Assignment 08

Due Time : 8:15, May 6, 2020 (Wednesday)

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Score : ________

Problem 1 Score: ________. 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.

Solution: (a) The 2-fold rotation axis corresponds to rotation C_2. The inversion center corresponds to spatial inversion I. Combining C_2 and I, we get reflection in a horizontal plane $\sigma_h = C_2 I = I C_2$, which is perpendicular to the 2-fold rotation axis. Therefore, the point group is $C_{2h} = \{E, I, C_2, \sigma_h\}$.

(b) The two mirror planes corresponds to two reflection operations σ_v and σ_d, respectively. Since the two mirror planes are at right angles, combining σ_v and σ_d, we get a 2-fold rotation $C_2 = \sigma_v\sigma_d = \sigma_d\sigma_v$, which is about the intersecting line of the two mirror planes. Therefore, the point group is $C_{2v} = \{E, C_2, \sigma_v, \sigma_d\}$.

(c) The mirror plane must be perpendicular to the 2-fold rotation plane, or the combination of the 2-fold rotation and the reflection does not satisfy the associativity of the point group. The 2-fold rotation axis corresponds to rotation C_2. The intersecting mirror plane corresponds to reflection σ_h. Combining C_2 and σ_h, we get a spatial reflection $I = C_2\sigma_h = \sigma_h C_2$. Therefore, the point group is $C_{2h} = \{E, I, C_2, \sigma_h\}$.

□

Problem 2 Score: ________. Let a rotation about an axis passing through the original 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

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

Solution: Let the coordinates of a fixed point P before the operation be $r = \left(\begin{smallmatrix} x \\ y \end{smallmatrix}\right)$, and the coordinates after be $r' = \left(\begin{smallmatrix} x' \\ y' \end{smallmatrix}\right)$. If the operation is rotation about the axis passing through the original and perpendicular to the xOy plane, the relations between the coordinates before and after the operation are (see figure 1(a))

$$x' = x\cos\theta - y\sin\theta, \tag{1}$$
$$y' = x\sin\theta + y\cos\theta. \tag{2}$$

The above relations in the matrix form is

$$r' = R_\theta r. \tag{3}$$

Therefore, the expression of R_θ is

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{4}$$

If the operation is reflection in the line passing through the origin and making angle of $\theta/2$ with the positive x axis, the relations between the coordinates before and after the operation are (see figure 1(b))

$$x' = x\cos\theta + y\sin\theta, \tag{5}$$
$$y' = x\sin\theta - y\cos\theta. \tag{6}$$

The above relations in the matrix form is

$$r' = S_\theta r. \tag{7}$$

Therefore, the expression of S_θ is

$$S_\theta = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{8}$$

□

Problem 3 Score: ________. Continue from the above problem.

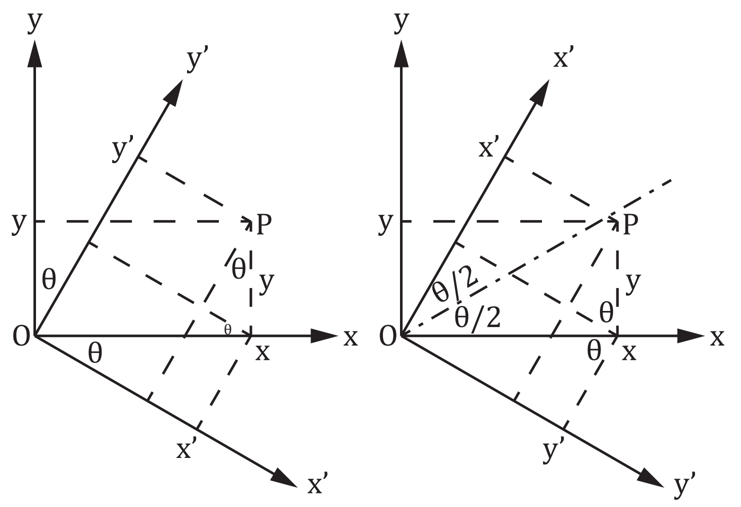

Figure 1: The scheme of two kinds of operations. Rotating of a point about an axis through an angle of θ is equivalent to rotating of the coordinate system about the same axis inversely through the angle of θ. Reflecting of a point in a line is equivalent to reflecting of the coordinate system in the same line.

(a) Compute the effect of rotating the vector $2e_x+3e_y$ conterclockwise about the origin through an angle of $\pi/2$ radians.

(b) Compute the effect of reflecting the vector e_x+e_y through the line $y=2x$.

