## Chapter 3

# Some Finite and Discrete Groups

We have have encountered several finite groups in the previous chapter: the cyclic group  $Z_n$ , the symmetric group  $S_n$ , and its subgroup the alternating group  $A_n$ . The properties of these groups will be elaborated in this chapter. We will also discuss three other groups obtained by incorporating 'reflections' into  $Z_n$ , the dihedral group  $D_n$ , the generalized quaterion group  $Q_n$ , and the dicyclic group  $DZ_n$ . These three groups differ from one another in the way 'reflections' are introduced.

A large class of finite groups is obtained from matrices over a finite field. In mathematics, a field is collection of objects that can mutually multiply, divide, add, and subtract. **REAL** numbers  $\mathbb{R}$  and **COMPLEX** numbers  $\mathbb{C}$  are two familiar fields, each having an infinite number of elements. Thus matrix groups over these fields similarly have an infinite order. Integers  $\mathbb{Z}$  do **NOT** form a field because we cannot divide them, but integers modulo a **PRIME NUMBER** pdo form finite fields which we shall denote by  $\mathbb{F}_p$ . As a result, matrix groups over these finite fields also have a finite orders.

Let me illustrate how to carry out the four arithmetic operations in the field  $\mathbb{F}_7$ :  $2 \times 5 = 10 \equiv 3 \pmod{7}$ ,  $6 + 8 = 14 \equiv 0$ ,  $8 - 11 = -3 \equiv 4$ , and  $6/5 \equiv 4$  (because  $4 \times 5 = 20 \equiv 6 \pmod{7}$ ).

There are also finite fields  $\mathbb{F}_{p^n}$  with  $p^n$  elements, but the four arithmetic operations  $(+, -, \times, /)$  are much more complicated.

Finite subgroups of O(3) are symmetry groups of MOLECULES and CRYS-TALS. They are known as point groups. Some of them may also be symmetry groups for the THREE GENERATIONS of elementary fermions. (Crystal) lattices give rise to a discrete translational symmetry group of infinite order. Point groups incorporating this translational symmetry is known as **space groups**, but we will not discuss these in detail.

Since integers (Z) do not form a field,  $n \times n$  matrices with integer entries generally do not form a group. There is however an exception when n = 2. The set of  $2 \times 2$  matrices with unit determinant and integer entries form a group known as SL(2, Z). This modular group is isomorphic to the group of linear fractional transformations in a complex plane  $[z \rightarrow (az + b)/(cz + d), a, b, c, d \in \mathbb{Z}, ad - bc = 1]$ . It is useful in STRING THEORY, and in the study of MODULAR FUNCTIONS (Jacobi  $\theta$ -functions) in mathematics. This group is clearly not finite, but it is discrete.

Another infinite discrete group useful in integrable models in statistical physics [the YANG-BAXTER EQUATION, for example] is the braid group.

These then are some examples of finite and infinite discrete groups. For finite groups, there is a general Sylow theorem, which yields information on the structure of a finite group G merely from its order |G|. If |G| = pis a prime number, then the only possible group is  $Z_p$ . If  $|G| = \prod p_i^{m_i}$  is decomposed into products of prime numbers  $p_i$ , then the theorem states that G must contain subgroups  $Z_{p_i^{m_i}}$  for all i (known as Sylow p-subgroup), and many of the known properties of these p-subgroups can be used to elucidate the structure of G. For example, it can shown that the smallest nonabelian SIMPLE group is the  $A_5$  group of order |G| = 60.

## **3.1** cyclic group

## $Z_n$ ( $C_n$ )

It is the rotational symmetry group of an *n*-sided REGULAR POLYGON. This group was previously discussed in  $\S1.2.1(1)$ , and here are some more of its properties:

- 1. It is a finite subgroup of SO(2) generated by  $e^{2\pi i/n}$ .
- 2. Being an abelian group, every element is a class, hence |C| = n.
- 3. If n = p is a **PRIME NUMBER**, then there are no non-trivial subgroups, and it is the only group of order n. This also means that  $Z_p$  is simple if p is prime.



Figure 3.1: *n*-sided regular polygons

If n is not prime and m **DIVIDES** n, then  $H = Z_m$  is a (normal) subgroup of  $G = Z_n$ , with the quotient group  $G/H = Z_{n/m}$ .

4. If n = pq is a product of two primes which are MUTUALLY COPRIME, then  $Z_n \cong Z_p \times Z_q$ .

**Proof** : Since p and q are coprime, one can find integers a, b via the 'extended Euclid algorithm' so that  $aq + bp = 1 \pmod{n}$ , with a, b unique modulo p, q respectively. The correspondence  $Z_n \leftrightarrow Z_p \times Z_q$  is

 $e^{2\pi ik/n} \leftrightarrow e^{2\pi ika/p} \times e^{2\pi ikb/q} = e^{2\pi ik(aq+bp)/pq}$ 

For example, in  $Z_{15} \cong Z_3 \times Z_5$ , since 1 = -1 \* 5 + 2 \* 3, we have  $e^{2\pi i k/15} = e^{-2\pi i k/3} \times e^{2\pi i (2k)/5}$ .

5. This is no longer true if p and q are NOT COPRIME. For example, it is not possible to have  $G = Z_{p^2}$  to be the same as the direct product

 $Z_p \times Z_p$ . In the case when p, q are coprime, although (x, e) has order p and (e, y) has order q, some element  $(x, y) \in (Z_p, Z_q)$  may have order pq, the order of the generator of  $Z_{pq}$ . In the case when p = q, every element (x, y) has order p, so it is impossible to get to the generator of  $Z_{p^2}$  which has order  $p^2$ .

6.  $\boxtimes$  Aut $(Z_p) = Z_{p-1}$  if p is prime.

**Proof** : Let  $\epsilon = e^{2\pi i/p}$ , and  $\varphi \in \operatorname{Aut}(Z_p) := G$ . Then  $\varphi(\epsilon)$  must be a generator of  $Z_p$ , so it must be  $\epsilon^m$ , for some 0 < m < p. We shall denote this  $\varphi$  by  $\varphi_m$ . Now  $\varphi_1$  is the identity of G, and |G| = p - 1because that is the number of  $\varphi_m$ . Moreover, G is abelian because  $\varphi_k \varphi_\ell(\epsilon) = \varphi_\ell \varphi_k(\epsilon) = \epsilon^{k+\ell}$ . Thus G is either  $Z_{p-1}$ , or  $Z_{a_1} \times \cdots \times Z_{a_r}$ if  $p - 1 = a_1 \times \cdots \times a_r$ . It can be proven that it is the former but I will skip the proof. For a proof, see Proposition 2, p.15 of 'Groups and Representations' by J.L. Alperin and R.B. Bell.

7.  $\boxtimes$  **Example.** At the end of last chapter, we showed that  $S_3 = Z_3 \rtimes_{\varphi} Z_2$ . Let us show that this semi-direct product is unique.

Since  $\varphi \in \operatorname{Aut}(Z_3) = Z_2$ , either  $\varphi(\epsilon) = \epsilon$ , or  $\varphi(\epsilon) = \epsilon^2$ , where  $\epsilon = e^{2\pi i/3}$ . Since  $\varphi_h$  is a homomorphism in H, we must have  $\varphi_{(12)}^2(\epsilon) = \varphi_e(\epsilon) = \epsilon$ , hence either  $\varphi_{(12)}(\epsilon) = \epsilon$ , leading to the direct product  $Z_3 \times Z_2$ , or  $\varphi_{(12)}(\epsilon) = \epsilon^2$ , leading to the semi-direct product  $S_3 = Z_3 \rtimes_{\varphi} Z_2$  discussed at the end of the last chapter.

## 3.2 $\boxtimes$ Sylow *p*-subgroups

#### $\boxtimes$ $\boxtimes$ $\boxtimes$

Every group G has many abelian subgroups: if m is the order of any  $g \in G$ , then |G| is divisible by m, and  $Z_m$  is an abelian subgroup of G. One might also want to know whether the converse is also true. That is, given m which divides |G|, does G have an abelian subgroup  $Z_m$ ? The answer is, not necessarily. However, if  $|G| = p_1^{m_1} p_2^{m_2} \cdots p_k^{m_k}$ , where  $p_i$  are prime numbers that are mutually prime, then G does have abelian subgroups  $Z_{p_i^{m_i}}$  for every i. These are called the Sylow p-subgroups. They have very interesting

properties that can tell us a great deal about G, just from its order |G|. Specifically, the Sylow theorem tells us that (see Ref [10], pp. 64 for a proof):

#### 3.2.1 Sylow's theorem

- 1. G has at least one Sylow p-subgroup for every prime factor p of |G|; every  $Z_p$  subgroup is contained in a Sylow p-subgroup
- 2. The number  $n_p$  of Sylow *p*-subgroups (called the Sylow number) is 1 mod *p*, and it divides  $|G|/p^m$
- 3. All the Sylow *p*-subgroups are conjugate, meaning that a similarity transformation from some  $g \in G$  takes one to another. In particular, if  $n_p = 1$ , then the Sylow *p*-subgroup is a normal subgroup.
- 4. If N is a normal subgroup of G, and P a Sylow p-subgroup of G. Then P/N is a Sylow p-subgroup of G/N, and  $P \cap N$  is a Sylow p-subgroup of N.

