Principles and Applications of Symmetry in Magnetism (PASM), Summer School
Fort Collins, Colorado

Invariant Theory and Symmetry Analysis of Magnetism and Spin-Orbitronics

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Outline

Lecture 1: A primer on spin-orbitronics

Spin-orbit coupling in crystals, Dzyaloshinskii-Moriya interaction, spin-orbit torques

Lecture 2: Representation Theory applied to crystals

Group of symmetries, reducible and irreducible representations, orthogonality theorem, characters

Lecture 3: Character tables of crystal point groups

Salient features of the character table, invariant functions, decomposition theorem, product group

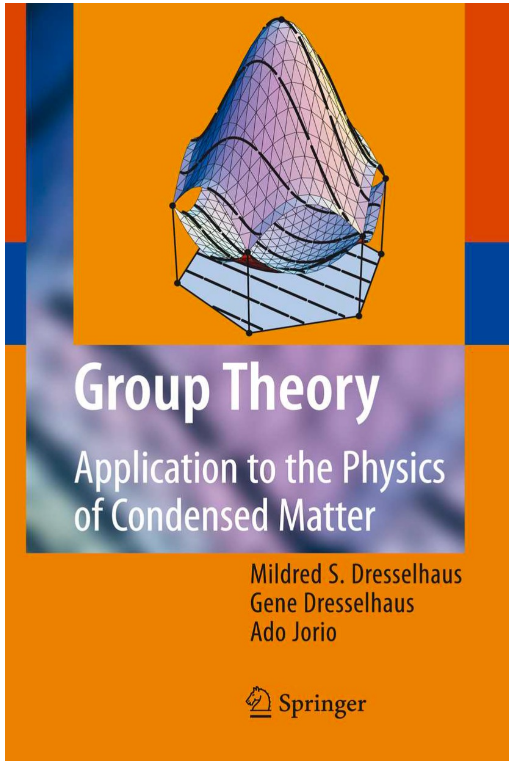
Lecture 4: Application to the C_{3v} point group

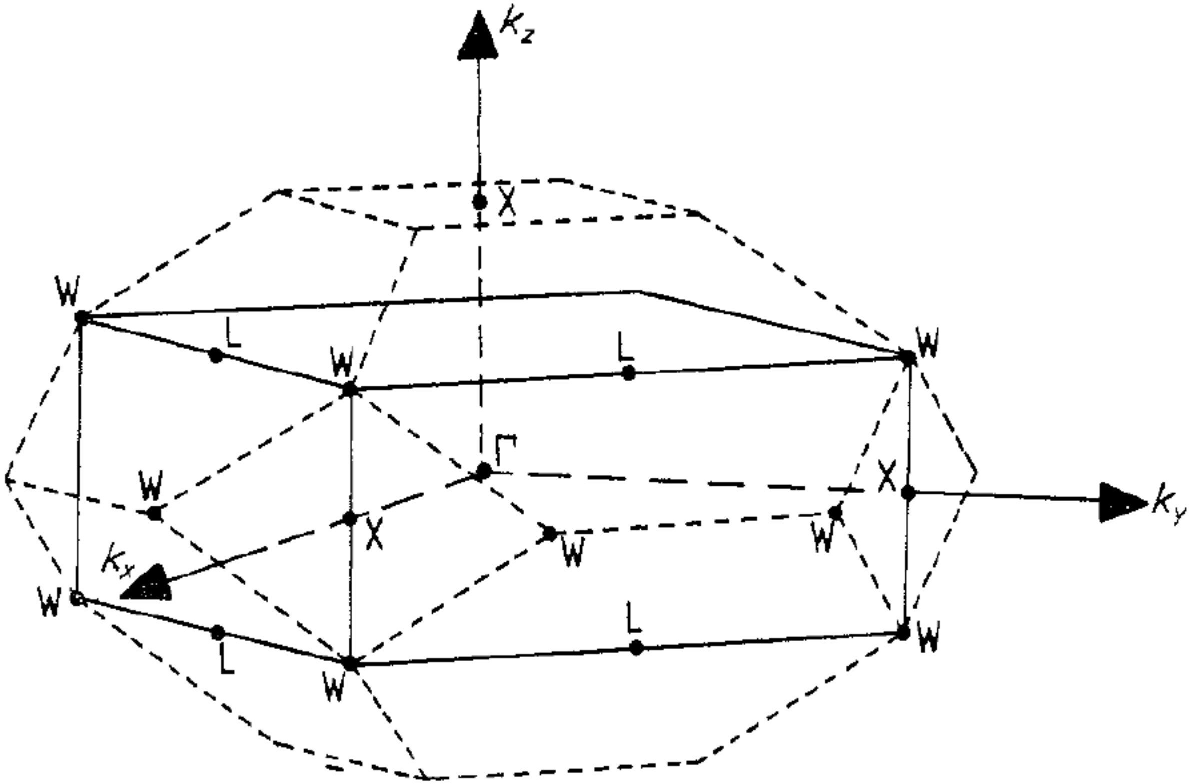
Hamiltonian, conductivity tensor, DMI and SOT

