by two reflections

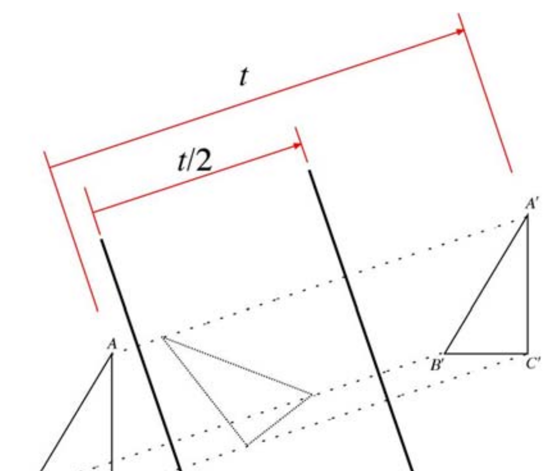
Consider a sequence of reflections across parallel lines, m_1 and m_2. The locations of the lines can be specified by coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. Both reflections are generated by the same matrix m_θ. The complete transformation can be written as

$$\mathbf{r}' = m_\theta \cdot \{[m_\theta \cdot (\mathbf{r} - \mathbf{r}_1) + \mathbf{r}_1] - \mathbf{r}_2\} + \mathbf{r}_2$$

Using $m_\theta \cdot m_\theta = I$ (identity), we have

$$\mathbf{r}' = \mathbf{r} + (I - m_\theta) \cdot (\mathbf{r}_2 - \mathbf{r}_1)$$

This represents a pure translation, with translation vector $\mathbf{t} = (I - m_\theta) \cdot (\mathbf{r}_2 - \mathbf{r}_1)$.



We saw previously that

$$I - m_\theta = 2\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \cdot (\cos\theta \quad \sin\theta) = 2N \cdot N^T$$

where N describes the normal unit vector $\mathbf{n}$. In the case

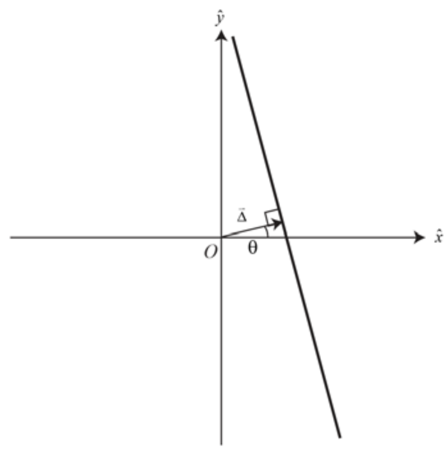
$$\mathbf{t} = 2 \cdot (\mathbf{r}_2 - \mathbf{r}_1)^{(\perp)}\, \hat{\mathbf{n}}$$

The translation vector is normal to the lines, and has a length of twice their separation.

Equation for a line in 2-D

We saw earlier that the equation for a line could be developed by rotating points along the y axis CW by an angle θ. More generally, we want to include an offset from the origin $\vec{\Delta} = (\delta_x \quad \delta_y)^T$, giving

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} 0 \\ s \end{pmatrix} + \begin{pmatrix} \delta_x \\ \delta_y \end{pmatrix} = \begin{pmatrix} -\sin\theta \cdot s + \delta_x \\ \cos\theta \cdot s + \delta_y \end{pmatrix}$$



This represents two equations

$$-\sin\theta \cdot x + \cos\theta \cdot y = s + (-\sin\theta \cdot \delta_x + \cos\theta \cdot \delta_y)$$

$$\cos\theta \cdot x + \sin\theta \cdot y = \cos\theta \cdot \delta_x + \sin\theta \cdot \delta_y$$