#### 3.2.2 Sample applications

As a sample application of the Sylow theorem, let us use it to obtain information about whether the groups below could be simple or not.

- 1. If |G| = 15 = 3.5, then G is not simple for the following reason.  $n_3$  must divide 5 and be 1 mod 3, so it has to be 1. Thus the Sylow 3-group is a normal subgroup so G is not simple.
- 2. If  $|G| = 30 = 2 \cdot 3 \cdot 5$ , then it is also not simple for the following reason. In that case  $n_3$  divides 10 and must be 1 (mod 3), so it must be 1 or 10. If  $n_3 = 1$  then the Sylow 3-subgroup is normal and G is not simple, so let us suppose  $n_3 = 10$ , in which case there would be  $2 \times 10 = 20$ distinct elements of order 3. Now  $n_5$  must divide 6 and be 1 (mod 5), so it could be 1 or 6. Again if G were simple we must rule out 1, so  $n_5 = 6$  and there are  $4 \times 6 = 24$  elements of order 5. Altogether they give 44 elements which cannot be accommodated if |G| = 30. Hence G must not be simple because we have ruled out all the possibilities for its being simple.

- 3. G with  $|G| = 42 = 2 \cdot 3 \cdot 7$  cannot be simple.  $n_7$  must divide 6 and be 1 (mod 7), so it is 1, so the Sylow 7-subgroup is normal and G is not simple.
- 4. Suppose G with  $|G| = 60 = 2^2 \cdot 3 \cdot 5$  is simple. This group has  $n_5 = 6$  so there are 24 elements of order 5. Moreover,  $n_3 = 10$  so there are 20 elements of order 3. Since the group G contains |G| 1 = 59 nonidentity elements, this fixes the number of elements of order 2 and 4 to be 59 - 24 - 20 = 15. The Sylow 2-subgroups of G has order 4, and there are two possible groups of that order (see a systematic discussion of low-order groups later):  $Z_2 \times Z_2$ , and  $Z_4$ . Since all the Sylow p-groups must be isomorphic to each other, these Sylow 2-groups must all be of the same kind. Now  $Z_2 \times Z_2$  has 3 elements of order 2, and none of order 4, and  $Z_4$  has 2 elements of order 4 and 1 of order 2. Either has 3 elements of order 2 or order 4, hence  $n_2 = 5$  to make a total of 15 such elements.

The alternating group  $A_5$  has 60 elements and contains all the even permutations (odd cycles) of 5 objects. The 5-cycle elements have order 5, and there are 4! = 24 of them, precisely what  $n_5 = 6$  gives. The three cycles contain  $C_3^5 2! = 20$  elements of order 3, precisely what  $n_3 = 10$  requires. The remaining elements are 2<sup>2</sup>-cycles, and there are  $5 \times 3 = 15$  of them, each having order 2, so its Sylow 2-group must be  $Z_2 \times Z_2$ . Indeed, the elements  $K_4 = (e, (12)(34), (13)(24), (14)(23))$ forms a normal subgroup of  $A_4$ , sometimes known as Klein's 4-group (K<sub>4</sub>), and  $A_5$  contains 5 such  $K_4$  groups, corresponding to each of the 5 choices of 4 numbers out of 1,2,3,4,5. There are 3 order 2 elements in  $K_4$ , as required. Actually  $K_4 \cong Z_2 \times Z_2$  with the correspondence  $K_4 \leftrightarrow (Z_2, Z_2)$  to be  $e \leftrightarrow (1,1), (12)(34) \leftrightarrow (1,-1), (13)(24) \leftrightarrow$  $(-1,1), and (-1,-1) = (1,-1)(-1,1) \leftrightarrow (12)(34)(13)(24) = (14)(23).$ We conclude that  $A_5$  passes all the Sylow *p*-group tests to be simple.

To show that it is really simple, suppose N is a proper normal subgroup of  $A_5$ , whose order must then be |N| must be 30, 20, 15, 12, 5, 4, 3, 2, 1. Since it is normal, if it contains one Sylow *p*-subgroup of  $A_5$ , then it contains all of them. Using a prime to denote the Sylow numbers of N and no prime to denote the Sylow number of  $A_5$ , this implies that  $n'_p = n_p$  if  $n'_p \neq 0$ . Now if 5||N|, then  $n'_5 = n_5 = 6$  and it must contain 24 elements of order 5, hence |N| = 30. Since 3|30, it must have  $n'_3 = n_3 = 10$  and contains also 20 elements of order 3, so the order of N cannot be 30 and |N| cannot be divisible by 5. That leaves  $|N| \leq 12$ . If 3||N|, then  $n'_3 = n_3 = 10$  so there are 20 elements of order 3, leading to a contradiction, so that leaves |N| = 4, 2, 1 as remaining possibilities. If  $|N| = 4 = 2^2$ , then  $n'_2 = n_2 = 5$ , also a contradiction. Finally,  $|N| \neq 2$  because there are many elements in  $A_5$  that are conjugate to a 2-cycle in N, so that leaves |N| = 1, proving that  $A_5$  is simple.

It can be shown that any simple group of order 60 is isomorphic to  $A_5$ , and that  $A_5$  is the lowest-order group that is simple.

## 3.3 dihedral group

## D<sub>n</sub>

If we incorporate the reflections, the group  $Z_n$  enlarges into the dihedral group  $D_n$  of order 2n. See Fig. 3.2. If n is odd, the reflections are taken about the lines passing through a vertex but perpendicular to the opposite edge. If n is even, then half of these reflection lines are those joining opposite vertices, and half are those joining the midpoints of opposing edges. Since reflections do not commute with rotations,  $D_n$  is nonabelian. It is subgroup of O(2), though not SO(2) because reflections are involved.



Figure 3.2: Reflection axes of regular polygons

Here are some properties of the dihedral group.

- 1. Let  $\theta_k$  be the *k*th vertex of an *n*-sided polygon,  $k = 1, 2, \dots, n$ , and *r* be the elementary ROTATION rotating  $\theta_k$  to  $\theta_{k+1}$ . See Fig. 3.2. Then  $Z_n = \{r | r^n = 1\}$ . Let  $\sigma := \sigma_1$  be an elementary REFLECTION changing  $\theta_k$  to  $\pi \theta_k$ , namely, a reflection about the vertical axis. Then it is easy to see that  $\sigma = r\sigma r$ , and hence  $r^p \sigma r^p = \sigma$ .
- 2. As a result,  $\sigma_p := \sigma r^{p-1}$  are reflections satisfying  $\sigma_p^2 = 1$ , and  $\sigma \sigma_p = r^{p-1}$  are rotations. This also tells us that a **PRESENTATION** of  $D_n$  is  $\{\sigma_1, \sigma_2 | \sigma_1^2 = \sigma_2^2 = (\sigma_1 \sigma_2)^n = 1\}.$
- 3.  $Z_n$  forms a normal subgroup of  $D_n$ . The quotient group  $D_n/Z_n \cong Z_2$  is generated by the reflection  $\sigma$ .
- 4.  $\boxtimes$  In fact,  $D_n = Z_n \rtimes_{\varphi} Z_2$ .

Let us discuss the automorphism  $\varphi_h(n)$ , with  $h \in Z_2$  and  $n \in Z_n$ . All that we have to do is to specify it on the generator h = -1 of  $Z_2$ , and the generator  $\epsilon = e^{2\pi i/n}$  of  $Z_n$ . We know that  $h_{-1}(\epsilon) = \epsilon^m$  for some *m* which has no common divisor with *n*. We also know that  $\varphi_{h_1}(n_2) = h_1 n_2 h_1^{-1}$ , hence  $\varphi_{-1}(\epsilon) = \epsilon^m = \sigma \epsilon \sigma^{-1} = \epsilon^{-1}$ , hence m = -1.