Lecture 5: Your turn, with the C_{4v} point group

Surprise me ☺

Lecture II
Representation Theory applied to crystals





Very quick reminder about crystal symmetries and point groups

system	Schoenflies symbol	Hermann–Mauguin symbol[b] full	Hermann–Mauguin symbol[b] abbreviated	examples
triclinic	C_1	1	1	
	$C_i, (S_2)$	$\bar{1}$	$\bar{1}$	Al_2SiO_5
monoclinic	$C_{1h}, (S_1)$	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	C_4	4	4	
	S_4	$\bar{4}$	$\bar{4}$	
	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, β-Sn

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

i: inversion, C_n: n-fold rotation, $\sigma_{h,v,d}$: reflection
S_n: n-fold improper rotation (rotation+reflection)

A few definitions

Definition of a group A collection of elements $A, B, C, \ldots$ form a group when the following four conditions are satisfied:

1. The product of any two elements of the group is itself an element of the group. For example, relations of the type $AB = C$ are valid for all members of the group.
2. The associative law is valid – i.e., $(AB)C = A(BC)$.
3. There exists a unit element E (also called the identity element) such that the product of E with any group element leaves that element unchanged $AE = EA = A$.
4. For every element A there exists an inverse element A^{-1} such that $A^{-1}A = AA^{-1} = E$.

In general, the elements of a group will not commute, i.e., $AB \neq BA$. But if all elements of a group commute, the group is then called an *Abelian* group.

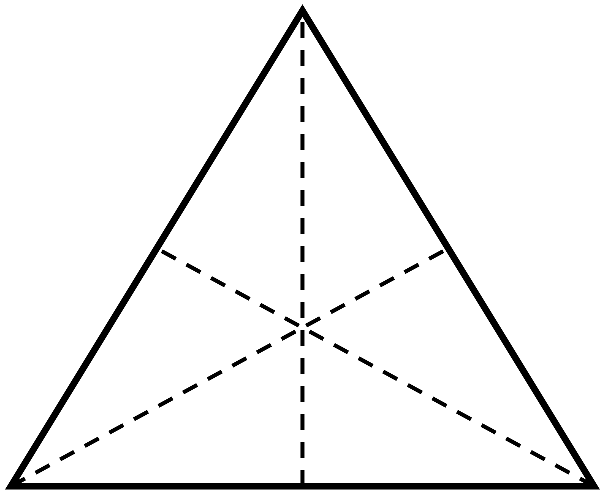
Conjugation *An element B conjugate to A is by definition $B \equiv XAX^{-1}$, where X is an arbitrary element of the group.*

Definition of a class

A class is the totality of elements which can be obtained from a given group element by conjugation

The symmetries of a crystal form a group: The equilateral triangle

Rhombohedral D_3 (32)



- 1 Identity
- 2 C_3 rotations around the origin
- 3 C_2 rotations around the three axes

