Group Theory

Solutions to Problems in Homework Assignment 08

Spring, 2020

1. Identify the point group that is obtained by combining the two symmetry elements in each case.
   (a) A 2-fold rotation axis and an inversion center.
   (b) Two mirror planes at right angles to each other.
   (c) A 2-fold rotation axis and an intersecting mirror plane.

(a) Noting that $IC_2 = \sigma_h$ with σ_h a mirror plane perpendicular to the 2-fold rotation axis, we see that the point group has four elements E, C_2, I, and σ_h. Thus, the group is C_{2h} $(2/m)$

$$C_{2h} = \{E, C_2, I, \sigma_h\}.$$

(b) Let σ_v and $\sigma_{v'}$ denote the two mirror planes perpendicular to each other. Noting that $\sigma_v \sigma_{v'}$ gives a result that can be obtained through a pure rotation through π about an axis passing through the intersection of the two mirror planes, we see that the group contains C_2. Thus, the group is C_{2v} $(mm2)$

$$C_{2v} = \{E, C_2, \sigma_v, \sigma_{v'}\} = \{E, C_2, 2\sigma_v\}.$$

(c) Let σ_h denote the mirror plane intersecting the 2-fold rotation axis. Since $C_2\sigma_h = I$, the group is the same as in (a), *i.e.*, it is C_{2h} $(2/m)$

$$C_{2h} = \{E, C_2, I, \sigma_h\}.$$

2. Let a rotation about an axis passing through the origin and perpendicular to the xOy plane through an angle of θ be represented by the matrix R_θ and a reflection in the line passing through the origin and making an angle of $\theta/2$ with the positive x axis be represented by the matrix S_θ. Show that R_θ and S_θ can be expressed as

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \quad S_\theta = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}.$$

We first consider a counterclockwise rotation about the z axis through an angle of θ. Assume that the position vector $\vec{\rho}$ in the xOy plane makes an angle of φ with the x axis before the rotation. We then have $\vec{\rho} = x\,\vec{e}_x + y\,\vec{e}_y = \rho\cos\varphi\,\vec{e}_x + \rho\sin\varphi\,\vec{e}_y$. After the rotation, the position vector makes an angle of $\varphi + \theta$ with the x axis. Thus,

$$\begin{aligned} \vec{\rho}\,' &= \rho\cos(\varphi+\theta)\,\vec{e}_x + \rho\sin(\varphi+\theta)\,\vec{e}_y \\ &= \big(x\cos\theta - y\sin\theta\big)\vec{e}_x + \big(x\sin\theta + y\cos\theta\big)\vec{e}_y. \end{aligned}$$

Comparing the above result with $\vec{\rho}\,' = x'\,\vec{e}_x + y'\,\vec{e}_y$, we obtain

$$\begin{aligned} x' &= x\cos\theta - y\sin\theta, \\ y' &= x\sin\theta + y\cos\theta. \end{aligned}$$

Writing the above relations in matrix form, we have

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

Comparing the above equation with $\begin{pmatrix} x' \\ y' \end{pmatrix} = R_\theta \begin{pmatrix} x \\ y \end{pmatrix}$, we obtain

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

We now consider the reflection in the line passing through the origin and making an angle of $\theta/2$ with the positive x axis. The direction of the line is given by $\vec{n} = \cos(\theta/2)\vec{e}_x + \sin(\theta/2)\vec{e}_y$. Let us write the position vector as the sum of the component in the direction of $\vec{n}$, $\vec{r}_{\parallel} = (\vec{r}\cdot\vec{n})\vec{n}$, and the component in the direction perpendicular to $\vec{n}$, $\vec{r}_{\perp} = \vec{r} - \vec{r}_{\parallel} = \vec{r} - (\vec{r}\cdot\vec{n})\vec{n}$,

$$\vec{r} = \vec{r}_{\parallel} + \vec{r}_{\perp}.$$

Under the reflection, $\vec{r}_{\perp}$ changes sign while $\vec{r}_{\parallel}$ remains unchanged. We then have

