PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 6:

Examples of point groups and their characters

Reading: Chapter 3 in DDJ

1. **Schoenflies notation**
2. **Hermann-Mauguin notation**
3. **Relationships between symmetries**

Note: In this lecture, some materials are taken from an electronic version of the Dresselhaus, Dresselhaus, Jorio text

PHY 745 Group Theory

MWF 11-11:50 AM	OPL 102	http://www.wfu.edu/~natalie/s17phy745/

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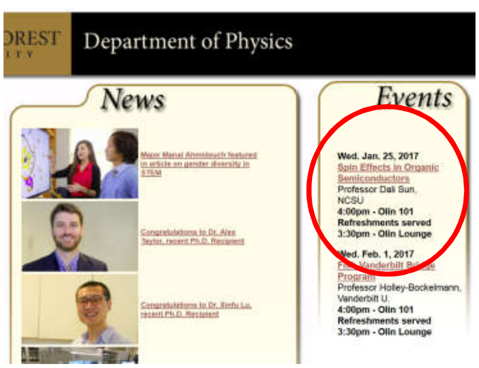
Course schedule for Spring 2017

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	DDJ Reading	Topic	HW	Due date
1	Wed: 01/11/2017	Chap. 1	Definition and properties of groups	#1	01/20/2017
2	Fri: 01/13/2017	Chap. 1	Theory of representations		
	Mon: 01/16/2017		*MLK Holiday - no class*		
3	Wed: 01/18/2017	Chap. 2	Theory of representations		
4	Fri: 01/20/2017	Chap. 2	Proof of the Great Orthonality Theorem	#2	01/23/2017
5	Mon: 01/23/2017	Chap. 3	Notion of character of a representation	#3	01/25/2017
6	Wed: 01/25/2017	Chap. 3	Examples of point groups	#4	01/30/2017
7	Fri: 01/27/2017				
8	Mon: 01/30/2017				



Point group symmetry elements in the Schoenflies notation

- E = Identity
- C_n = rotation through $2\pi/n$. For example C_2 is a rotation of 180°. Likewise C_3 is a rotation of 120°, while C_6^2 represents a rotation of 60° followed by another rotation of 60° about the same axis so that $C_6^2 = C_3$. In a Bravais lattice it can be shown that n in C_n can only assume values of n=1, 2, 3, 4, and 6. The observation of a diffraction pattern with five-fold symmetry in 1984 was therefore completely unexpected, and launched the field of quasicrystals.
- σ = reflection in a plane.
- σ_h = reflection in a "horizontal" plane. The reflection plane here is perpendicular to the axis of highest rotational symmetry.
- σ_v = reflection in a "vertical" plane. The reflection plane here contains the axis of highest symmetry.

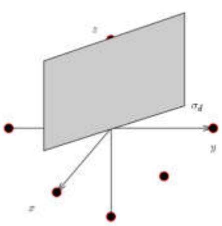


Figure 3.1: Schematic illustration of a dihedral symmetry axis. The reflection plane containing the diagonal of the square and the four-fold axes is called a dihedral plane. For this geometry $\sigma_d(x, y, z) = (-y, -x, z)$.

- σ_d = reflection in a diagonal plane. The reflection plane here is a vertical plane which bisects the angle between the two fold axes ⊥ to the principal symmetry axis. An example of a diagonal plane is shown in Fig. 3.1. σ_d is also called a dihedral plane.

- i = inversion which takes

$$\begin{cases} x \rightarrow -x \\ y \rightarrow -y \\ z \rightarrow -z \end{cases}$$

- S_n = improper rotation through $2\pi/n$, which consists of a rotation by $2\pi/n$ followed by a reflection in a horizontal plane.
- iC_n = compound rotation-inversion, which consists of a rotation followed by an inversion.

There are 32 distinct point groups generated by combinations of these operations

Point group symmetry elements in the Hermann-Mauguin notation

Table 3.5: Comparison between Schoenflies and Hermann-Mauguin notation.

	Schoenflies	Hermann-Mauguin
rotation	C_n	n
rotation-inversion	iC_n	$\bar{n}$
mirror plane	σ	m
horizontal reflection plane $\perp$ to $n-$fold axes	σ_h	n/m
$n-$fold axes in vertical reflection plane	σ_v	nm
two non $-$ equivalent vertical reflection planes	$\sigma_{v'}$	nmm

Table 3.6: Comparison of notation for proper and improper rotations in the Schoenflies and International systems.