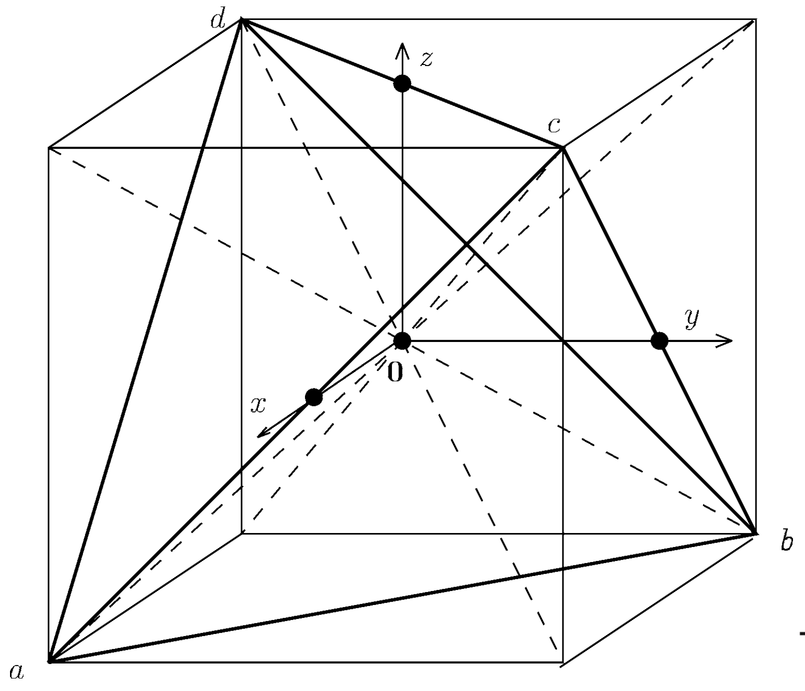
D_3 is a group of order 6
It possesses 3 classes

Very important because #irrep = #classes

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	-1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	2	-1	0

Crystal symmetries form a group: The tetrahedron

Cubic T_d ($\bar{4}3m$)



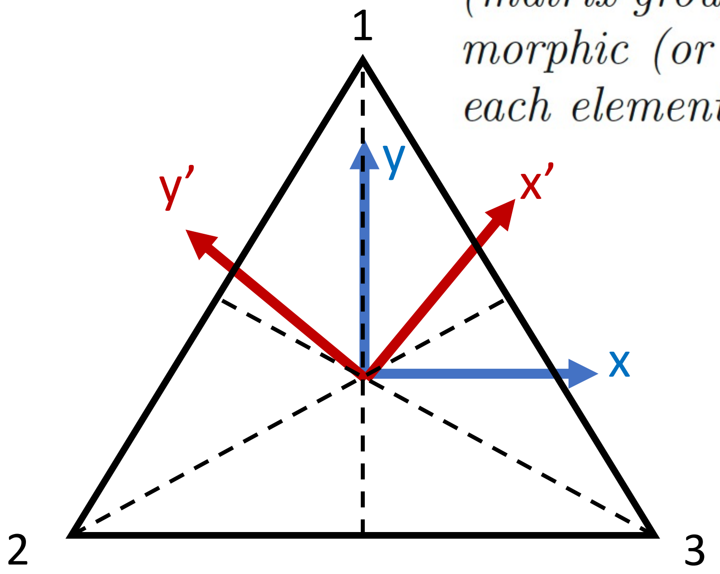
- 1 Identity
- 8 C_3 rotations around {111}
- 3 C_2 rotations around {001}
- 6 σ_d reflections on the diagonal plane
- 6 S_4 improper rotations

T_d is a group of order 24
It possesses 5 classes

T_d ($\bar{4}3m$)		E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
$x^2+y^2+z^2$	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) $yz, zx, xy)$	T_1	3	0	−1	−1	1
(x, y, z)	T_2	3	0	−1	1	−1

Introducing representations

Definition 13. *A* representation *of an abstract group is a substitution group (matrix group with square matrices) such that the substitution group is homomorphic (or isomorphic) to the abstract group. We assign a matrix $D(A)$ to each element A of the abstract group such that $D(AB) = D(A)D(B)$.*