- 5. As a consequence of the properties in item (1),  $\sigma r^p \sigma = r^{-p}$ , hence  $\{r^p, r^{-p}\}$  forms a class. There are n/2 such classes if n is even, (n-1)/2 such classes if n is odd.
- 6. Moreover,  $r^{-1}\sigma_p r = r^{-1}\sigma r^p = \sigma r^{p+1} = \sigma_{p+2}$ . If *n* is odd, then all  $\sigma_p$  together form a class, but if *n* is even, then they separate into two classes.
- 7. HENCE  $|\mathcal{C}| = n/2 + 3$  if *n* is even,  $|\mathcal{C}| = (n-1)/2 + 2$  if *n* is odd.
- 8. Suppose n is a prime, then it has n Sylow 2-subgroups each generated by a  $\sigma_i$ , and one Sylow n-subgroup  $Z_n$  of the rotations.

## **3.4** symmetric group

## S<sub>n</sub>

The permutations of n objects form a symmetric group, of order n!, denoted as  $S_n$ . Other than  $S_2$  which is isomorphic to  $Z_2$ , they are NONABELIAN.

This is the most important finite group because every finite group can be considered as a subgroup of some  $S_n$  (see the 'regular representation' of a group in the next chapter).

Any subgroup of a symmetric group is called a **permutation group**. Most finite groups are isomorphic to a permutation group. A permutation group of n objects is **transitive** if every object can be reached from any other object by some group element; otherwise **intransitive**.

Here are some facts about the symmetric group.

- 1. If s, t are permutations,  $sts^{-1}$  has the same cycle structure as t, hence all elements having the same cycle structure form a CLASS. For example,  $S_2$  has two classes,  $\{e\}$ , and  $\{(12)\}$ .  $S_3$  has three classes, the identity class, the 2-cycle class, and the 3-cycle class.  $S_4$  has five classes: the identity class, 2-cycles, 3-cycles, 4-cycles, and  $2^2$ -cycles.
- 2.  $D_3 \cong S_3$ . To see that, first note that both have order 6. Next, take the regular triangle which is invariant under  $D_3$  and label the vertices by 1,2,3. Then the three  $Z_3$  rotations correspond to the even permutations e = (1), (123), and (132). The three reflections correspond to the odd permutations (12), (13), and (23).
- 3.  $\boxtimes$  There are three Sylow 2-subgroups generated by (12), (13), (23) respectively, and one Sylow 3-subgroup generated by (123).
- 4.  $S_4$  leaves the CUBE invariant. To see that, label the vertices on the top surface 1,2,3,4, and the corresponding vertices at the bottom surface also 1,2,3,4. Suppose the 6 surfaces of the cube locate at  $x = \pm 1$ ,  $y = \pm 1$ ,  $z = \pm 1$ , respectively. Then rotations about the z-axis correspond to (1234), (1432), (1324), rotations about the x-axis correspond to (12)(34), and rotations about the y-axis corresponds to (14)(23). Now (1234) is an odd permutation and (12)(34) is an even permutation. Multiplying the three odd permutations and the two even permutations together in all possible ways, meaning rotating about these three axes repeatedly one after another, one can generate the whole  $S_4$  group.

Since the octahedron is dual to the cube,  $S_4$  is also the rotational symmetry group of the octahedron, which is why it is also known as the octahedral group O.

## 3.5 alternating group

A<sub>n</sub>

Even permutations of n objects form a subgroup of the symmetric group of order n!/2, known as the alternating group  $A_n$ .

- 1.  $A_n$  is a normal subgroup of  $S_n$ .
- 2.  $A_n$  for n > 4 is simple.
- 3. The Klein group  $K_4 = [e, (12)(34), (13)(24), (14)(23)] \cong Z_2 \times Z_2$ is a normal subgroup of  $A_4$ .
- 4.  $A_3 \cong Z_3$ .
- 5.  $A_4$  is the rotational symmetry group of the regular TETRAHEDRON (pyramid). See Fig. 1.2. Label the four vertices by 1,2,3,4. Then (123) and (132) correspond to rotations about an axis perpendicular to the 1,2,3 plane going through vertex 4. The other 3-cycle permutations can all be interpreted in a similar way. Finally, the remaining even permutations, (12)(34) corresponds to a 180° rotations about an axis joining the midpoints of lines (12) and (34), and similarly (13)(24). The odd permutations such as (12) can never leave the solid tetrahedron invariant.

For that reason,  $A_4$  is also known as the tetrahedral group T.

- A<sub>5</sub> is the rotational symmetry group of the icosahedron and the dodecahedron. For that reason it is also known as the icosahedral group I.
- 7. The number of classes |C| of  $S_n$  and  $A_n$  are tabulated in the following table. Note that a class in  $S_n$  can split up into several classes of  $A_n$ , or else  $|C|_{A_n}$  would generally be smaller than what is listed below.

n	1	<b>2</b>	3	4	5	6	7	8	9	10
$S_n$	1	<b>2</b>	3	<b>5</b>	7	11	15	22	30	42
$A_n$	1	<b>1</b>	3	4	<b>5</b>	<b>7</b>	9	<b>14</b>	<b>18</b>	<b>24</b>

Table 3.2 The number of classes in  $S_n$  and  $A_n$ 

## **3.6** Quaternion groups

 $Q, \ Q_n$ 

- 1. A quaternion is a generalization of a complex number, with one real component and three imaginary components i, j, k. They obey the multiplication rule  $i^2 = j^2 = k^2 = -1$ , ij = -ji = k, jk = -kj = i, ki = -ik = j. They can be represented by the Pauli matrices  $i = i\sigma_1, j = -i\sigma_2, k = i\sigma_3$ , if 1 is represented by the 2-dim identity matrix e.
- 2. The Pauli matrices generate a group P of order 16, consisting of  $(1, -1, +i, -i) * (e, \sigma_1, \sigma_2, \sigma_3)$ , with a center Z(P) consisting of  $\pm e, \pm ie$ . The quotient group  $P/Z(P) \cong K_4$ .
- 3. It also contains a larger subgroup Q of order 8, called the quaternion group, consisting of  $\pm(e, i, j, k)$ , where so that  $ij = k, jk = i, ki = j, i^2 = j^2 = k^2 = -e$ .
- 4. The generalized quaternion group  $Q_n$  is generated by

$$a = \begin{pmatrix} e^{\pi i/n} & \\ & e^{-\pi i/n} \end{pmatrix}, \quad j = \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} = -i\sigma_2$$

Its order is 4n, and  $Q_2 \cong Q$ .

## 3.7 Dicyclic groups

 $\mathsf{DZ}_n\ (\mathsf{DC}_n)$ 

1. It is generated by  $a = e^{\pi i/n}$  and j. Note that  $aj = ja^{-1}$ .

- 2. Its order is 4n.
- 3. Suppose we use the representation  $i \to i\sigma_3$ ,  $j \to i\sigma_1$ ,  $k = -i\sigma_2$ , then the generators in terms of  $2 \times 2$  matrices are

$$a = \begin{pmatrix} e^{\pi i/n} \\ e^{-\pi i/n} \end{pmatrix}, \quad j = i \begin{pmatrix} 1 \\ 1 \end{pmatrix} = i\sigma_1$$

- 4.  $DC_1 \cong Z_4, DC_2 \cong Q$
- 5. If n = 2m is even, then  $a^m = i\sigma_3$ , so the group contains  $i\sigma_3 i\sigma_1 = -i\sigma_2$ , and hence it contains  $Q_n$ . Conversely, the group  $Q_n$  contains  $-i\sigma_2 i\sigma_3 = i\sigma_1$ , so  $Q_n$  contains  $DC_n$ . Consequently,  $DC_{2m} \cong Q_{2m}$ .
- 6. COMPARISON: The orders of  $D_{2n}, Q_n, DZ_n$  are all equal to 4n. All three of them are generated by a common rotation

$$r = \begin{pmatrix} e^{\pi i/n} & \\ & e^{-\pi i/n} \end{pmatrix},$$

but individual 'reflections'  $\sigma$ . For  $D_{2n}$ ,  $\sigma = \sigma_1$ , for  $Q_n$ ,  $\sigma = -i\sigma_2$ , and for  $DZ_n$ ,  $\sigma = i\sigma_1$ . Note that in the last two cases,  $\sigma$  is really not a reflection because  $\sigma^2 = -1$  rather than +1.

## 3.8 Classical groups over a finite field

- 1. The set of  $m \times m$  non-singular matrices over a finite field  $\mathbb{F}$  forms a group called the general linear group over the finite field  $\mathbb{F}$ , and is denoted as  $GL(m, \mathbb{F})$  or GL(m, q), if  $|\mathbb{F}| = q = p^n$ . This group and some of its subgroups are usually called the classical subgroups over a finite field. Since the matrix elements are all numbers in  $\mathbb{F}$ , the number of possible matrices is finite, so every such group is always a finite group.
- 2. The subgroup of  $GL(m, \mathbb{F})$  consisting of matrices of determinant 1 is called the special linear group, and is denoted by  $SL(m, \mathbb{F})$  or SL(m,q). It has a center Z consisting of all multiple of the identity matrix with determinant 1, namely, matrices of the form  $\alpha \mathbf{1}_m$  with  $\alpha^m = 1$ . The group SL(m,q)/Z is called the projected special

#### 3.8. CLASSICAL GROUPS OVER A FINITE FIELD

linear group and is denoted by PSL(m,q), or simply L(m,q). It is a classic theorem, proven by L.E. Dickson in his 1896 Ph.D. theis at the University of Chicago, that all PSL(m,q) groups are simple unless m = 2 and q = 2 or 3.