(c) Compute the effect of rotating the vector e_y conterclockwise about the origin through an angle of $\pi/3$ radians and then reflecting through the line $y=2x$.

Solution: (a) The coordinates after rotating the vector $2e_x+3e_y$ conterclockwise about the origin through an angle of $\pi/2$ radians is

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\frac{\pi}{2} & -\sin\frac{\pi}{2} \\ \sin\frac{\pi}{2} & \cos\frac{\pi}{2} \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} -3 \\ 2 \end{pmatrix}. \tag{9}$$

Therefore, the effect of the rotation is to transform the vector $2e_x+3e_y$ into $-3e_x+2e_y$.

(b) The line $y=2x$ make angle of $\theta/2=\arctan 2$ with the positive x axis. The coordinates after reflecting the vector e_x+e_y through this line is

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -\frac{3}{5} & \frac{4}{5} \\ \frac{4}{5} & \frac{3}{5} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{5} \begin{pmatrix} 1 \\ 7 \end{pmatrix}. \tag{10}$$

Therefore, the effect of the reflecting is to transform the vector e_x+e_y into $\frac{1}{5}e_x+\frac{7}{5}e_y$

(c) The coordinates after rotating the vector e_y conterclockwise about the origin through an angle of $\pi/3$ radians is

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\frac{\pi}{3} & -\sin\frac{\pi}{3} \\ \sin\frac{\pi}{3} & \cos\frac{\pi}{3} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix}. \tag{11}$$

The coordinates after reflecting through the line $y=2x$ is

$$\begin{pmatrix} x'' \\ y'' \end{pmatrix} = \begin{pmatrix} -\frac{3}{5} & \frac{4}{5} \\ \frac{4}{5} & \frac{3}{5} \end{pmatrix} \frac{1}{2} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix} = \frac{1}{5} \begin{pmatrix} -3\sqrt{3}+4 \\ 4\sqrt{3}+3 \end{pmatrix}. \tag{12}$$

Therefore, the effect of the reflecting after the rotating is to transform the vector e_y into $\frac{-3\sqrt{3}+4}{5}e_x+\frac{4\sqrt{3}+3}{5}e_y$. □

Problem 4 Score: ________. Continue from the above problem.

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

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

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

Solution: (a) Since

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

$S_\theta S_\psi$ is a rotation and the angle of the rotation is $\theta - \psi$ (counterclockwise).

(b)

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

(c) Operating $T_{R_\theta v} R_\theta$ on an arbitrary vector $(x, y)^T$, we get

$$\begin{aligned} T_{R_\theta v} R_\theta \begin{pmatrix} x \\ y \end{pmatrix} =& R_\theta \begin{pmatrix} x \\ y \end{pmatrix} + R_\theta v = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x + v_x \\ y + v_y \end{pmatrix} \\ =& \begin{pmatrix} (x+v_x)\cos\theta - (y+v_y)\sin\theta \\ (x+v_x)\sin\theta + (y+v_y)\cos\theta \end{pmatrix}. \end{aligned}$$

Operating $R_\theta T_v$ on $(x, y)^T$, we get

$$R_\theta T_v \begin{pmatrix} x \\ y \end{pmatrix} = R_\theta \begin{pmatrix} x + v_x \\ y + v_y \end{pmatrix} = \begin{pmatrix} (x+v_x)\cos\theta - (y+v_y)\sin\theta \\ (x+v_x)\sin\theta + (y+v_y)\cos\theta \end{pmatrix}. \tag{13}$$

We find that

$$T_{R_\theta v} R_\theta \begin{pmatrix} x \\ y \end{pmatrix} = R_\theta T_v \begin{pmatrix} x \\ y \end{pmatrix}. \tag{14}$$

Due to the arbitrariness of $(x, y)^T$, $T_{R_\theta v} R_\theta = R_\theta T_v$.

□

Problem 5 Score: ________. 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}.

Solution: (a) The group C_{2v} is

$$C_{2v} = \{E, C_2, \sigma_v, \sigma_d\}. \tag{15}$$

The multiplication table of C_{2v} is shown in table 1.
From the multiplication table, we get the subgroups of C_{2v}, as shown in table 2.
From the multiplication table, we get the inverse of each element in C_{2v} is itself:

$$E^{-1} = E, \quad C_2^{-1} = C_2, \quad \sigma_v^{-1} = \sigma_v, \quad \sigma_d^{-1} = \sigma_d.$$

Table 1: The multiplication table of C_{2v}.

	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

Table 2: The subgroups of C_{2v}.