In other words, any symmetry operation can be represented by a square matrix, called a representation

$$E = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} \quad A = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} \quad B = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$$

identity, C_2, C_2

$$C = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \quad D = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \quad F = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$

C_2, C_3, C_3

In 2d, (x,y), we naturally get the following representation

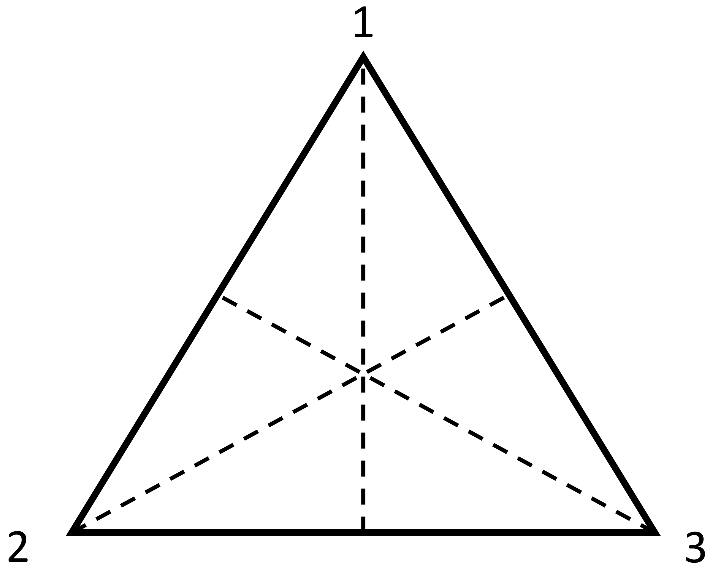
$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad A = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad B = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$C = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad D = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad F = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

This representation is NOT unique!

Introducing representations

We can also build a representation of dimension 1



$E = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}$ identity

$A = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}$ C_2

$B = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$ C_2

$C = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}$ C_2

$D = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$ C_3

$F = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$ C_3

Multiplication table

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

$$(E, D, F) = \mathcal{E}$$

is a self-conjugated subgroup

$$(A, B, C) = \mathcal{A}$$

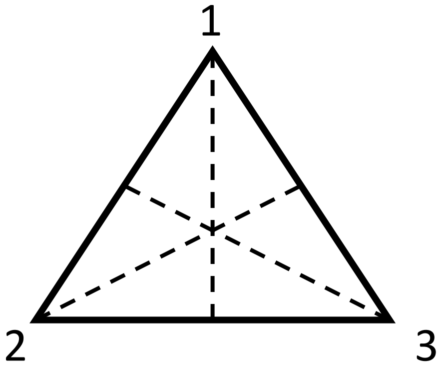
is called a *coset* of this subgroup

	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{E}$	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{A}$	$\mathcal{A}$	$\mathcal{E}$

This group (called the factor group) is isomorphic to the permutation group P(2). In 1d, z, the representation is

$$\left.\begin{matrix} E \\ D \\ F \end{matrix}\right\} \rightarrow (1) \qquad z \rightarrow z$$

$$\left.\begin{matrix} A \\ B \\ C \end{matrix}\right\} \rightarrow (-1) \qquad z \rightarrow -z$$



Introducing representations

In summary, for D_3, we have found 3 representations

fully invariant

parity

2d

$$
\begin{array}{cccccc}
E & A & B & C & D & F \\
(1) & (1) & (1) & (1) & (1) & (1) \\
(1) & (-1) & (-1) & (-1) & (1) & (1) \\
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &
\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} &
\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} &
\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
\end{array}
$$

In principle, we could also build 4d representations, for instance

$$
\Gamma_{\mathrm{R}} : \quad
\overset{E}{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}
\overset{A}{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}
\overset{B}{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}}
\cdots, \quad \Rightarrow \quad
\left(\begin{array}{c|c|c} \Gamma_1 & 0 & \mathcal{O} \\ \hline 0 & \Gamma_{1'} & \mathcal{O} \\ \hline \mathcal{O} & \mathcal{O} & \Gamma_2 \end{array}\right)
$$