Defining $\Delta = \sqrt{\delta_x{}^2 + \delta_y{}^2}$, we have $\cos\theta = \delta_x/\Delta$, $\sin\theta = \delta_y/\Delta$, or $\delta_x = \cos\theta \cdot \Delta$, $\delta_y = \sin\theta \cdot \Delta$. These give $\cos\theta \cdot \delta_x + \sin\theta \cdot \delta_y = \Delta$ and $-\sin\theta \cdot \delta_x + \cos\theta \cdot \delta_y = 0$. Now the line can be described by

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -\sin\theta & \cos\theta \\ \cos\theta & \sin\theta \end{pmatrix} \cdot \begin{pmatrix} s \\ \Delta \end{pmatrix}$$

All points on the line satisfy $\cos\theta \cdot x + \sin\theta \cdot y = \Delta$. The squared distance from the origin of any point on the line is $x^2 + y^2 = s^2 + \Delta^2$. The point of closes approach occurs when

$$\frac{d}{ds}(x^2 + y^2)\bigg|_{s=s_{\min}} = 2s_{\min} = 0$$

Therefore, $s_{\min} = 0$, and the point of closest approach has coordinates

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \delta_x \\ \delta_y \end{pmatrix}$$

We can further write $(\cos\theta \cdot \Delta) \cdot x + (\sin\theta \cdot \Delta) \cdot y = \Delta^2$, which gives the form

$$\delta_x \cdot x + \delta_y \cdot y = \Delta^2$$

A line can be described by its axis intercepts as

$$\frac{x}{x_i} + \frac{y}{y_i} = 1$$

We see that

$$\frac{x}{\left(\frac{\Delta^2}{\delta_x}\right)} + \frac{y}{\left(\frac{\Delta^2}{\delta_y}\right)} = 1$$

So the intercepts are

$$x_i = \frac{\Delta^2}{\delta_x}, \; y_i = \frac{\Delta^2}{\delta_y}$$

We know that $\cos\theta \cdot x + \sin\theta \cdot y = \Delta$. Notice that $\cos\theta \cdot \delta_x + \sin\theta \cdot \delta_y = \Delta$, so points on the line satisfy

$$\cos\theta \cdot (x - \delta_x) + \sin\theta \cdot (y - \delta_y) = 0$$

Equation for a line through two points

We sometimes wish to know the equation for a line passing through two points (x_1, y_1) and (x_2, y_2). Using the following three equations

1) $\cos\theta \cdot (x - \delta_x) + \sin\theta \cdot (y - \delta_y) = 0$

2) $\cos\theta \cdot (x_1 - \delta_x) + \sin\theta \cdot (y_1 - \delta_y) = 0$

3) $\cos\theta \cdot (x_2 - \delta_x) + \sin\theta \cdot (y_2 - \delta_y) = 0$

We can take the differences 1)-2) and 1)-3) and separate x and y terms to obtain

$$\cos\theta \cdot (x - x_1) = -\sin\theta \cdot (y - y_1)$$

$$\cos\theta \cdot (x - x_2) = -\sin\theta \cdot (y - y_2)$$

The ratio of the LHS equals that of the RHS:

$$\frac{x - x_1}{x - x_2} = \frac{y - y_1}{y - y_2}$$

Expand and simplify

$$(y_2 - y_1) \cdot x - (x_2 - x_1) \cdot y = x_1 \cdot y_2 - x_2 \cdot y_1$$

The angle θ is found by

$$\cos\theta = \frac{y_2 - y_1}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}, \quad \sin\theta = \frac{-(x_2 - x_1)}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$

and delta is

$$\Delta = \frac{x_1 \cdot y_2 - x_2 \cdot y_1}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$

with components

$$\delta_x = \frac{(x_1 \cdot y_2 - x_2 \cdot y_1) \cdot (y_2 - y_1)}{(x_2 - x_1)^2 + (y_2 - y_1)^2}, \quad \delta_y = \frac{-(x_1 \cdot y_2 - x_2 \cdot y_1) \cdot (x_2 - x_1)}{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