$$\begin{aligned}
\vec{r}\,' &= \vec{r}_{\parallel} - \vec{r}_{\perp} = 2(\vec{r}\cdot\vec{n})\vec{n} - \vec{r}\\
&= 2\big[\,x\cos(\theta/2) + y\sin(\theta/2)\,\big]\big[\cos(\theta/2)\vec{e}_x + \sin(\theta/2)\vec{e}_y\,\big]\\
&\quad - x\,\vec{e}_x - y\,\vec{e}_y\\
&= \Big\{x\big[\,2\cos^2(\theta/2) - 1\,\big] + 2y\sin(\theta/2)\cos(\theta/2)\Big\}\,\vec{e}_x\\
&\quad + \Big\{2x\sin(\theta/2)\cos(\theta/2) - y\big[\,1 - 2\sin^2(\theta/2)\,\big]\Big\}\,\vec{e}_y\\
&= \big(x\cos\theta + y\sin\theta\big)\vec{e}_x + \big(x\sin\theta - y\cos\theta\big)\vec{e}_y.
\end{aligned}$$

Writing the above equation in matrix form, we have

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

Comparing the above equation with $\begin{pmatrix} x' \\ y' \end{pmatrix} = S_\theta \begin{pmatrix} x \\ y \end{pmatrix}$, we obtain

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

3. Continue from the above problem.
   (a) Compute the effect of rotating the vector $2\vec{e}_x + 3\vec{e}_y$ counterclockwise about the origin through an angle of $\pi/2$ radians.
   (b) Compute the effect of reflecting the vector $\vec{e}_x + \vec{e}_y$ through the line $y = 2x$.
   (c) Compute the effect of rotating the vector $\vec{e}_y$ counterclockwise about the origin through an angle of $\pi/3$ radians and then reflecting through the line $y = 2x$.

(a) For $\theta = \pi/2$, we have

$$R_{\pi/2} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

The vector $2\vec{e}_x + 3\vec{e}_y$ is expressed in matrix form as

$$2\vec{e}_x + 3\vec{e}_y = \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$

We then have

$$R_{\pi/2}(2\vec{e}_x + 3\vec{e}_y) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} -3 \\ 2 \end{pmatrix}.$$

Thus, $R_{\pi/2}(2\vec{e}_x + 3\vec{e}_y) = -3\vec{e}_x + 2\vec{e}_y$.

(b) The slope of the line $y = 2x$ is $\tan^{-1} 2$, that is, $\tan(\theta/2) = 2$ with $\theta/2$ the angle the line makes with the positive x axis. We then have $\sin\theta = 4/5$, $\cos\theta = -3/5$, and

$$S_\theta = \frac{1}{5}\begin{pmatrix} -3 & 4 \\ 4 & 3 \end{pmatrix}.$$

The effect of S_θ on $\vec{e}_x + \vec{e}_y$ is then given by

$$S_\theta(\vec{e}_x + \vec{e}_y) = \frac{1}{5}\begin{pmatrix} -3 & 4 \\ 4 & 3 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{5}\begin{pmatrix} 1 \\ 7 \end{pmatrix} = \frac{1}{5}(\vec{e}_x + 7\vec{e}_y).$$

(c) The effect of rotating the vector $\vec{e}_y$ counterclockwise about the origin through an angle of $\pi/3$ radians and then reflecting through the line $y = 2x$ is given by

$$\begin{aligned} S_\theta R_{\pi/3}\vec{e}_y &= \frac{1}{10}\begin{pmatrix} -3 & 4 \\ 4 & 3 \end{pmatrix}\begin{pmatrix} 1 & -\sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{10}\begin{pmatrix} -3 & 4 \\ 4 & 3 \end{pmatrix}\begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix} \\ &= \frac{1}{10}\begin{pmatrix} 4+3\sqrt{3} \\ 3-4\sqrt{3} \end{pmatrix} = \frac{1}{10}\big[(4+3\sqrt{3})\vec{e}_x + (3-4\sqrt{3})\vec{e}_y\big]. \end{aligned}$$

4. Continue from the above problem.

(a) Show that $S_\theta S_\psi$ is a rotation and find the angle of rotation.

(b) Show that $S_\theta R_\psi S_\theta = R_{-\psi}$.

(c) Let $T_{\vec{v}}$ be a translation through $\vec{v}$, $T_{\vec{v}}\vec{w} = \vec{w} + \vec{v}$. Show that $T_{R_\theta \vec{v}} R_\theta = R_\theta T_{\vec{v}}$.