This is called a *reducible* representation, which can be written in terms of the *irreducible* ones

$$
\Gamma_{\mathrm{R}} = \Gamma_1 + \Gamma_{1'} + \Gamma_2
$$

Schur's lemma – for real

Lemma. *A matrix which commutes with all matrices of an irreducible representation is a constant matrix, i.e., a constant times the unit matrix. Therefore, if a non-constant commuting matrix exists, the representation is reducible; if none exists, the representation is irreducible.*

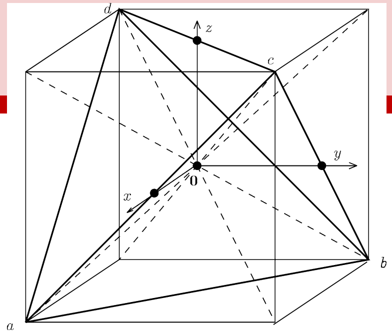
Lemma. *If the matrix representations* $D^{(1)}(A_1), D^{(1)}(A_2), \ldots, D^{(1)}(A_h)$ *and* $D^{(2)}(A_1), D^{(2)}(A_2), \ldots, D^{(2)}(A_h)$ *are two irreducible representations of a given group of dimensionality* ℓ_1 *and* ℓ_2*, respectively, then, if there is a matrix of* ℓ_1 *columns and* ℓ_2 *rows* M *such that*

$$MD^{(1)}(A_x) = D^{(2)}(A_x)M \tag{2.38}$$

for all A_x*, then* M *must be the null matrix* ($M = \mathcal{O}$) *if* $\ell_1 \neq \ell_2$*. If* $\ell_1 = \ell_2$*, then either* $M = \mathcal{O}$ *or the representations* $D^{(1)}(A_x)$ *and* $D^{(2)}(A_x)$ *differ from each other by an equivalence (or similarity) transformation.*

Introducing representations

Definition 16. *If by one and the same equivalence transformation, all the matrices in the representation of a group can be made to acquire the same block form, then the representation is said to be* reducible*; otherwise it is* irreducible. *Thus, an irreducible representation cannot be expressed in terms of representations of lower dimensionality.*



Character of a representation

The concrete matrix representation of a point group can be very heavy to handle
Fortunately, the matrices of the irreducible representations obey a number of rules

1. Unitarity *Every representation with matrices having nonvanishing determinants can be brought into unitary form by an equivalence (similarity) transformation.*

2. Wonderful orthogonality theorem

$$\sum_R D^{(\Gamma_j)}_{\mu\nu}(R)\left[D^{(\Gamma'_j)}_{\mu'\nu'}(R)\right]^* = \frac{h}{\ell_j}\delta_{\Gamma_j,\Gamma_{j'}}\delta_{\mu\mu'}\delta_{\nu\nu'}$$

elements of the group (h)
Matrix element (D)
Irreducible representation (Γ_j)
Symmetry operation (R)
Dimensionality of the irreducible representation (ℓ_j)

3. Character Since the trace (or character) of a matrix remains invariant upon equivalence transformation, **the character of each element in a class is the same**..so a class can be tagged by its character

Character of a representation

Definition 17. *The* character *of the matrix representation* $\chi^{\Gamma_j}(R)$ *for a symmetry operation* R *in a representation* $D^{(\Gamma_j)}(R)$ *is the* trace *(or the sum over diagonal matrix elements) of the matrix of the representation:*

$$\chi^{(\Gamma_j)}(R) = \mathrm{trace}\, D^{(\Gamma_j)}(R) = \sum_{\mu=1}^{\ell_j} D^{(\Gamma_j)}(R)_{\mu\mu}\,, \tag{3.1}$$

Let's build the character table of D_3

	E	A	B	C	D	F
Γ_1 :	(1)	(1)	(1)	(1)	(1)	(1)
$\Gamma_{1'}$:	(1)	(-1)	(-1)	(-1)	(1)	(1)
Γ_2 :	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