Proper Rotations		Improper Rotations	
International	**Schoenflies**	**International**	**Schoenflies**
1	C_1	$\bar{1}$	S_2
2	C_2	$\bar{2}\equiv$m	σ
3	C_3	$\bar{3}$	S_6^{-1}
3_2	C_3^{-1}	$\bar{3}_2$	S_6
4	C_4	$\bar{4}$	S_4^{-1}
4_3	C_4^{-1}	$\bar{4}_3$	S_4
6	C_6	$\bar{6}$	S_3^{-1}
6_5	C_6^{-1}	$\bar{6}_5$	S_3

Some relationships between point symmetry elements

1. Inversion commutes with all point symmetry operations.
2. All rotations about the same axis commute.
3. All rotations about an arbitrary rotation axis commute with reflections across a plane perpendicular to this rotation axis.
4. Two two-fold rotations about perpendicular axes commute.
5. Two reflections in perpendicular planes will commute.
6. Any two of the symmetry elements σ_h, S_2, C_n ($n =$ even) implies the third.

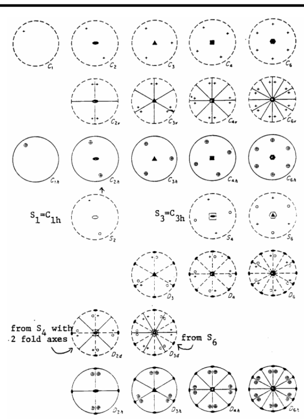
The 32 Point Groups and Their Symbols

System	Schoenflies symbol	Hermann-Mauguin symbol Full	Hermann-Mauguin symbol Abbreviated	Examples
Triclinic	C_1	1	1	
	$C_i, (S_2)$	$\bar{1}$	$\bar{1}$	Al_2SiO_5
Monoclinic	$C_{2v}, (C_{1h}), (S_1)$	m	m	KNO_2
	C_2	2	2	
	C_{2h}	$2/m$	$2/m$	
Orthorhombic	C_{2v}	$2mm$	mm	
	$D_2, (V)$	222	222	
	$D_{2h}, (V_h)$	$2/m\ 2/m\ 2/m$	mmm	I, Ga
Tetragonal	S_4	$\bar{4}$	$\bar{4}$	
	C_4	4	4	
	C_{4h}	$4/m$	$4/m$	$CaWO_4$
	$D_{2d}, (V_d)$	$\bar{4}2m$	$\bar{4}2m$	
	C_{4v}	$4mm$	$4mm$	
	D_4	422	42	
	D_{4h}	$4/m\ 2/m\ 2/m$	$4/mmm$	TiO_2, In, $\beta-$Sn

The 32 Point Groups and Their Symbols

System	Schoenflies symbol	Hermann-Mauguin symbol Full	Hermann-Mauguin symbol Abbreviated	Examples
Rhombohedral	C_3	3	3	AsI_3
	$C_{3i}, (S_6)$	$\bar{3}$	$\bar{3}$	$FeTiO_3$
	C_{3v}	$3m$	$3m$	
	D_3	32	32	Se
	D_{3d}	$\bar{3}2/m$	$\bar{3}m$	Bi, As, Sb, Al_2O_3
Hexagonal	$C_{3h}, (S_3)$	$\bar{6}$	$\bar{6}$	
	C_6	6	6	
	C_{6h}	$6/m$	$6/m$	
	D_{3h}	$\bar{6}2m$	$\bar{6}2m$	
	C_{6v}	$6mm$	$6mm$	ZnO, NiAs
	D_6	622	62	CeF_3
	D_{6h}	$6/m\ 2/m\ 2/m$	$6/mmm$	Mg, Zn, graphite
Cubic	T	23	23	$NaClO_3$
	T_h	$2/m\bar{3}$	$m3$	FeS_2
	T_d	$\bar{4}3m$	$\bar{4}3m$	ZnS
	O	432	43	β-Mn
	O_h	$4/m\ \bar{3}\ 2/m$	$m3m$	NaCl, diamond, Cu