3. Many of the finite groups we discussed before are isomorphic to some subgroups of GL(m,q). Here is a sample list:

$$S_{3} \cong L(2,2)$$

$$A_{4} \cong L(2,3)$$

$$S_{4} \cong PGL(2,)$$

$$A_{5} \cong L(2,4) \cong L(2,5)$$

$$A_{6} \cong L(2,9)$$

$$A_{8} \cong L(4,2)$$

$$GL(3,2) \cong L(2,7)$$
(3.1)

A very detailed list of the properties of finite groups can be found in the book 'Atlas of Finite Groups' by Conway, Curtis, Norton, Parker, Wilson, and also on the website http://brauer.maths.qmul.ac.uk/Atlas/v3/

4. The order of GL(m,q) is

$$|GL(m,q)| = q^{m(m-1)/2}(q^m - 1)(q^{m-1} - 1)\cdots(q - 1).$$
(3.2)

**Proof**: Let the *i*th coulumn of a matrix in GL(m,q) be denoted  $u_i$ . We will count the number of possible matrices in GL(m,q) by counting the total number of each column vector  $u_i$ . Start from  $u_1$ . Every of the *m* components of  $u_1$  could be one of the *q* numbers in  $\mathbb{F}$ , hence there are altogether  $q^m$  possible vectors. Since the matrices have to be non-singular, we must exclude the vector  $\vec{0}$  so there are  $q^m - 1$  possible vectors left for  $u_1$ . Now look at  $u_2$ . It must not be a multiple of  $u_1$ for the matrix to be non-singular, so there are  $q^m - q$  possibilities. For  $u_3$ , it cannot be any linear combinations of  $u_1$  and  $u_2$ , so its possible number is  $q^m - q^2$ . Proceeding thus, we get the order of the group to be

$$\prod_{k=0}^{m-1} (q^m - q^k) = q^{m(m-1)/2} (q^m - 1)(q^{m-1} - 1) \cdots (q - 1).$$

5. The order of SL(m,q) is

$$|SL(m,q)| = \frac{|GL(m,q)|}{q-1} = q^{m(m-1)/2}(q^m-1)(q^{m-1}-1)\cdots(q^2-1)(3.3)$$

- 6. The order of PSL(m,q) = L(m,q) is |SL(m,q)|/r, where r is the number of solutions of  $\alpha^m = 1$  in  $\mathbb{F}$ . For example, if m = 2, then the solution of  $\alpha^2 = 1$  is  $\alpha = \pm 1$ . If 2 divides q, then  $+1 \equiv -1$ , so r = 1. Otherwise r = 1.
- 7. We can check these order formulas against the examples in (3.1):

$$|S_3| = 3! = 6, |L(2,2)| = 2(2^2 - 1)/1 = 6;$$
  

$$|A_4| = 4!/2 = 12, |L(2,3)| = 3(3^2 - 1)/2 = 12;$$
  

$$|A_5| = 5!/2 = 60, |L(2,4)| = 4(4^2 - 1)/1 = 60,$$
  

$$|L(2,5)| = 5(5^2 - 1)/2 = 60;$$
  

$$|A_6| = 6!/2 = 360, |L(2,9)| = 9(9^2 - 1)/2 = 360;$$
  

$$|GL(3,2)| = 2^3(2^3 - 1)(2^2 - 1)(2 - 1) = 168,$$
  

$$|L(2,7)| = 7(7^2 - 1)/2 = 168.$$
  
(3.4)

## 3.9 Modular Group

#### $GL(2,\mathbb{Z}), SL(2,\mathbb{Z}), PSL(2,\mathbb{Z})$

The set of integers  $\mathbb{Z}$  is *not* a field, not even a group, because we can multiply and cannot divide. Yet,  $GL(2,\mathbb{Z}) \equiv GL_2(\mathbb{Z}) \equiv S^*L_2(\mathbb{Z})$  is a group if we confine ourselves to  $2 \times 2$  matrices of integer coefficients *and* determinant  $\pm 1$ . The latter condition is necessary because the determinant of the inverse is the inverse of the determinant, so unless the determinant is  $\pm 1$ , its inverse is not an integer.

This is also sufficient because  $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$  implies  $A^{-1} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} / \det(A)$ .  $SL(2,\mathbb{Z}) \equiv SL_2(\mathbb{Z})$  is the subgroup of  $S^*L_2(\mathbb{Z})$  with determinant +1, and  $PSL(2,\mathbb{Z}) \equiv PSL_2(\mathbb{Z})$  is the subgroup of  $SL_2(\mathbb{Z})$  with A and -A identified. It is also called the modular group. It generates the fractional linear transformation on the complex plane:

$$z \to z' = \frac{az+b}{cz+d}.\tag{3.5}$$

It has two generators,  $S: z \mapsto -1/z$ , and  $T: z \mapsto z+1$ . Note that  $ST: z \mapsto (z-1)/z$ ,  $(ST)^2: z \mapsto 1/(1-z)$ ,  $(ST)^3: z \mapsto z$ . In fact, the modular group has the PRESENTATION

$$\Gamma := PSL(2,\mathbb{Z}) = \{S, T | S^2, (ST)^3\}.$$
(3.6)

This group and its subgroups are important in many branches of mathematics, including number theory, the theory of modular functions, Monster group, etc. It is also useful in the string theory.

 $\Gamma(\mathbb{N})$  defined by restricting the matrix elements to  $a \equiv d \equiv 1 \pmod{N}$ and  $b \equiv c \equiv 0 \pmod{N}$  is a normal subgroup of  $\Gamma$ .  $\Gamma(N)$  is also a subgroup of  $\Gamma_0(\mathbb{N})$ , defined as a subgroup of  $\Gamma$  with  $c \equiv 0 \pmod{N}$ . These are some of the important subgroups of the modular group.

order	abelian group	non – abelian group
2	$Z_2 \cong S_2 \cong D_1$	_
3	$Z_3 \cong A_3$	_
4	$Z_4;  Z_2 \times Z_2 \cong K_4$	_
5	$Z_5$	_
6	$Z_6 \cong Z_3 \times Z_2$	$S_3$
7	$Z_7$	_
8	$Z_8; Z_4 \times Z_2; Z_2^3$	$D_4; \ Q$
9	$Z_9; Z_3^3$	_
10	$Z_{10} \cong Z_5 \times Z_2$	$D_5$
11	$Z_{11}$	_
12	$Z_{12} \cong Z_4 \times Z_3; \ Z_6 \times Z_2 \cong Z_3 \times Z_2^2$	$D_6; A_4$
13	$Z_{13}$	_
14	$Z_{14} \cong Z_7 \times Z_2$	$D_7$
15	$Z_{15} \cong Z_5 \times Z_3$	_
16	$Z_{16}; Z_8 \times Z_2; Z_4^2; Z_4 \times Z_2^2; Z_2^4$	$D_8; D_4 \times Z_2; Q_2 \times Z_2; Q_4 \cong DC_4$
		$P; Z_4 \rtimes Z_4; Z_2^2 \rtimes Z_4;$ two others

## **3.10** A list of groups of order $\leq 16$

Table 3.3 A list of group of small order

## 3.11 $\boxtimes$ A short list of group presentations

#### $\boxtimes$ $\boxtimes$ $\boxtimes$

Every group has a (abstract) presentation (see §1.3), but presentations are not necessarily unique. Here is a short list of examples.

	group	section	relation
1.	$Z_n$	3.1	$\{r r^n\}$
2.	$D_n$	3.3	$\{r,\sigma r^n,\sigma^2,(r\sigma)^2\}$
3.	$DC_n$	3.7	$\{r,\tau r^{2n}=1,r^n=\tau^2,\tau r\tau^{-1}=r^{-1}\}$
4.	Q	3.6	$\{i, j   i^4, i^2 j^2, i j i j^{-1}\}$
5.	$S_n$	3.4	$\left  \left\{ \sigma_1, \sigma_2, \cdots, \sigma_{n-1} \middle  \sigma_i^2 = 1, \sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}, \sigma_i \sigma_j = \sigma_j \sigma_i \right. (j \neq i \pm 1) \right\}$
6.	$B_n$		$\{\sigma_1, \sigma_2, \cdots, \sigma_{n-1}   \sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}, \sigma_i \sigma_j = \sigma_j \sigma_i \ (j \neq i \pm 1) \}$
7.	$S_3$	3.4	$\{F, G   F^3, G^2, (FG)^2\}$
8.	$A_4 = T$	3.5	$\{F, G   F^3, G^2, (FG)^3\}$
9.	$S_4 = O$	3.4	$\{F, G   F^3, G^2, (FG)^4\}$
10.	$A_5 = I$	3.5	$\{F,G F^3,G^2,(FG)^5\}$
11.	$PSL_2(\mathbb{Z})$	3.9	$\{F,G F^3,G^2\}$