Order	Subgroup(s)
$s=1$	$\{E\}$
$s=2$	$\{E,C_2\},\{E,\sigma_v\},\{E,\sigma_d\}$
$s=4$	$\{E,C_2,\sigma_v,\sigma_d\}$

For $X=E,C_2,\sigma_v,\sigma_d$,

$$XC_2X^{-1}=E, \tag{16}$$

so the class of C_{2v} constructed from E is $\{E\}$.
For $X=E,C_2,\sigma_v,\sigma_d$,

$$XC_2X^{-1}=C_2, \tag{17}$$

so the class of C_{2v} constructed from C_2 is $\{C_2\}$.
For $X=E,C_2,\sigma_v,\sigma_d$,

$$X\sigma_vX^{-1}=\sigma_v, \tag{18}$$

so the class of C_{2v} constructed from σ_v is $\{\sigma_v\}$.
For $X=E,C_2,\sigma_v,\sigma_d$,

$$X\sigma_dX^{-1}=\sigma_d, \tag{19}$$

so the class of C_{2v} constructed from σ_d is $\{\sigma_d\}$.
The invariant subgroups of C_{2v} are the subgroups consisting entirely of complete classes of C_{2v}:

$$\{E\},\quad \{E,C_2\},\quad \{E,\sigma_v\},\quad \{E,\sigma_d\},\quad \{E,C_2,\sigma_v,\sigma_d\}.$$

(b) The group D_{2h} is

$$D_{2h}=\{E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'\}. \tag{20}$$

The multiplication table of D_{2h} is shown in table 3.

Table 3: The multiplication table of D_{2h}

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

From the multiplication table, we get the subgroups of C_{2v}, as shown in table 4.
From the multiplication table, we get the inverse of each element in C_{2v} is itself:

$$E^{-1}=E,\quad I^{-1}=I,\quad C_2^{-1}=C_2,\quad (C_2')^{-1}=C_2',\quad (C_2'')^{-1}=C_2'',\quad \sigma_h^{-1}=\sigma_h,\quad \sigma_v^{-1}=\sigma_v,\quad (\sigma_v')^{-1}=\sigma_v.$$

Table 4: The subgroups of D_{2h}.

Order	Subgroup(s)
$s=1$	$\{E\}$
$s=2$	$\{E,I\},\{E,C_2\},\{E,C_2'\},\{E,C_2''\},\{E,\sigma_h\},\{E,\sigma_v\},\{E,\sigma_v'\}$
$s=4$	$\{E,C_2,C_2',C_2''\},\{E,I,C_2,\sigma_h\},\{E,I,C_2',\sigma_v'\},\{E,I,C_2'',\sigma_v\},\{E,C_2,\sigma_v,\sigma_v'\}$
$s=8$	$\{E,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'\}$

For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$XEX^{-1}=E, \tag{21}$$

so the class of D_{2h} constructed from E is $\{E\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$XIX^{-1}=E, \tag{22}$$

so the class of D_{2h} constructed from I is $\{I\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$XC_2X^{-1}=C_2, \tag{23}$$

so the class of D_{2h} constructed from C_2 is $\{C_2\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$XC_2'X^{-1}=C_2', \tag{24}$$

so the class of D_{2h} constructed from E is $\{C_2'\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$XC_2''X^{-1}=C_2'', \tag{25}$$

so the class of D_{2h} constructed from C_2'' is $\{C_2''\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$X\sigma_hX^{-1}=\sigma_h, \tag{26}$$

so the class of D_{2h} constructed from σ_h is $\{\sigma_h\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$X\sigma_vX^{-1}=\sigma_v, \tag{27}$$

so the class of D_{2h} constructed from σ_v is $\{\sigma_v\}$.
For $X=E,,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'$,

$$X\sigma_vX^{-1}=\sigma_v', \tag{28}$$

so the class of D_{2h} constructed from σ_v' is $\{\sigma_v'\}$.
The invariant subgroups of C_{2h} are the subgroups consisting entirely of complete classes of C_{2v}:

$$\{E\},\{E,I\},\{E,C_2\},\{E,C_2'\},\{E,C_2''\},\{E,\sigma_h\},\{E,\sigma_v\},\{E,\sigma_v'\},$$
$$\{E,C_2,C_2',C_2''\},\{E,I,C_2,\sigma_h\},\{E,I,C_2',\sigma_v'\},\{E,I,C_2'',\sigma_v\},\{E,C_2,\sigma_v,\sigma_v'\},\{E,I,C_2,C_2',C_2'',\sigma_h,\sigma_v,\sigma_v'\}$$

□