Group Theory
PHYS2102
Spring, 2020

Assignment 09

Due Time : 8:15, May 13, 2020 (Wednesday)

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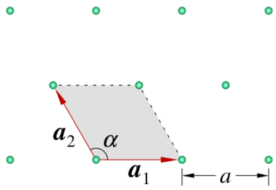
Score : ________

Consider the two-dimensional triangular Bravais lattice (also referred to as the hexagonal Bravais lattice) shown in the figure.



The basis lattice vectors are given by

$$a_1 = ae_x, \quad a_2 = -(a/2)e_x + (\sqrt{3}/2)e_y.$$

Problem 1 Score: ________. Find the crystallographic point group of the triangular Bravais lattice. What is the space group of the triangular Bravais lattice in the international system?

Solution: The allowed point symmetry operations of the triangular Bravais lattice are $\{E, C_6, C_6^2 = C_3, C_6^3 = C_2, C_6^4 = C_3^2, C_6^5, C_2^{'(1)}, C_2^{'(2)}, C_2^{'(3)}, C_2^{''(1)}, C_2^{''(2)}, C_2^{''(3)}, I, S_6, S_3, S_3^5, S_6^5, \sigma_h, \sigma_v, \sigma_v', \sigma_v'', \sigma_d, \sigma_d', \sigma_d''\}$, so the crystallographic point group is $\frac{6}{m}mm\,(D_{6h})$.

The bravais lattice type is primitive lattice (P), so the space group of the triangular Bravais lattice in the international system is $P\frac{6}{m}mm$. □

Problem 2 Score: ________. Construct the character table for the crystallographic point group of the triangular Bravais lattice.

Solution: The multiplication table of D_{6h} is so large that I have to omit it here. But I do construct the subgroups and classes of D_{6h}. The subgroups of D_{6h} are

$$C_1, C_s, C_i, C_2, C_3, C_6, D_2, D_3, D_6, C_{2v}, C_{3v}, C_{6v}, C_{2h}, C_{3h}, C_{6h}, D_{2h}, D_{3h}, S_6, D_{6h}.$$

The classes of D_{6h} are

$$\{E\}, \quad \{2C_6\}, \quad \{2C_3\}, \quad \{C_2\}, \quad \{3C_2'\}, \quad \{3C_2''\}, \quad \{I\}, \quad \{2S_6\}, \quad \{2S_3\}, \quad \{\sigma_h\}, \quad \{3\sigma_v\}, \quad \{3\sigma_d\}.$$

The number of inequivalent irreducible representations is equal to the number of classes of D_{6h}, so there are 12 inequivalent irreducible representations of D_{6h}. Suppose the dimension of the pth inequivalent irreducible representation of D_{6h} is d_p. The sum of the square of the dimensions of the inequivalent irreducible representations of D_{6h} is equal to the order of D_{6h}:

$$\sum_{p=1}^{12} d_p^2 = 24. \tag{1}$$

Solving the above equation, we get

$$d_1 = d_2 = \cdots = d_8 = 1, \quad d_9 = d_{10} = d_{11} = d_{12} = 2, \tag{2}$$

so D_{6h} has 8 inequivalent irreducible representations of order 1 and 4 inequivalent irreducible representations of order 2. The representation of the identity element is always identity matrix, so its character is equal to the dimension of the representation:

$$\chi^p(E) = d_p = \begin{cases} 1, & p = 1, 2, \cdots, 8, \\ 2, & p = 9, 10, 11, 12. \end{cases} \tag{3}$$

Since $C_2^2 = C_2'^2 = C_2''^2 = I = \sigma_h^2 = \sigma_v^2 = \sigma_d^2 = E$, we have

$$\chi^p(\{C_2\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{4}$$
$$\chi^p(\{3C_2'\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{5}$$
$$\chi^p(\{3C_2''\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{6}$$
$$\chi^p(\{I\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{7}$$

$$\chi^p(\{\sigma_h\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{8}$$
$$\chi^p(\{3\sigma_v\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{9}$$
$$\chi^p(\{3\sigma_d\}) = \pm 1, \quad p = 1, 2, \cdots, 8, \tag{10}$$

and thus

$$\chi^p(\{E\}) = 1, \quad p = 1, 2, \cdots, 8. \tag{11}$$

The equations above are not all independent:

- Since $C_2 \times C_2^{'(1)} = C_2^{''(1)}$, we have
$$\chi^p(\{C_2\})\chi^p(\{3C_2'\}) = \chi^p(\{3C_2''\}), \quad p = 1, 2, \cdots, 8. \tag{12}$$
- Since $I \times \sigma_h = C_2$, we have
$$\chi^p(\{I\})\chi^p(\{\sigma_h\}) = \chi^p(\{C_2\}), \quad p = 1, 2, \cdots, 8. \tag{13}$$
- Since $C_2 \times \sigma_v = \sigma_d'$, we have
$$\chi^p(\{C_2\})\chi^p(\{3\sigma_v\}) = \chi^p(\{3\sigma_d\}), \quad p = 1, 2, \cdots, 8. \tag{14}$$
- Since $\sigma_h \times \sigma_v = C_2'$, we have
$$\chi^p(\{\sigma_h\})\chi^p(\{\sigma_v\}) = \chi^p(\{3C_2'\}), \quad p = 1, 2, \cdots, 8. \tag{15}$$

The characters of other classes can be determined by the characters mentioned above

- Since $C_6 = C_2^{'(1)} \times C_2^{''(2)}$, we have
$$\chi^p(\{2C_6\}) = \chi^p(\{C_2'\})\chi^p(\{C_2''\}), \quad p = 1, 2, \cdots, 8. \tag{16}$$
- Since $C_3 = C_2^{''(1)} \times C_2^{''(3)}$, we have
$$\chi^p(\{2C_3\}) = \chi^p(\{3C_2''\})\chi^p(\{3C_2''\}) = 1, \quad p = 1, 2, \cdots, 8. \tag{17}$$
- Since $S_6 = C_6 \times \sigma_h$, we have
$$\chi^p(\{S_6\}) = \chi^p(\{2C_6\})\chi^p(\{\sigma_h\}), \quad p = 1, 2, \cdots, 8. \tag{18}$$
- Since $S_3 = C_3 \times \sigma_h$, we have
$$\chi^p(\{S_3\}) = \chi^p(\{2C_3\})\chi^p(\{\sigma_h\}), \quad p = 1, 2, \cdots, 8. \tag{19}$$

In this way, for $p = 1, 2, \cdots, 8$, we can determine the characters of all the classes by only knowing $\chi^p(\{C_2\}), \chi^p(\{3C_2'\}), \chi^p(\{I\})$. There are 8 combinations of $\chi^p(\{C_2\}) = \pm 1, \chi^p(\{3C_2'\}) = \pm 1, \chi^p(\{I\}) = \pm 1$, which correspond to 8 inequivalent irreducible 1-dimensional representations.
As for the left four 2-dimensional inequivalent irreducible representations, we use the orthogonality relation for characters:

$$\frac{1}{g}\sum_{T \in D_{6h}} \chi^p(T)^* \chi^q(T) = \delta_{pq} \tag{20}$$

for $p = 1, 2, \cdots, 8$ and $q = 9, 10, 11, 12$, so

$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) + 3\chi^q(\{3C_2'\}) + 3\chi^q(\{3C_2''\}) + \chi^q(\{I\}) + 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) + 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \tag{21}$$
$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) + 3\chi^q(\{3C_2'\}) + 3\chi^q(\{3C_2''\}) - \chi^q(\{I\}) - 2\chi^q(\{2S_3\}) - 2\chi^q(\{2S_6\}) - \chi^q(\{\sigma_h\}) - 3\chi^q(\{3\sigma_v\}) - 3\chi^q(\{3\sigma_d\}) = 0, \tag{22}$$
$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) - 3\chi^q(\{3C_2'\}) - 3\chi^q(\{3C_2''\}) + \chi^q(\{I\}) + 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) - 3\chi^q(\{3\sigma_v\}) - 3\chi^q(\{3\sigma_d\}) = 0, \tag{23}$$
$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) - 3\chi^q(\{3C_2'\}) - 3\chi^q(\{3C_2''\}) - \chi^q(\{I\}) - 2\chi^q(\{2S_3\}) - 2\chi^q(\{2S_6\}) - \chi^q(\{\sigma_h\}) + 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \tag{24}$$