Stereographic projections of simple point groups



Some details

Table 22.2: Character Table for Group C_{2h}

C_{2h} (2/m)			E	C_2	σ_h	i
x^2, y^2, z^2, xy	R_z	A_g	1	1	1	1
	z	A_u	1	1	−1	−1
xz, yz	R_x, R_y	B_g	1	−1	−1	1
	x, y	B_u	1	−1	1	−1

More details from the Bilbao crystallographic server:
http://www.cryst.ehu.es/#pointop

For a specific case, choose a three-dimensional crystallographic point group from the next table:

C_1	1	C_i	-1	C_2	2	C_s	m	C_{2h}	2/m	D_2	222	C_{2v}	mm2	D_{2h}	mmm
C_4	4	S_4	-4	C_{4h}	4/m	D_4	422	C_{4v}	4mm	D_{2d}	-42m	D_{4h}	4/mmm	C_3	3
C_{3i}	-3	D_3	32	C_{3v}	3m	D_{3d}	-3m	C_6	6	C_{3h}	-6	C_{6h}	6/m	D_6	622
C_{6v}	6mm	D_{3h}	-62m	D_{6h}	6/mmm	T	23	T_h	m-3	O	432	T_d	-43m	O_h	m-3m

C_{2h} symmetry operations (for unique axis z)

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	1
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 0,0,z	2_{001}
3	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	-1 0,0,0	-1
4	x,y,-z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	m x,y,0	m_{001}

Another example

Table 22.3: Character Table for Group D_2

D_2 (222)			E	C_2^z	C_2^y	C_2^x
x^2, y^2, z^2		A_1	1	1	1	1
xy	R_z, z	B_1	1	1	−1	−1
xz	R_y, y	B_2	1	−1	1	−1
yz	R_x, x	B_3	1	−1	−1	1

$D_{2h} = D_2 \otimes i$

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	1
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 0,0,z	2_{001}
3	-x,y,-z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	2 0,y,0	2_{010}
4	x,-y,-z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	2 x,0,0	2_{100}

Tetrahedral group:

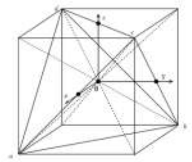


Figure 3.3: Schematic diagram for the symmetry operations of the group T_d.

For simple tetrahedron:

1	identity	
3	two-fold axes	(x, y, z)
4	three-fold axes	(body diagonals–positive rotation)
4	three-fold axes	(body diagonals–negative rotations)
12	symmetry elements	

Tetrahedral group:

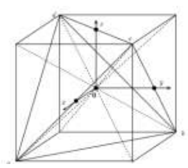


Figure 3.3: Schematic diagram for the symmetry operations of the group T_d.

For complex tetrahedron:

- Identity
- 8 C_3 about body diagonals corresponding to rotations of $\pm\frac{2\pi}{3}$
- 3 C_2 about x, y, z directions
- 6 S_4 about x, y, z corresponding to rotations of $\pm\frac{\pi}{2}$
- 6 σ_d planes that are diagonal reflection planes

24 symmetry elements

Table 3.32: Character Table for Group T

T (23)		E	$3C_2$	$4C_3$	$4C_3'$
	A	1	1	1	1
	E	1	1	ω	ω^2
		1	1	ω^2	ω
(R_x, R_y, R_z), (x, y, z)	T	3	-1	0	0

where $\omega = \exp(2\pi i/3)$

Table 3.34: Character Table for Group T_d

T_d ($\bar{4}3m$)		E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
	A_1	1	1	1	1	1
	A_2	1	1	1	-1	-1
	E	2	-1	2	0	0
(R_x, R_y, R_z)	T_1	3	0	-1	-1	1
(x, y, z)	T_2	3	0	-1	1	-1

Octahedral group

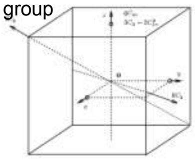


Figure 3.4: Schematic for the symmetry operations of the group O.

Table 3.33: Character Table for Group O

O (432)		E	$8C_3$	$3C_2 = 3C_4^2$	$6C_2'$	$6C_4$
$(x^2+y^2+z^2)$	A_1	1	1	1	1	1
	A_2	1	1	1	−1	−1
$(x^2-y^2, 3z^2-r^2)$	E	2	−1	2	0	0
(R_x, R_y, R_z), (x, y, z)	T_1	3	0	−1	−1	1
(xy, yz, zx)	T_2	3	0	−1	1	−1

$O_h = O \otimes i \ \ (m3m)$