Table 3.4 A short list of group presentations

#### **Concrete** representations

- 1. The elementary rotation  $r = e^{2\pi i/n}$  satisfies  $r^n = 1$ .
- 2. If  $r = \begin{pmatrix} e^{2\pi i/n} & 0 \\ 0 & e^{-2\pi i/n} \end{pmatrix}$  is the elementary rotation and  $\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is the elementary reflection, then calculation shows that  $r\sigma = \begin{pmatrix} 0 & e^{2\pi i/n} \\ e^{-2\pi i/n} & 0 \end{pmatrix}$ , hence  $(r\sigma)^2 = 1$ .
- 3.  $DC_n$  in §3.7 is generated by  $a = e^{\pi i/n}$  and the second imaginary unit j anticommuting with i. We need to show that they satisfy the the generator and relation above.

Let  $a = \sqrt{r} = e^{\pi i/n}$ . Thus  $r^{2n} = 1$ . Let  $\tau = j$ , then it is easy to show that the relations in the table are satsified.

4. The group Q in §3.6 is defined by three mutually anticommuting imaginary units i, j, k so that ij = k, etc. We shall show that the i, j defined in the table above are the same as two of those imaginary units.

From  $i^2 j^2 = 1$  we know that  $i^2 = j^{-2}$ . Together with  $i^4 = 1$ , one deduces  $i^2 = j^2$ ,  $j^4 = 1$ ,  $i^2 j = j^3 = j^2 i$ ,  $j^2 i = i^3 = ij^2$ . We can therefore identify  $i^2 = j^2$  with -1.

Let k := ij. Then  $k^2 = ijijj^{-2} = j^{-2} = j^2 = i^2 = -1$ , hence  $k^2i = i^3 = ik^2, k^2j = j^3 = jk^2, k^4 = 1$ .

Moreover,  $ijij^{-1} = 1 \Rightarrow ji = i^{-1}j = i^3j = -ij$ . Similarly,  $kj = ij^2 = -jij = -jk$ , etc.

5. The concrete representations of the generators  $\sigma_i$  in the table are  $\sigma_i = (i, i+1)$ . Then  $\sigma_i^2 = 1$  and  $\sigma_i$  and  $\sigma_j$  commutes if  $j \neq i \pm 1$ . Moreover,  $\sigma_i \sigma_{i+1} \sigma_i = (i, i+1)(i+1, i+2)(i, i+1) = (i, i+2)$  and  $\sigma_{i+1} \sigma_i \sigma_{i+1} = (i+1, i+2)(i, i+1)(i+1, i+2) = (i, i+2)$ , hence these two are equal. This finishes the verification of the relations in the table.

Note that abstractly  $(\sigma_i \sigma_{i+1})^3 = (\sigma_i \sigma_{i+1} \sigma_i)(\sigma_{i+1} \sigma_i \sigma_{i+1}) = (\sigma_i \sigma_{i+1} \sigma_i)(\sigma_i \sigma_{i+1} \sigma_i) = 1$ . This shows that the relation  $\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}$  is needed to show that  $\sigma_i \sigma_{i+1} = (i, i+1, i+2)$  is of order 3.

In the same way, it can be used to show that  $\sigma_i \sigma_{i+1} \sigma_{i+2}$  is a four cycle, etc.

6.  $B_n$  is called the **braid group**. Its generators and relations are almost identical with  $S_n$ , except for the absence of the relation  $\sigma_i^2 = 1$ .  $S_n$  is the group permuting *n* objects, and  $B_n$  is the group braiding *n* threads. When you exchange two objects twice, you get back to the unexchanged configuration, which is why  $\sigma_i^2 = 1$  in  $S_n$ . On the other hand, when you braid two threads twice, you do not get back to the unbraided configuration–just look at girls with braided pony-tails.

Note from Fig. 3.3 that  $\sigma_i$  braids two threads one way, and  $\sigma_i^{-1}$  braids it another way.

Multiplication from left to right corresponds to joining the threads together from top to bottom. For example,  $\sigma_1 \sigma_2 \sigma_1$  is given by the

The following figure shows why the relation  $\sigma_a \sigma_{a+1} \sigma_a = \sigma_{a+1} \sigma_1 \sigma_{a+1}$ is true. For example, thread *a* is above the other two threads in both figures, and thread (a+2) is below the other two threads in both figures.



Figure 3.3: An elementary braid and its inverse braid. Note that  $\sigma_a$  are called  $g_a$  in this and the subsequent figures.



Figure 3.4: The braid multiplication of  $\sigma_1 \sigma_2 \sigma_1$ 

This relation is also known as the Yang-Baxter relation because it is a special case of the YB relation used in integrable statistical models.

- 7. Let F = (123) = (12)(23), G = (12). Then FG = (13) has order 2. Since GF = (23), all the 2-cycles, and hence all of  $S_3$ , can be generated from F and G.
- 8. Let F = (123) = (12)(23), G = (13)(24). Then FG = (243) = (24)(43) is of order 3. Since the signatures of F and G are both even, together they must generate a subgroup of  $A_4$ . By direct calculation it is easy to see that the whole  $A_4$  is generated.
- 9. Let F = (123) = (12)(23), G = (34). Then FG = (1234) is of order 4. The signature of G is odd and that of F is even, so F, G together generate a subgroup of  $S_4$ . Direct calculation shows that it is the entire  $S_4$ .



Figure 3.5: The relation  $\sigma_a \sigma_{a+1} \sigma_a = \sigma_{a+1} \sigma_a \sigma_{a+1}$ 

- 10. Let F = (123) = (12)(23), G = (34)(45). Then FG = (12345) is of order 5. Since both generators have even signature, they generate a subgroup of  $A_5$ . Direct calculation shows that it is the entire  $A_5$ .
- 11. See §3.9, with the substitution G = S and F = ST.

## **3.12** Horizontal Symmetry of Leptons

 $\beta$ -decay gives rise to one of the three charged leptons  $(e, \mu, \tau)$  and a corresponding neutrino  $(\nu_e, \nu_\mu, \nu_\tau)$ . In general, none of these particles have a definite mass, but one can always choose a basis to diagonalize the  $3 \times 3$  (left-handed effective) mass matrix  $\overline{M}_e$  of the charged leptons. In that case the charged leptons have a definite mass but the neutrinos still do not. If the neutrino mass eigenstates are denoted as  $\nu_1, \nu_2, \nu_3$ , and if

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = U \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}, \qquad (3.7)$$

then the unitary matrix U is called the (PMNS) neutrino mixing matrix. From neutrino oscillation experiments, U is equal to

$$U = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 & \sqrt{2} & 0\\ -1 & \sqrt{2} & \sqrt{3}\\ -1 & \sqrt{2} & -\sqrt{3} \end{pmatrix}$$
(3.8)

to within 1 standard deviation. Such a mixing is usually known as tri-bimaximal mixing.

It can be verified that each of

$$G_{1} = \frac{1}{3} \begin{pmatrix} 1 & -2 & -2 \\ -2 & -2 & 1 \\ -2 & 1 & -2 \end{pmatrix}$$

$$G_{2} = -\frac{1}{3} \begin{pmatrix} 1 & -2 & -2 \\ -2 & 1 & -2 \\ -2 & -2 & 1 \end{pmatrix}$$

$$G_{3} = - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
(3.9)

has one +1 eigenvalue and two -1 eigenvalues, and that he eigenvector of  $G_i$  with +1 eigenvalue is the *i*th column of the mixing matrix U. Since these columns are also the eigenvectors of the neutrino mass matrix  $\overline{M}_{\nu}$ , every  $G_i$  commutes with  $\overline{M}_{\nu}$  and they constitute a symmetry of the neutrino mass matrix.

Since the charged-lepton mass matrix  $M_e$  is diagonal, any diagonal  $3 \times 3$  matrix commutes with it and constitutes a symmetry. In particular,

$$F = \begin{pmatrix} 1 & & \\ & \omega & \\ & & \omega^2 \end{pmatrix}, \qquad \omega := e^{2\pi i/3}$$
(3.10)

is such a symmetry. The group  $\mathcal{G}_i$  generated by F and  $G_i$  is then a horizontal symmetry group of the leptons at high energy. Later on, this group breaks spontaneously into separate symmetries F and  $G_i$  for the charged leptons and the neutrinos, respectively.