(a) Evaluating the matrix product $S_\theta S_\psi$, we have

$$\begin{aligned} S_\theta S_\psi &= \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \cos\psi & \sin\psi \\ \sin\psi & -\cos\psi \end{pmatrix} \\ &= \begin{pmatrix} \cos\theta\cos\psi + \sin\theta\sin\psi & \cos\theta\sin\psi - \sin\theta\cos\psi \\ \sin\theta\cos\psi - \cos\theta\sin\psi & \sin\theta\sin\psi + \cos\theta\cos\psi \end{pmatrix} \\ &= \begin{pmatrix} \cos(\theta-\psi) & -\sin(\theta-\psi) \\ \sin(\theta-\psi) & \cos(\theta-\psi) \end{pmatrix} = R_{\theta-\psi}. \end{aligned}$$

Thus, $S_\theta S_\psi$ is a rotation through an angle of $\theta - \psi$.

(b) Evaluating the matrix product $S_\theta R_\psi S_\theta$, we have

$$\begin{aligned} S_\theta R_\psi S_\theta &= \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \cos\psi & -\sin\psi \\ \sin\psi & \cos\psi \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \\ &= \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \cos(\psi+\theta) & \sin(\psi+\theta) \\ \sin(\psi+\theta) & -\cos(\psi+\theta) \end{pmatrix} \\ &= \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix} = R_{-\psi}. \end{aligned}$$

(c) For $T_{R_\theta \vec{v}} R_\theta \vec{w}$ with $\vec{w}$ an arbitrary vector, we have

$$T_{R_\theta \vec{v}} R_\theta \vec{w} = R_\theta \vec{w} + R_\theta \vec{v} = R_\theta(\vec{w} + \vec{v}) = R_\theta T_{\vec{v}} \vec{w}.$$

Thus, $T_{R_\theta \vec{v}} R_\theta = R_\theta T_{\vec{v}}$.

5. Consider the point groups C_{2v} and D_{2h}.

(a) Find all invariant subgroups of C_{2v}.

(b) Find all invariant subgroups of D_{2h}.

(a) The elements of C_{2v} are E, C_2, σ_v, and σ_d. The multiplication table of C_{2v} is given by

	E	C_2	σ_v	σ_d
E	E	C_2	σ_v	σ_d
C_2	C_2	E	σ_d	σ_v
σ_v	σ_v	σ_d	E	C_2
σ_d	σ_d	σ_v	C_2	E

The multiplication table can be obtained by taking as in Fig. 1, for example, the C_2 axis along the z axis, the σ_v mirror plane as the zOx plane, and the σ_d mirror plane as the yOz plane. The effects of the symmetry operations in group C_{2v} on a general point with coordinates (x, y, z) are then given by

$$
\begin{aligned}
&E(x, y, z) = (x, y, z),\\
&C_2(x, y, z) = (-x, -y, z),\\
&\sigma_v(x, -y, z) = (x, y, z),\\
&\sigma_d(x, y, z) = (-x, y, z).
\end{aligned}
$$

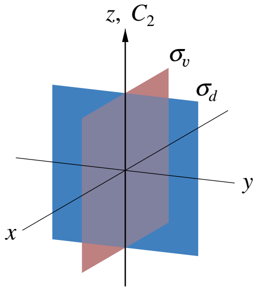

FIG. 1: Symmetry operations in point group C_{2v}.

The result of the product of any two symmetry operations can be obtained by using the above results for individual symmetry operations. For example,

$$C_2\sigma_v(x, y, z) = C_2(x, -y, z) = (-x, y, z) = \sigma_d(x, y, z).$$

Thus, $C_2\sigma_v = \sigma_d$.

From the multiplication table, we see that the inverses of all the elements of C_{2v} are themselves, respectively, since the product of any element with itself is equal to the identity element E. Making use of the multiplication table, we find the following subgroups of C_{2v} with the two trivial subgroups included: C_1, C_s, C_2, C_{2v}, where C_s can represent either $\{E, \sigma_v\}$ or $\{E, \sigma_d\}$ and C_2 represents $\{E, C_2\}$.