Equation for a perpendicular line through a point

Let's find a line perpendicular to $\cos\theta \cdot (x - \delta_x) + \sin\theta \cdot (y - \delta_y) = 0$ that passes through a point (x_0, y_0). The new line will satisfy

$$\cos(\theta + 90°) \cdot (x - x_0) + \sin(\theta + 90°) \cdot (y - y_0) = 0$$

which gives

$$-\sin\theta \cdot (x - x_0) + \cos\theta \cdot (y - y_0) = 0$$

Casting the new line in the form $\delta'_x \cdot x + \delta'_y \cdot y = (\Delta')^2$, we have

$$\delta'_x = \sin^2\theta \cdot x_0 - \sin\theta \cdot \cos\theta \cdot y_0$$

$$\delta'_y = -\sin\theta \cdot \cos\theta \cdot x_0 + \cos^2\theta \cdot y_0$$

and

$$\Delta' = -\sin\theta \cdot x_0 + \cos\theta \cdot y_0$$

Intersection of two lines

Let's find the point of intersection (x_0, y_0) of lines $\delta_{x1} \cdot x + \delta_{y1} \cdot y = (\Delta_1)^2$ and $\delta_{x2} \cdot x + \delta_{y2} \cdot y = (\Delta_2)^2$. The system of equations

$$\delta_{x1} \cdot x_0 + \delta_{y1} \cdot y_0 = (\Delta_1)^2$$

$$\delta_{x2} \cdot x_0 + \delta_{y2} \cdot y_0 = (\Delta_2)^2$$

can be written

$$\begin{pmatrix} \delta_{x1} & \delta_{y1} \\ \delta_{x2} & \delta_{y2} \end{pmatrix} \cdot \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} {\Delta_1}^2 \\ {\Delta_2}^2 \end{pmatrix}$$

so

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} \delta_{x1} & \delta_{y1} \\ \delta_{x2} & \delta_{y2} \end{pmatrix}^{-1} \cdot \begin{pmatrix} {\Delta_1}^2 \\ {\Delta_2}^2 \end{pmatrix}$$

Taking the inverse

$$\begin{pmatrix} \delta_{x1} & \delta_{y1} \\ \delta_{x2} & \delta_{y2} \end{pmatrix}^{-1} = \frac{1}{\delta_{x1} \cdot \delta_{y2} - \delta_{x2} \cdot \delta_{y1}} \cdot \begin{pmatrix} \delta_{y2} & -\delta_{y1} \\ -\delta_{x2} & \delta_{x1} \end{pmatrix}$$

The point of intersection is

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \frac{1}{\delta_{x1} \cdot \delta_{y2} - \delta_{x2} \cdot \delta_{y1}} \cdot \begin{pmatrix} \delta_{y2} & -\delta_{y1} \\ -\delta_{x2} & \delta_{x1} \end{pmatrix} \cdot \begin{pmatrix} \Delta_1^2 \\ \Delta_2^2 \end{pmatrix}$$

Reorienting vectors and matrices

We can reorient an object so that its properties at a vector $\mathbf{r}$ become those at a vector $\mathbf{q}$ by multiplying by a matrix T that transforms the coordinates from one orientation into another, i.e., $\mathbf{q} = T \cdot \mathbf{r}$. Often our objective is to apply a symmetry transformation that has a known form in the orientation with coordinates $\mathbf{q}$, for example, $\mathbf{q}' = M \cdot \mathbf{q}$, so $\mathbf{q}' = M \cdot T \cdot \mathbf{r}$. Now we reorient the transformed object back to the original coordinates by applying the inverse transformation T^{-1}, i.e., $\mathbf{r}' = T^{-1} \cdot \mathbf{q}' = T^{-1} \cdot M \cdot T \cdot \mathbf{r}$. Apparently, the symmetry operation could be performed in the original orientation with multiplication by the matrix