$$\chi^q(\{E\}) - 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) - \chi^q(\{C_2\}) + 3\chi^q(\{3C_2'\}) - 3\chi^q(\{3C_2''\}) + \chi^q(\{I\}) - 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) - \chi^q(\{\sigma_h\}) - 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \tag{25}$$

$$\chi^q(\{E\}) - 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) - \chi^q(\{C_2\}) + 3\chi^q(\{3C_2'\}) - 3\chi^q(\{3C_2''\}) - \chi^q(\{I\}) + 2\chi^q(\{2S_3\}) - 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) + 3\chi^q(\{3\sigma_v\}) - 3\chi^q(\{3\sigma_d\}) = 0, \tag{26}$$

$$\chi^q(\{E\}) - 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) - \chi^q(\{C_2\}) - 3\chi^q(\{3C_2'\}) + 3\chi^q(\{3C_2''\}) + \chi^q(\{I\}) + 2\chi^q(\{2S_3\}) - 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) - 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \tag{27}$$

$$\chi^q(\{E\}) - 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) - \chi^q(\{C_2\}) - 3\chi^q(\{3C_2'\}) + 3\chi^q(\{3C_2''\}) - \chi^q(\{I\}) - 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) - \chi^q(\{\sigma_h\}) + 3\chi^q(\{3\sigma_v\}) - 3\chi^q(\{3\sigma_d\}) = 0, \tag{28}$$

and

$$\begin{aligned}\left|\chi^q(\{E\})\right|^2 + 2\left|\chi^q(\{2C_6\})\right|^2 + 2\left|\chi^q(\{2C_3\})\right|^2 + \left|\chi^q(\{C_2\})\right|^2 + 3\left|\chi^q(\{3C_2'\})\right|^2 + 3\left|\chi^q(\{3C_2''\})\right|^2 + \left|\chi^q(\{I\})\right| + 2\left|\chi^q(\{2S_3\})\right|^2 + 2\left|\chi^q(\{2S_6\})\right|^2 \\ + \left|\chi^q(\{\sigma_h\})\right|^2 + 3\left|\chi^q(\{3\sigma_v\})\right|^2 + 3\left|\chi^q(\{3\sigma_d\})\right|^2 = 24,\end{aligned} \tag{29}$$

for $q = 9, 10, 11, 12$. We already know that the character of the identity element is always equal to the dimension of the representation, $\chi^q(\{E\}) = 2$ for $q = 9, 10, 11, 12$. Adding the equation (21)∼(28), we get

$$\chi^q(\{E\}) + 2\chi^q(\{2C_3\}) = 0, \quad q = 9, 10, 11, 12, \tag{30}$$

so

$$\chi^q(\{2C_3\}) = -1, \quad q = 9, 10, 11, 12. \tag{31}$$

Adding equations (21)∼(24), we get

$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) = 0, \quad q = 9, 10, 11, 12, \tag{32}$$

so

$$2\chi^q(\{2C_6\} + \chi^q(\{C_2\}) = 0, \quad q = 9, 10, 11, 12. \tag{33}$$

Adding equations (21) and (22), we get

$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) + 3\chi^q(\{3C_2'\}) + 3\chi^q(\{3C_2''\}) = 0, \quad q = 9, 10, 11, 12, \tag{34}$$

so

$$\chi^q(\{3C_2'\}) + \chi^q(\{3C_2''\}) = 0, \quad q = 9, 10, 11, 12 \tag{35}$$

Adding equation (21), (22), (25) and (26), we get

$$\chi^q(\{E\}) + 2\chi^q(\{2C_3\}) + 3\chi^q(\{3C_2'\}) = 0, \quad q = 9, 10, 11, 12, \tag{36}$$

so

$$\chi^q(\{3C_2'\}) = 0, \quad q = 9, 10, 11, 12, \tag{37}$$

and

$$\chi^q(\{3C_2''\}) = 0, \quad q = 9, 10, 11, 12. \tag{38}$$

Adding equations (21) and (24), we get

$$\chi^q(\{E\}) + 2\chi^q(\{2C_6\}) + 2\chi^q(\{2C_3\}) + \chi^q(\{C_2\}) + 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \quad q = 9, 10, 11, 12, \tag{39}$$

so

$$\chi^q(\{3\sigma_v\}) + \chi^q(\{3\sigma_d\}) = 0, \quad q = 9, 10, 11, 12. \tag{40}$$