Since all the elements of C_{2v} commute with one another, all of its subgroups are invariant subgroups.

(b) Point group D_{2h} is given by $D_{2h} = \{E,\ C_2,\ C_2',\ C_2'',\ I,\ \sigma_h,\ \sigma_v,\ \sigma_v'\}$ in which σ_h is perpendicular to C_2 (the major rotation axis) and σ_v and σ_v' are parallel to C_2 with σ_v and σ_v' contain respectively C_2' and C_2'' which are perpendicular to each other and are both perpendicular to C_2. The multiplication table of D_{2h} is given by

	E	C_2	C_2'	C_2''	I	σ_h	σ_v	σ_v'
E	E	C_2	C_2'	C_2''	I	σ_h	σ_v	σ_v'
C_2	C_2	E	C_2''	C_2'	σ_h	I	σ_v'	σ_v
C_2'	C_2'	C_2''	E	C_2	σ_v'	σ_v	σ_h	I
C_2''	C_2''	C_2'	C_2	E	σ_v	σ_v'	I	σ_h
I	I	σ_h	σ_v'	σ_v	E	C_2	C_2''	C_2'
σ_h	σ_h	I	σ_v	σ_v'	C_2	E	C_2'	C_2''
σ_v	σ_v	σ_v'	σ_h	I	C_2''	C_2'	E	C_2
σ_v'	σ_v'	σ_v	I	σ_h	C_2'	C_2''	C_2	E

Similarly to what was done regarding point group C_{2v} in the above, the multiplication table for point group D_{2h} can be obtained by taking as in Fig. 2, for instance, the C_2 axis along the z axis, the C_2' axis along the x axis, and the C_2'' axis along the y axis and, correspondingly, the σ_h mirror plane as the xOy plane, the σ_v mirror plane as the zOx plane, and the σ_v' mirror plane as the yOz plane. The effects of the symmetry operations in point group D_{2h} on a general point with coordinates (x, y, z) are given by

$$\begin{array}{ll}
E(x,y,z) = (x,y,z), & C_2(x,y,z) = (-x,-y,z), \\
C_2'(x,y,z) = (x,-y,-z), & C_2''(x,y,z) = (-x,y,-z), \\
I(x,y,z) = (-x,-y,-z), & \sigma_h(x,y,z) = (x,y,-z), \\
\sigma_v(x,-y,z) = (x,y,z), & \sigma_v'(x,y,z) = (-x,y,z).
\end{array}$$

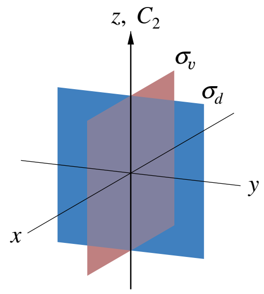

FIG. 2: Symmetry operations in point group D_{2h}.

The result of the product of any two symmetry operations can be obtained by using the above results for individual symmetry operations.
Using the multiplication table, we find the following subgroups of D_{2h} with the two trivial subgroups included

$$C_1,\ C_I,\ C_s,\ C_2,\ C_{2h},\ D_2,\ C_{2v},\ D_{2h}.$$

where $C_1 = \{E\}$, $C_I = \{E, I\}$, $C_2 = \{E, C_2\}$, $C_s = \{E, \sigma_h\} = \{E, \sigma_v\} = \{E, \sigma_v'\}$, $D_2 = \{E,\ C_2,\ C_2',\ C_2''\}$, and

$$\begin{array}{l}
C_{2h} = \{E,\ C_2,\ I,\ \sigma_h\} = \{E,\ C_2',\ I,\ \sigma_v'\} = \{E,\ C_2'',\ I,\ \sigma_v\}, \\
C_{2v} = \{E,\ C_2,\ \sigma_v,\ \sigma_v'\} = \{E,\ C_2',\ \sigma_v,\ \sigma_h\} = \{E,\ C_2'',\ \sigma_v',\ \sigma_h\}.
\end{array}$$

Because D_{2h} is an Abelian group and because the inverses of all the elements are themselves, respectively, we have $a^{-1}ba = b$ for any elements a and b of D_{2h}. Therefore, all the subgroups of D_{2h} are its invariant subgroups.