$$M' = T^{-1} \cdot M \cdot T$$

Reorienting objects and functions

Let's consider transforming an object within space, rather than the vectors that describe the space. Say an object has a property described by the function $P(\mathbf{r})$. After transformation of the object, the property is described by the function $Q(\mathbf{r})$, where $Q(T \cdot \mathbf{r}) = P(\mathbf{r})$, where T is the matrix used above to transform a vector. Now assume a transformation of the object turns the function $Q(\mathbf{r})$ into $Q'(\mathbf{r})$, such that $Q'(M \cdot \mathbf{r}) = Q(\mathbf{r})$. After this transformation, we transform back to the original orientation using $P'(T^{-1} \cdot \mathbf{r}) = Q'(\mathbf{r})$. Then $P'(T^{-1} \cdot M \cdot T \cdot \mathbf{r}) = P(\mathbf{r})$. If this is a symmetry operation, then $P'(\mathbf{r}) = P(\mathbf{r})$, so $P(\mathbf{r}) = P(T^{-1} \cdot M \cdot T \cdot \mathbf{r}) = P(M' \cdot \mathbf{r})$. The transformation matrix for this symmetry operation is again $M' = T^{-1} \cdot M \cdot T$.

Proper, isometric transformations about the origin in 3-D

In 2-D, a rotation is performed about a point; in 3-D, a rotation is performed about an axis, i.e., a line. A rotation about an axis in 3-D does not affect coordinates parallel to the axis, so the generalization of our 2-D result is straightforward. A vector can be rotated by angle ω about the z-axis by multiplying by the matrix

$$R_{z,\omega} = \begin{pmatrix} \cos\omega & -\sin\omega & 0 \\ \sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Rotation about an arbitrary axis

Let's find the matrix to rotate a vector about an arbitrary axis $\hat{\mathbf{n}}$ by an angle ω, written $R_{\hat{\mathbf{n}},\omega}$. Assume $\hat{\mathbf{n}}$ makes an angle θ (the polar angle) wrt the z axis and its projection on the x-y plane makes an angle ϕ (the azimuthal angle) wrt the x axis. Note that

$$R_{z,\phi} \cdot R_{y,\theta} = \begin{pmatrix} \cos\theta \cdot \cos\phi & -\sin\phi & \sin\theta \cdot \cos\phi \\ \cos\theta \cdot \sin\phi & \cos\phi & \sin\theta \cdot \sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

It is useful to note that $(R_{z,\phi} \cdot R_{y,\theta})^{-1} = (R_{z,\phi} \cdot R_{y,\theta})^T$ This gives

$$\hat{\mathbf{n}} = R_{z,\phi} \cdot R_{y,\theta} \cdot \hat{\mathbf{z}} = \begin{pmatrix} \sin\theta \cdot \cos\phi \\ \sin\theta \cdot \sin\phi \\ \cos\theta \end{pmatrix}$$

A rotation $R_{\hat{\mathbf{n}},\omega}$ of any vector can be performed by rotating the object to bring $\hat{\mathbf{n}}$ along the z axis, applying $R_{z,\omega}$, then rotating back to bring z along $\hat{\mathbf{n}}$

$$R_{\hat{\mathbf{n}},\omega} = (R_{z,\phi} \cdot R_{y,\theta}) \cdot R_{z,\omega} \cdot (R_{z,\phi} \cdot R_{y,\theta})^{-1}$$

It is not very helpful to write out the full product in the general case. Notice that

$$\begin{aligned} R_{\hat{\mathbf{n}},\omega} \cdot \hat{\mathbf{n}} &= (R_{z,\phi} \cdot R_{y,\theta}) \cdot R_{z,\omega} \cdot \cancel{(R_{z,\phi} \cdot R_{y,\theta})^{-1}} \cdot \cancel{R_{z,\phi} \cdot R_{y,\theta}} \cdot \hat{\mathbf{z}} \\ &= (R_{z,\phi} \cdot R_{y,\theta}) \cdot R_{z,\omega} \cdot \hat{\mathbf{z}} = (R_{z,\phi} \cdot R_{y,\theta}) \cdot \hat{\mathbf{z}} = \hat{\mathbf{n}} \end{aligned}$$

Points on the axis are unchanged by the rotation about the axis.