Subtracting (21) from (22), we get

$$\chi^q(\{I\}) + 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) + 3\chi^q(\{3\sigma_v\}) + 3\chi^q(\{3\sigma_d\}) = 0, \quad q = 9, 10, 11, 12, \tag{41}$$

so

$$\chi^q(\{I\}) + 2\chi^q(\{2S_3\}) + 2\chi^q(\{2S_6\}) + \chi^q(\{\sigma_h\}) = 0, \quad q = 9, 10, 11, 12. \tag{42}$$

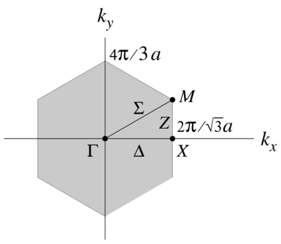
$\cdots$ There 48 unknown characters for $q = 9, 10, 11, 12$, and 42 equations from the orthogonality relation for characters plus the fact that $\chi^q(\{E\}) = 2$ for $q = 9, 10, 11, 12$, technically, we may obtain all the characters for the four 2-dimensional inequivalent irreducible representations. $\cdots$
The character table of D_{6h} is shown in table 1.

Table 1: The character table of D_{6h}.

	$\{E\}$	$\{2C_6\}$	$\{2C_3\}$	$\{C_2\}$	$\{3C_2'\}$	$\{3C_2''\}$	$\{I\}$	$\{2S_3\}$	$\{2S_6\}$	$\{\sigma_h\}$	$\{3\sigma_v\}$	$\{3\sigma_d\}$
Γ^1	1	1	1	1	1	1	1	1	1	1	1	1
Γ^2	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
Γ^3	1	1	1	1	-1	-1	1	1	1	1	-1	-1
Γ^4	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1
Γ^5	1	-1	1	-1	1	-1	1	-1	1	-1	-1	1
Γ^6	1	-1	1	-1	1	-1	-1	1	-1	1	1	-1
Γ^7	1	-1	1	-1	-1	1	1	1	-1	1	-1	1
Γ^8	1	-1	1	-1	-1	1	-1	-1	1	-1	1	-1
Γ^9	2	1	-1	-2	0	0	2	1	-1	-2	0	0
Γ^{10}	2	-1	-1	2	0	0	2	-1	-1	2	0	0
Γ^{11}	2	1	-1	-2	0	0	-2	-1	1	2	0	0
Γ^{12}	2	-1	-1	2	0	0	-2	1	1	-2	0	0

□

Problem 3 Score: _________. Find the basis lattice vectors of the reciprocal lattice of the triangular Bravais lattice. Show that the first Brillouin zone of the triangular Bravais lattice is as given in the following figure.



Solution: The basis lattice vectors of the reciprocal lattice of the triangular Bravais lattice are

$$\boldsymbol{b}_1 = \frac{2\pi \boldsymbol{a}_2 \times \hat{e}_z}{\hat{e}_z \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)} = \frac{4\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{2}\hat{e}_x + \frac{1}{2}\hat{e}_y), \tag{43}$$

$$\boldsymbol{b}_2 = \frac{2\pi \hat{e}_z \times \boldsymbol{a}_1}{\hat{e}_z \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)} = \frac{4\pi}{\sqrt{3}a}\hat{e}_y. \tag{44}$$

As shown in figure 1, we construct the reciprocal lattice of the triangular Bravais. We join the original point $\vec{k} = 0$ of the reciprocal lattice and the six nearest reciprocal lattice points around it with dash line. We draw the perpendicular bisectors of these lines with dotty line. The region enclosed by these dotty line is the first Brillouin region, which is the same as figure given above.

