Notes of Group Theory and Physics

Taper

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Abstract

Notes of Group Theory and Physics written by Sternberg [Ste94].

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1 Basic definitions and examples (Ch 1)

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1.1 The Classification of the finite subgroups of SO(3) (1.8)

Previous section established one important formula for this section. Suppose a group G acts on a set M. Define the **fix point set** $\mathrm{FP}(a)$ of an element $a \in G$ as the set of all $m \in M$ such that $am = m$, i.e. left invariant under a. Denote G_m for $m \in M$ as the isotropy subgroup of m. Then we have

$$\sum_{a \neq e} \# \, \mathrm{FP}(a) = \sum_{\text{orbits}} \frac{\# G}{\# G_m} (\# G_m - 1) \tag{1.1.1}$$

eq:fp-orbit-formula

The proof is on section 1.7 of [Ste94].

This section classifies all possible finite subgroups of SO(3). The classification of finite subgroups of O(3) is on the next section. We basically study the action of $G = \mathrm{SO}(3)$ on $M = S^2$, the unit sphere. The first interesting discovery is

Theorem 1.1 ((Euler))**.** *When the dimension n is odd, any $a \in \mathrm{SO}(n)$ leaves at least one non-zero vector invariant, i.e. any $a \in \mathrm{SO}(n)$, $\mathrm{Ker}(a - I) \neq \varnothing$, or there is always a $\mathbf{v} \neq 0$, such that $a\mathbf{v} = \mathbf{v}$.*

This implies that any rotation in odd dimensional space is a rotation about some fixed axis (since $a\mathbf{v} = \mathbf{v}$ implies $(a\mathbf{p}) \cdot \mathbf{v} = (a\mathbf{v}) \cdot (a\mathbf{p}) = \mathbf{v} \cdot \mathbf{p} = 0$).

Then the book analyses the formula counting fix point sets and orbits 1.1.1. Use new symbols for three numbers:

ree-symbols-for-3-numbers

$$\begin{aligned} n &= \#G \\ r &= \text{number of orbits of } G \\ n_i &= \#G_m, \text{ where } m \in i\text{th orbit.} \end{aligned}$$

Then we have

$$2 - \frac{2}{n} = r - \sum_{1}^{r} \frac{1}{n_i} \tag{1.1.2}$$

This equation can be simplified by considering the practical numerical values of n, r and n_i, with $n_i \leq n$. By eliminating case by case, he finally arrived at five sets of possible values:

tab:Finite-rot-g

Table 1: Finite rotation groups

r	(n_1, n_2, n_3)	$\#G$	Schoenflies	Hermann-Mauguin	Note
2	(n,n,0)	n	C_n	n	Cyclic group
3	$(2, 2, k), k \geq 2$	$2k$	D_k	222 for D_2, $k2$ otherwise	Dihedral group
3	$(2, 3, 3)$	12	T	23	of regular tetrahedron
3	$(2, 3, 4)$	24	O	432	of regular octahedron
3	$(2, 3, 5)$	60	I	not mentioned	of icosahedron, of Fullerene[1]

For details about derivation please visit pp. 28 to 31 of [Ste94]. But we need to exclude some subgroups from the list of crystallographic groups. The result is that, on the first row, n is restricted to be $1, 2, 3, 4$ and 6; on the second row, k is restricted to be $2, 3, 4$ and 6. And I is excluded from the list of crystallographic groups.

The reason is the common one on Solid States classes about possible space-filling polygons (see pp.31 of [Ste94]). Also, a good proof about possible rotation angles in three-dimension for a lattice is provided on pp.31 to 32 of [Ste94]. The key is that the rotation matrix could be made of integers, and hence its characteristic (trace) should be an integer.

Next the author mentioned the **atomic hypothesis** , an interesting historical account of our view on crystals. The essence is that because only above mentioned angles occurred in rotational symmetries of crystals, we can presume that a crystal is not a continuum, but is "built up from discrete subunits in a regular repetitive pattern" (pp.32).

He also mentions the **law of rational indices** which found a basis for modern way of labeling different faces of a lattice (the (100) side, etc.). But this law is too long to be typed here.

In sum, we have only following finite subgroups of SO(3) that is interested for crystals:

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

[1]See section 1.10 about Fullerene and icosahedron for details.

1.2 Classification of finite subgroups of $\mathrm{O}(3)$

sec:Classif-subg-O3

This section based on the work of previous section 1.1. To use the result of those groups of matrices with $\det = 1$ in that section, the author first discuss the example of T_d and O.