If can be verified that  $F^3 = 1$ ,  $G_i^2 = 1$ . Moreover,  $(FG_1)^4 = 1$ ,  $(FG_2)^3 = 1$ ,  $(FG_3)^2 = 1$ , hence from the last section, we conclude that  $\mathcal{G}_1 = S_4$ ,  $\mathcal{G}_2 = A_4$ , and  $\mathcal{G}_3 = S_3$ .

## 3.13 Crystal Point Groups and Space Groups

Crystals are interesting (and sometimes very expensive) objects, especially those of gem quality. If you drop and break it, it will break into pieces with facets always the same as the original ones. Continued thus, one can imagine eventually breaking a crystal down to its fundamental unit with a particular shape. What we would like to do in this section is to discuss the possible shapes and symmetries of the crystals. This is a big subject, so we will only summarize the salient points from the symmetry point of view.

Some of these crystals are shown in the following pictures to remind you how beautiful they can be. It should be cautioned that the shape of the macroscopic crystal shown depends on how the gem is cut and is **NOT** necessarily the shape of the fundamental unit cell.



Figure 3.6: Various gemstones

#### 3.13.1 Point groups

The symmetry of a unit cell should be found among the finite groups, but not all finite groups are suitable because the individual units must be able to fit and stack together to form a crystal. Only certain angles between crystal faces are allowed, and that translates into a restriction on the ALLOWED ROTATION ANGLES about a single axis to be  $2\pi/n$  with n = 1, 2, 3, 4, 6. The allowed rotational symmetry groups with this restriction are

$$C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T, O,$$

where  $C_1$  is just the trivial group containing the identity, meaning that there is no symmetry at all. Note that the reflections in  $D_n$  are actually 180°rotations about an axis in the *xy*-plane, if  $C_n$  represents rotations about the *z*-axis. We shall use the notation  $r_n$  to denote a rotation of  $2\pi/n$  about the z-axis:

$$r_n = \begin{pmatrix} \cos(2\pi/n) & \sin(2\pi/n) & 0\\ -\sin(2\pi/n) & \cos(2\pi/n) & 0\\ 0 & 0 & 1 \end{pmatrix}.$$

Thus  $C_2, C_3, C_4, C_6$  are generated respectively by  $r_2, r_3, r_4, r_6$ .

We will also use X, Y, Z to denote reflections about the yz-, zx-, xy-planes respectively, namely,

$$X = \begin{pmatrix} -1 & \\ & 1 & \\ & & 1 \end{pmatrix}, \ Y = \begin{pmatrix} 1 & \\ & -1 & \\ & & 1 \end{pmatrix}, \ Z = \begin{pmatrix} 1 & \\ & 1 & \\ & & -1 \end{pmatrix},$$

so that XYZ = -1 is the inversion and

$$X_n := r_n X r_n^{-1} = \begin{pmatrix} -\cos(4\pi/n) & \sin(4\pi/n) & 0\\ \sin(4\pi/n) & \cos(4\pi/n) & 0\\ 0 & 0 & 1 \end{pmatrix}$$

performs a reflection about the  $r_n z$ -plane, where  $r_n$  is the x-axis rotated by  $2\pi/n$  in the xy-plane. In particular,  $X_4 = Y$ .

Correspondingly, -X, -Y, -Z are  $\pi$  rotations about the x, y, z axes respectively.

With reflections and inversions, it turns out there are 32 SYMMETRY GROUPS allowed. They are called point groups because they refer to the symmetry about a central point in a unit crystal cell. These groups are listed in TABLE 3.4 in the Schoenflies (S) notation, with the generators between parentheses. The comparison with the Herman-Mauguin (H-M) scheme of nameing these groups can be found in TABLE 3.5.

The first two columns list those with ROTATION symmetry only, belonging to SO(3), the next four columns list groups including REFLECTIONS or INVERSIONS, belonging to O(3). Columns 3 and 4 are groups containing the inversion -1, and columns 5 and 6 are groups that do not contain an inversion.

Some of these groups are **CONGRUENT** to one another as an abstract group, but as a finite subgroup of O(3), no two of them are equivalent, in the sense that they cannot be related by an O(3) similarity transformation.

SO(3)		w/ inversion		w/o inversion	
G	G	G	G	G	G
$C_1$ (1)	1	$C_i \ (\pm 1)$	2		
$C_2(r_2)$	2	$C_{2h}(r_2,-1)$	4	$C_s(Z)$	2
$C_3(r_3)$	3	$S_6(r_3, -1)$	6		
$C_4(r_4)$	4	$C_{4h} (r_4, -1)$	8	$S_4 (-r_4)$	4
$C_6(r_6)$	6	$C_{6h} (r_6, -1)$	12	$C_{3h}\left(r_{3},Z ight)$	6
$D_2(r_2, -X)$	4	$D_{2h}(r_2, -X, -1)$	8	$C_{2v}$ $(r_2, X)$	4
$D_3(r_3, -X)$	6	$D_{3d}(r_3, -X, -1)$	12	$C_{3v}$ $(r_3, X)$	6
$D_4(r_4, -X)$	8	$D_{4h}(r_4, -X, -1)$	16	$C_{4v}(r_4, X), D_{2d}(r_2, -X, -r_4)$	8
$D_6(r_6, -X)$	12	$D_{6h}(r_6, -X, -1)$	24	$C_{6v}(r_6, X), D_{3h}(r_3, -X, -r_6)$	12
T	12	$T_h (T, -1)$	24		
0	24	$O_h(O, -1)$	48	$T_d (T, -O/T)$	24

Table 3.4 The list of 32 point groups, with generators in parentheses. Columns 1 and 2 are pure rotation groups, columns 3 and 4 have inversions incorporated, and columns 5 and 6 have reflections but no inversions incorporated

In the S-scheme, a SUBSCRIPT h indicates the presence of reflection about the <u>h</u>orizontal (*xy*-) plane, generated by Z, and a SUBSCRIPT v indicates the presence of a reflection about a <u>vertical</u> plane, such as the *yz*-plane the reflection about which is generated by X. The SUBSCRIPT d indicates the presence of a reflection about some <u>d</u>iagonal plane, neither horizontal nor vertical. Since  $r_2 = -Z$  is contained in  $C_{nh}$  and  $D_{nh}$  for even n and in T and O, these groups contain both Z and -Z, hence the inversion -1. For these groups, we can use -1 instead of Z as one of the generators, as is done in the third column of Table 3.4.

TABLE 3.6 gives a list of sample molecules with these point-group symmetries, with pictures for some of them shown below the table. For more examples, see HTTP://EN.WIKIPEDIA.ORG/WIKI/MOLECULAR\_SYMMETRY.

S	SO(3)	w/ i	inversion	w/o inversion		
S	$\mathrm{H}-\mathrm{M}$	S	H - M	S	H - M	
$C_1$	1	$C_i$	1			
$C_2$	2	$C_{2h}$	2/m	$C_s$	m	
$C_3$	3	$S^6$	$\overline{3}$			
$C_4$	4	$C_{4h}$	4/m	$S^4$	$\overline{4}$	
$C_6$	6	$C_{6h}$	6/m	$C_{3h}$	3/m	
$D_2$	222	$D_{2h}$	mmm	$C_{2v}$	mm2	
$D_3$	32	$D_{3d}$	$\bar{3}m$	$C_{3v}$	3m	
$D_4$	422	$D_{4h}$	4/mmm	$C_{4v}, D_{2d}$	$4mm, \ \bar{4}2m$	
$D_6$	62	$D_{6h}$	6/mmm	$C_{6v}, D_{3h}$	$6mm, \ \bar{6}2m$	
T	23	$T_h$	m3			
O	432	$O_h$	m3m	$T_d$	$\bar{4}3m$	

Table 3.5 A dictionary for the Schoenflies (S) and Hermann-Mauguin (H-M) notations of the 32 point groups

S	Molecule	generators
$C_1$	CHFClBr	1
$C_s$	$H_2C_2ClBr$	Z
$C_i$	HClBrC - CHClBr	-1
$C_n$	$H_2O_2$	$r_n$
$C_{nv}$	$H_2O$	$r_n, X$
$C_{nh}$	$B(OH)_3$	$r_n, Z$
$S_4$	1, 3, 5, 7 - tetrafluro -	$-r_4$
	acyclooctatetrane	
$D_{nh}$	$BF_3$	$r_n, -X, -1$
$T_d$	$CCl_4$	T, -O/T
$O_h$	$SF_6$	O, - <b>1</b>

Table 3.6 Sample molecules with different symmetries. See also Fig. 3.4.