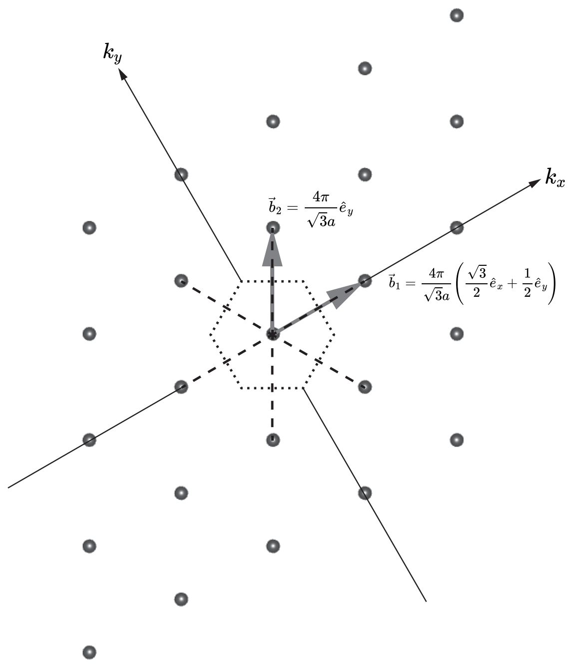


Figure 1: The reciprocal lattice and the first Brillouin of triangular Bravais lattice.

□

Problem 4 Score: _________. Find the point groups for the $\vec{k}$-vectors: $\vec{k}_\Gamma = \vec{0}$, $\vec{k}_X$, and $\vec{k}_M$.

Solution: $\vec{k}_\Gamma$ remains invariant under all the point symmetry operations of D_{6h}, so the point groups for $\vec{k}_\Gamma$ is D_{6h}.
$\vec{k}_X$ remains invariant under the point symmetry operations $\{E, C_2, C_2', C_2'', I, \sigma_h, \sigma_v, \sigma_d\}$, so the point group for $\vec{k}_X$ is D_{2h}.
$\vec{k}_M$ remains invariant under the point symmetry operations $\{E, C_3, C_3^2, C_2', C_2'', C_2''', S_3, S_3^5, \sigma_h, \sigma_v, \sigma_v', \sigma_v''\}$, so the point group for $\vec{k}_M$ is D_{3h}. □

Problem 5 Score: _________. Identify the symmetry axes and their point groups in the first Brillouin zone of the triangular Bravais lattice.

Solution: The symmetry axes in the first Brillouin zone of the triangular Bravais lattice is shown in figure 2.

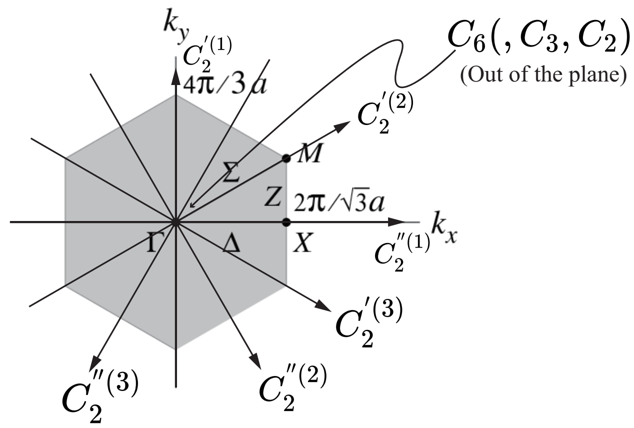


Figure 2: The first Brillouin zone and the symmetry axes.

The $C_2^{'(j)}$ and $C_2^{''(j)}$ axes ($j = 1, 2, 3$) remain invariant under the point symmetry operations $\{E, I, C_2, C_2', C_2'', \sigma_h, \sigma_v, \sigma_v'\}$, so the point group of the $C_2^{'(j)}$ and $C_2^{''(j)}$ axes ($j = 1, 2, 3$) are all D_{2h}.
The C_6 axis remains invariant under all the point symmetry operations of D_{6h}, so the point group of the C_6 axis is D_{6h}. □