T_d is the group of all symmetries(including those that does not preserve the chirality, i.e. with $\det = -1$) of tetrahedron. As abstract groups, T_d and O are all isomorphic to S_4, the symmetric group of order 4. Note that in the context of crystal symmetry, the isomorphic class of group is not enough to characterize a behavior. For example, the C_2 containing π rotation is not the same as $\{e, i\}$ where i is the inversion, but they are isomorphic.[2] The link between T_d and O can be seen from the following:

> " we can consider our tetrahedron as situated inside a cube, with its vertices at the diagonally opposite vertices of each face of the cube. For a given cube there are two such tetrahedra, as shown in Fig. 1.13 (Figure 1 here). One tetrahedron is carried into the other by the inversion, $-I$. "

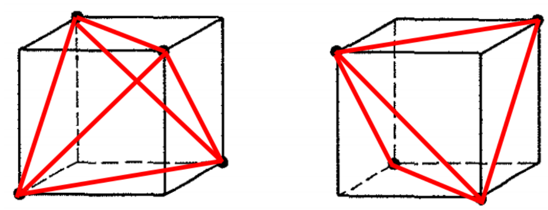

Figure 1: Fig 1.13 in [Ste94], with modification

fig:fig1.13

Written mathematically, we have

$$T_d = S_4 = T \cup T' \tag{1.2.1}$$

where T is mentioned in Table 1.1. And T' contains those matrices with $\det = -1$.

$$T_d \overset{\phi}{\cong} O \tag{1.2.2}$$

where ϕ is defined as

$$\begin{aligned} A &\to A \quad \text{for } A \in T \\ B &\to -B \quad \text{for } B \in T' \end{aligned}$$

In general case, for a finite subgroup G of $\mathrm{O}(3)$, we have the following. Let G_+ denote the subgroup of G with positive determinant. Let G_- denote the set of elements of G with negative determinant. We have two cases.

Case 1, $-I \in G_-$, then $G_- = (-I)G_+$, and the structure is simple.

[2] Perhaps representation classes of groups is more precise in describing the behavior.

Case 2, $-I \notin G_-$. Then the author defines $G^\vee := G_+ \cup (-I)G_-$, and shows that

$$G^\vee = G_+ \cup aG_+ \tag{1.2.3}$$
$$G_- = (-I)aG_+ \tag{1.2.4}$$

where a is some matrix in $G^\vee \setminus G_+$.

Then,

> “ From the 11 rotation groups listed at the end of the preceding section, we obtain 11 non-rotation groups by including $-I$. In addition, we must check for the normat subgroups of index two in each rotation group in order to construct non-rotation groups which do not include $-I$. ”

The rest of this section carries out this analysis, culminating in the table 4 on pp. 40 of [Ste94]. I reproduce the table with some addition in the Table 2.

Table 2: The 32 point groups

tab:point-g-32

Rotation groups		Non-rotation groups containing $-I$		Non-rotation groups not containing $-I$	
S	H–M	S	H–M	S	H–M
C_1	1	C_i	$\bar{1}$		
C_2	2	C_{2h}	2/m	C_s	m
C_3	3	S^6	$\bar{3}$		
C_4	4	C_{4h}	4/m	S^4	$\bar{4}$
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}	4mm
				D_{2d}	$\bar{4}2m$
D_6	62	D_{6h}	6/mmm	C_{6v}	6mm
				D_{3h}	$\bar{6}2m$
T	23	T_h	m3		
O	432	O_h	m3m	T_d	$\bar{4}3m$

The detailed derivation could be found on pp.35 to 39 of [Ste94]. Note that $S^6 \neq S_6$, and $S^4 \neq S_4$. Here is some explanations for subscripts:

h:	there is a horizontal reflection plane.
v:	there is a vertical reflection plane.
d:	there is diagonal vertical planes.
m:	there is a vertical mirror plane (in H-M notation).
$/m$:	there is a horizontal mirror plane (in H-M notation).

Note also that the online engine WolframAlpha is a very good source for details about certain groups. For example, this link is a good description of group S^4 (thouhg it is denoted S_4 on the webpage). Searching "crystallographic point group C4h" will get one a good description of C_{4h}. One can also found the book reference from that page by clicking the "Source information" link.

Then the author goes on to mention some historical methods in "determination of the actual symmetry groups of a given substance", "available to 19th century crystallographers". One method is "to attack the crystal with an acid, and to study the etch figures induced on the faces". Another is to study the "piezoelectricity", or to test the "rotatory optical activity".

He also gives a helpful graphical display of 32 point groups in Fig 1.19 on [Ste94](from pp.42 to 44), which is too long to be included here.

References

[Ste94] Shlomo. Sternberg. *Group theory and physics.* Cambridge University Press, 1994.

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