## 3.13.2 Space groups and the Bravais lattices

The unit cells in a crystal arrange themselves into a lattice. The unit cells are parallelopipeds bounded by three independent vectors  $\vec{e_1}, \vec{e_2}, \vec{e_3}$ , and we



Figure 3.7: Sample molecules with different symmetries. For an animated version showing the various

shall assume  $\vec{e_1}, \vec{e_2}$  lie in the *xy*-plane. The lattice points are located at integral multiple combinations of these vectors,  $\vec{r} = n_1\vec{e_1} + n_2\vec{e_2} + n_3\vec{e_3}$ , with integers  $n_i$ . The lattices commensurate to the point group structures are known as Bravais lattices. The extended point-group symmetry including translations along the lattice is known as a space group.

Bravais lattices differ from one another only in the ANGLES and the LENGTHS of the edges in their unit parallelepipeds.

A unit parallelepiped is defined by a unit parallelogram in the xy-plane, plus a third vector  $\vec{e}_3$  off the plane. However, it is possible to choose another basis to alter the unit parallelogram, so if no restriction is placed on the shape of the parallelogram, it is not necessarily uniquely defined. For example, in the illustration below, a parallelogram is outlined, but there is another way to define a basic parallelogram



Figure 3.8: A crystal lattice

The 32 POINT GROUPS can be classified into 7 LATTICE SYSTEMS, each of which may correspond to one or more Bravais lattices, making a total of 14 POSSIBLE BRAVAIS LATTICES, as shown in the tables below. Let us now analyze what the corresponding Bravais lattices look like for each point group [see Appendix A of Ref. [16]].

Since a lattice is invariant under inversion -1, it would be simpler to start out with the point groups in the middle two columns of Table 3.5. There are 11 point groups there which are inversion symmetric, but it turns out that the pairs  $(C_{4h}, D_{4h})$ ,  $(D_{3d}, S^6)$ ,  $(C_{6h}, D_{6h})$ ,  $(T_h, O_h)$  give rise to the same lattice, which is why we are left with only 7 crystal systems. Each system however may contain more than one Bravais lattices.

#### $\boxtimes$ $\boxtimes$ $\boxtimes$

1.  $C_i$ . The only non-trivial symmetry is the inversion -1, but every lattice is inversion invariant anyway, hence there is no restriction in this case on the angles nor the lengths of the lattice vectors. We therefore end up with the triclinic system, which has three arbitrary angles (hence the name).

 $C_1$  has no symmetry and obviously belongs to this class as well.

2.  $C_{2h}$ . The generators are  $r := r_2$  and -1. Let u' be a lattice vector not along the z-axis. Then u = u' - ru' is another lattice vector so that ru = -u, so it lies in the xy-plane. Choose in this way two independent lattice vectors u, v in the plane, and by making linear combinations if necessary, we can assume their lengths to be the smallest and the next smallest. Let w be a third lattice vector not in the plane, and choose its length to be as small as possible. By the same argument,  $w - rw := 2\bar{w}$ is a lattice vector in the plane. If  $\bar{w}$  is also a lattice vector, then by adding suitable combinations of u and v if necessary, we can assume wto be along the z-axis. In this case we obtain the simple monoclinic system where the parallelogram in the layer above is directly on top of the parallelogram in the xy-plane. If  $\bar{w}$  is not a lattice vector, then by changing the bases from u, v to u, u + v or v, u + v if necessary, we may consider a w so that  $\bar{w} = (u + v)/2$ , in which case we end up with the centered monoclinic system where the parallelogram in the layer above to have its left-lower corner shifted to the center of the base parallelogram.

I think the pictures in Fig. 3.10 may be a bit misleading.

From Table 3.4,  $C_2$  also contains a  $r_2$ , so it belongs to this class.  $C_s$  contains a Z, so it is of the simple monoclinic type.

3.  $C_{4h}$ . The generators contains  $r_4$ . Since  $r_4^2 = r_2$ , the arguments before show the existence of u, v, w, with u, v in the base xy-plane. Applying  $r_4$ , we see that u, v must have equal length and be orthogonal to each other, so the base parallelogram is a square. As before,  $\bar{w} = 0$  or  $\bar{w} = (u + v)/2$ . The resulting **tetragonal** system now has a square in the xy-plane, and the square in the upper layer may be right above the one below (simple), or slide to the center of the square below (body-centered. Note that a  $\pi$  rotation about the x- or the y-axis is automatically invariant.

From the generators in Table 3.4, we see that  $C_4, S_4, D_4, C_{4v}, D_{2d}$  also belong to the system.

4.  $D_{2h}$ . In addition to  $r_2$ , there is now an invariance upon reflection through some line in the plane. In that case the basic cell in the plane has to be either a rectangle, or a diamond (rhombus).

If it is rectangular, then  $\bar{w} = 0, u/2, v/2$ , or  $\bar{w} = (u+v)/2$ , so the situation is very similar to the tetragonal case, except that the basis square can now be a more general rectangle.

If it is a rhombus, it is one symmetrically placed about the x-axis because -X is a generator of  $D_{2h}$ . With this additional symmetry, we must confine  $\bar{w}$  to 0 or (u + v)/2, so the situation is a bit like the monoclinic case except that the base parallelogram must now be a diamond.

This system is known as **orthorhombic** because the basis parallelogram is either a rectangle or a rhombus. There are four kinds, and hence four different Bravais lattices. Primitive  $(P, \bar{w} = 0 \text{ for rectangle})$ , basecentered  $(C, \bar{w} = 0 \text{ for diamond})$ , body-centered  $(I, \bar{w} = (u+v)/2 \text{ for})$ rectangle or diamond), and phase-centered  $(F, \bar{w} = u/2 \text{ or } v/2)$ . They are shown in the following figure.

 $D_2, C_{2v}$  also belong to the system.



Figure 3.9: The four versions of an orthorhombic system

Remarks on the figures:

- (a) i. Four half-diamonds are shown in the base plane of C; that is how this type is usually drawn
  - ii. Two layers each are drawn in each of I and F. It is also the case in Fog. 3.11, for the body-centered tetragonal case.
- 5.  $D_{6h}$  and  $D_{3d}$ . They both contain  $r_3$ , hence the base parallelogram is made up of two 60° equilateral triangles with sides u and  $v = r_6 u$ . We may assume  $\|\bar{w}\| \leq \|u\|$ . Since  $r_3 w - w = r_3 \bar{w} - \bar{w} := v$  is a lattice vector in the base plane with length  $\|\xi\| = \|r_3 \bar{w} - \bar{w}\| = \sqrt{3} \|\bar{w}\| \leq \sqrt{3} \|u\|$ , either  $\bar{w} = 0$  or  $\xi = r_6^m u$  (for some m) is equal to a spoke of the hexagon generated by  $r_6$  on u. Let that be -u, which yields  $\bar{w} = (2u + v)/3$ . In the first case the lattice is invariant under  $D_{6h}$  and the system is called hexagonal, and in the second case the system is invariant under  $D_{3d}$ and is called trigonal.

The other groups belonging to these systems are listed in Fig. 3.11.

6.  $T_h$ . Since  $T = A_4 \supset K'_4 \cong D_2$ , this must be a special case of the orthorhomic system. Let u be the shortest of the three lattice vectors.

The presence of several abstract  $r_3$  in T tells us that we must be able to choose one so that  $r_3u \neq -u$ . Then  $v = r_3u$  and  $w = r_3^2u$  must be lattice vectors of the same length as u. In the case of primitive orthorhombic, the rectangle must be a square and the unit cell must be a cube. Let us rename the orthonormal set of lattice vectors of equal length in this case  $e_1, e_2, e_3$ . The base-centered orthorhombic does not give anything different.

In the case of body-centered orthorhombic, Fig. 3.10 suggests that the body-centered point be  $u = (-e_1 + e_2 + e_3)/2$ . Then  $v = r_3 u = (-e_2 + e_3 + e_1)/2$  and  $w = r_3^2 u = (-e_3 + e_1 + e_2)/2$  are also lattice vectors of the same length. The binary combination of these vectors produce  $e_1, e_2, e_3$  which are longer lattice vectors, thus confirming that case (c) of Fig. 3.10, based on a cube, is indeed a valid configuration for this system. This system is known as **body-centered cubic**, or **bcc** for short.

In the case of the face-centered orthorhombic exhibited in (d) of Fig. 3.10, once again the outside shape is a cube. The demonstration is the same as the case above, except this time by taking  $u = (e_1 + e_2)/2$ ,  $v = (e_2 + e_3)/2$ , and  $w = (e_3 + e_1)/2$ . This system is known as face-centered cubic, or fcc for short.

The resulting 7 systems and 14 Bravais lattices, as well as the point groups they correspond to, are summarized in the following figure.