Rotations about the x and y axes

Say we want to rotate an object by ω about the x-axis, with $\theta = 90°$, $\phi = 0°$:

$$R_{z,0°} \cdot R_{y,90°} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \text{ and } \hat{\mathbf{n}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{\mathbf{x}}$$

We find

$$R_{x,\omega} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\omega & -\sin\omega \\ 0 & \sin\omega & \cos\omega \end{pmatrix}$$

To rotate about the y-axis, we use $\theta = 90°$, $\phi = 90°$:

$$R_{z,90°} \cdot R_{y,90°} = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \text{ and } \hat{\mathbf{n}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hat{\mathbf{y}}$$

This gives

$$R_{y,\omega} = \begin{pmatrix} \cos\omega & 0 & \sin\omega \\ 0 & 1 & 0 \\ -\sin\omega & 0 & \cos\omega \end{pmatrix}$$

Some other useful rotation matrices

Let's assume $\theta = 90°$, $\phi = 45°$, and $\omega = 180°$. Then

$$R_{z,45°} \cdot R_{y,90°} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -1 & 0 & 0 \end{pmatrix}, \; R_{z,180°} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ and } \hat{\mathbf{n}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

We can refer to the axis as $[110]$. The transformation corresponds to

$$R_{[110],180°} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = 2_{[110]}$$

Now consider the special case $\theta = 54.7°$ (i.e., $\sin\theta = \sqrt{2/3}$, $\cos\theta = 1/\sqrt{3}$), $\phi = 45°$, and $\omega = 120°$. Then

$$R_{z,45°} \cdot R_{y,54.7°} = \begin{pmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} \end{pmatrix}, \; R_{z,120°} = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{2}} & 0 \\ \sqrt{\frac{3}{2}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ and } \hat{\mathbf{n}} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

This axis is along $[111]$. The transformation corresponds to

$$R_{[111],120°} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = 3_{[111]}$$

Reflections in x and y

Similarly, reflections across a plane only change the coordinate normal to the plane. So, for example, reflections in x (across the y-z plane), or y (across the x-z plane), involve

$$m_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } m_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Let's perform the sequence of all three reflections.

$$M = m_z \cdot m_y \cdot m_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

What is the effect of the combined transformation?

$$\mathbf{r}' = M \cdot \mathbf{r} = -\mathbf{r}$$

This is an inversion ($M = -I$) through the origin, which we can call $\overline{1}$. Clearly $\det(\overline{1}) = -1$, so it is an improper transformation.

Improper, isometric transformations about the origin in 3-D

Consider a rotation by ω about the z axis coupled with an inversion

$$\overline{R}_{z,\omega} = \begin{pmatrix} -\cos\omega & \sin\omega & 0 \\ -\sin\omega & -\cos\omega & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Obviously $\overline{R}_{z,0^\circ} = -I$ and $\overline{R}_{z,180^\circ} = m_z$. We transform this to other orientations in the same manner as that used for rotations:

$$\overline{R}_{\hat{\mathbf{n}},\omega} = \left(R_{z,\phi} \cdot R_{y,\theta}\right) \cdot \overline{R}_{z,\omega} \cdot \left(R_{z,\phi} \cdot R_{y,\theta}\right)^{-1}$$

For example, $\theta = 90^\circ$, $\phi = 45^\circ$, and $\omega = 180^\circ$ give

$$\overline{R}_{[110],180^\circ} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = m_{[110]}$$

Likewise, $\theta = 54.7^\circ$, $\phi = 45^\circ$, and $\omega = 120^\circ$ give

$$\overline{R}_{[111],120^\circ} = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} = \overline{3}_{[111]}$$