## 3.13. CRYSTAL POINT GROUPS AND SPACE GROUPS

hexagonal (centered regular hexagon)		
cubic (isometric; cube)	simple	body-centered face-centered

crystal family	crystal system	Schönflies			C <sub>3</sub>
trialinia		C <sub>1</sub>			S <sub>6</sub> (C <sub>3i</sub> )
Inclinic		Ci		trigonal	D <sub>3</sub>
		C <sub>2</sub>			C <sub>3v</sub>
monoclinic		Cs			D <sub>3d</sub>
		C <sub>2h</sub>	haverenal		C <sub>6</sub>
		D <sub>2</sub>	hexagonal		C <sub>3h</sub>
orthorhombic		C <sub>2v</sub>			C <sub>6h</sub>
		D <sub>2h</sub>		hexagonal	D <sub>6</sub>
		C4			Cev
		S4			D <sub>3h</sub>
		C <sub>4h</sub>			D <sub>6h</sub>
tetragonal		D4			Т
		C <sub>4v</sub>			Th
		D <sub>2d</sub>	cubic		0
		D <sub>4h</sub>			Td
					Oh

Figure 3.10: Point groups and lattice systems

# 3.14 Piezoelectricity, optical activity, and dipole moments of crystals

## 3.14.1 Dipole moments

A crystal may be polar only when all its symmetry operations leave the dipole moment invariant. Am inversion symmetry -1 reverses the dipole moment, so NO CRYSTAL WITH THIS SYMMETRY MAY BE POLAR. This eliminates all

the them in the middle column of Table 3.4. Any crystal with two rotation axis cannot be polar either, so that eliminates the  $D_n, T, O$  series. That leaves  $C_n, C_{nv}$ , AND  $C_s$  as possible polar crystals.

## 3.14.2 Piezoelectricity

A crystal is piezoelectric if an electric voltage can result from a mechanical stress. Polar crystals are of this class, but dipole moments maybe produced from certain non-polar crystals under stress as well. The electric field  $E_i$  of a piezoelectric crystal is related to the stress tensor  $T_{jk}$  by the relation  $E_i = d_{ijk}T_{jk}$ . Under inversion -1, the piezoelectric tensor  $d_{ijk}$  changes a sign, so if the crystal has inversion as a symmetry,  $d_{ijk} = 0$  and it cannot be piezoelectric. THE OTHER 21 MAY BE PIEZOELECTRIC.

## 3.14.3 Optical activity

Crystals that can rotate the polarization direction of a linearly polarized light is called CHIRAL. Their molecules must be left-right asymmetric, and chirality behaves somewhat like a dipole moment under inversion and reflection. Hence we can find CHIRAL CRYSTALS AMONG POLAR CRYSTALS.

## 3.15 Brillouin zone

1. A unit cell surrounding a crystal lattice point is known as a Wigner-Seitz cell. The following picture illustrates its construction in the 2-dimensional case: draw dotted lines to all neighboring lattice points, draw solid lines bisecting and perpendicular to the middle of all the dotted lines, then the unit cell (orange) is the Wigner-Seitz cell. In 3-dimensions, the solid lines become solid planes.



Figure 3.11: Wigner-Seitz cells for a 2D and two 3D crystals

2. If  $\vec{e_1}, \vec{e_2}, \vec{e_3}$  are the lattice vectors defining a unit parallelepiped of a crystal, then their orthonormal complements  $\vec{f_1}, \vec{f_2}, \vec{f_3}$  defined through  $\vec{f_i} \cdot \vec{e_j} = \delta_{ij}$ , or explicitly by

$$\vec{f}_i = \vec{e}_j \times \vec{e}_k / \vec{e}_i \cdot (\vec{e}_j \times \vec{e}_k), \qquad (3.11)$$

where i, j, k is a cyclic permutation of 1,2,3, define a lattice called the reciprocal lattice. The Wigner-Seitz cell of a reciprocal lattice is known as the (first) Brillouin zone.

The reciprocal lattice of a body-centered cubic lattice (Fig. 3.6) is a face-centered cubic lattice, and vice versa. To see that, let u, v, w be three mutually orthogonal unit vectors along the three sides of the unit cube. These are lattice vectors but not the shortest. The shortest are those from the center to the middle of the cube, e.g.,  $e_1 = (u + v + w)/2$ ,  $e_2 = (u - v + w)/2$ ,  $e_3 = (u - v - w)/2$ . Using (3.11), we find the basis for the reciprocal lattice to be  $f_1 = u + v$ ,  $f_2 = w - v$ ,  $f_3 = u - w$ . These are vectors from the origin to the center of a face of a cube in a faced-centered cubic lattice, whose three sides along the cube are  $f_1 + f_2 = 2u$ ,  $f_1 - f_2 = 2v$ , and  $f_2 - f_3 = 2w$ . Notice that these three sides are all longer than  $f_i$ .



Figure 3.12: Brillouin zones of two crystals

3. The reciprocal lattice and the Brillouin zone derive their importance from the Bloch theorem, according to which the wave function  $\psi(\vec{r})$ of a particle in a crystal has a basis which can be expressed in the form  $\psi(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})\phi_{\vec{k}}(\vec{r})$ , with  $\vec{k}$  a parameter, and  $\phi_{\vec{k}}(\vec{r})$  is periodic:  $\phi_{\vec{k}}(\vec{r} + \vec{e}_i) = \phi_{\vec{k}}(\vec{r})$  for all *i*.

**Proof** : We need to use a fact to be explained in the next chapter: an abelian group has only 1-dimensional 'irreducible representation'. What that means in the present context is the following. Let  $T_i$  be a Hilbert-space operator which translates the argument of every function by an amount  $\vec{e_i}$ :  $T_i\psi(\vec{r}) = \psi(\vec{r} + \vec{e_i})$ . Then we can choose a suitable basis so that every  $\psi$  in that basis satisfies the relation  $T_i\psi(\vec{r}) = t_i\psi(\vec{r})$ , where  $t_i$  is a number independent of  $\vec{r}$  that satisfies the group composition law:  $t_{i+j} = t_i t_j$ . The logarithm of  $t_i$  is therefore additive in i, and hence a linear function of  $\vec{e_i}$ . This implies that  $t_i = \exp(i\vec{k}\cdot\vec{e_i})$  for some  $\vec{k}$ . Therefore, if we define a function  $\phi_{\vec{k}}(\vec{r})$  by  $\psi(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})\phi_{\vec{k}}(\vec{r})$ , then  $T_i\phi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}+\vec{e_i})$  so  $\phi_{\vec{k}}(\vec{r})$  is periodic in the crystal lattice. This concludes the proof.

Note: this gives rise to the expected result that the probability  $|\psi(\vec{r})|^2$  is the same in every lattice cell.

- 4. The allowed momenta in the crystal,  $\vec{k} + \vec{p}_m$ , can then be divided into different Brillouin zones, with the first Brillouin zone correspond to those with m = 0.
- 5. Being periodic,  $\phi(\vec{r})$  can be expanded into a Fourier series, namely, linear combinations of  $\exp(\vec{p}_m \cdot \vec{r})$ , where  $\vec{p}_m = m_1 \vec{f_1} + m_2 \vec{f_2} + m_3 \vec{f_3}$  is a vector in the reciprocal lattice. With that, we can interpret Bloch's theorem in the following way. Let  $\vec{k}$  be the momentum of the particle in the absence of the crystal. With the crystal present, the particle can scatter from the molecules in the crystal and alter its momentum to  $\vec{k} + \vec{p}_m$  for some m. This is called a Bragg diffraction. Experiments can be carried out to verify this Bragg diffraction law using any beam that can penetrate the crystal. Examples are x-ray, neutrons, and electrons.
- 6. We are familiar with the rule of reflection of a beam of light from the plane surface of a media: the reflection angle is equal to the incident angle. It turns out that Bragg diffraction can be interpreted in a more intuitive way as the reflection of the beam from some appropriate **crystal plane** that depend on m. To see that, let  $\vec{k}' = \vec{k} + \vec{p}_m$ . In order for the incident angle to be equal to the reflected angle,  $\vec{k}' - \vec{k} = \vec{p}_m$ must be normal to the reflection plane. If I write  $\underline{m} = (m_1, m_2, m_3), \underline{f} =$  $(f_1, f_2, f_3), \underline{e} = (e_1, e_2, e_3)$ , where  $e_i$  and  $f_j$  really stand for  $\vec{e}_i$  and  $\vec{f}_j$ , then  $p_m = \underline{m} \cdot f$ . If  $r = \underline{n} \cdot \underline{e}$  is a lattice point in the crystal, then the

plane of crystal lattice points satisfying the condition  $\vec{p}_m \cdot \vec{r} = \underline{m} \cdot \underline{n} = 0$  would be the reflection plane.