Character of a representation

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$$\chi^{(\Gamma_j)}(R) = \mathrm{trace}\, D^{(\Gamma_j)}(R) = \sum_{\mu=1}^{\ell_j} D^{(\Gamma_j)}(R)_{\mu\mu}\,, \tag{3.1}$$

Let's build the character table of D_3

class $\rightarrow$ IR $\downarrow$	$\mathcal{C}_1$ $\chi(E)$	$3\mathcal{C}_2$ $\chi(A, B, C)$	$2\mathcal{C}_3$ $\chi(D, F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Character of a representation

The characters also obey a number of very useful rules

1. First orthogonality theorem for characters

$$\sum_k N_k \chi^{(\Gamma_j)}(\mathcal{C}_k) \left[\chi^{(\Gamma_{j'})}(\mathcal{C}_k)\right]^* = h\delta_{\Gamma_j,\Gamma_{j'}} ,$$

elements in a class (N_k)

class ($\mathcal{C}_k$)

This equality sets the relation between the row of the χ-table

2. Second orthogonality theorem for characters

$$\sum_{\Gamma_j} \chi^{(\Gamma_j)}(\mathcal{C}_k) \left[\chi^{(\Gamma_j)}(\mathcal{C}_{k'})\right]^* N_k = h\delta_{kk'}$$

This equality sets the relation between the columns of the χ-table

Theorem. *A necessary and sufficient condition that two irreducible representations be equivalent is that the characters be the same.*

Salient features of a character table

C_{6v}

C_{6v} (6mm)			E	C_2	$2C_3$	$2C_6$	$3\sigma_d$	$3\sigma_v$
x^2+y^2, z^2	z	A_1	1	1	1	1	1	1
	R_z	A_2	1	1	1	1	−1	−1
		B_1	1	−1	1	−1	−1	1
		B_2	1	−1	1	−1	1	−1
(xz, yz)	(x, y), (R_x, R_y)	E_1	2	−2	−1	1	0	0
(x^2-y^2, xy)		E_2	2	2	−1	−1	0	0

$$\sum_k N_k \chi^{(\Gamma_i)}(\mathcal{C}_k) = 0$$

$$\chi^{(\Gamma_i)}(E) = \ell_i$$

$$\sum_{\Gamma_i} \chi^{(\Gamma_i)}(\mathcal{C}_k)\ell_i = 0$$

Character of a representation

Now let's build the character table for two cases

Group D_3

	$\mathcal{C}_1$	$3\mathcal{C}_2$	$2\mathcal{C}_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1		
Γ_2	2		

Group C_3

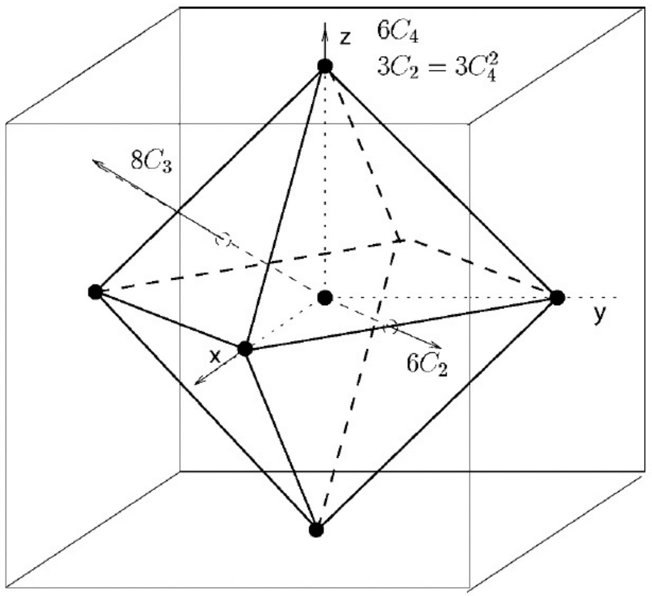
?

Decomposition of a reducible representation

Any reducible representation can be expressed in terms of irreducible ones
Not only very useful for computational purpose but also informative from a physics standpoint

Let's consider spherical orbitals in a cubic environment (group O)

$$Y_{\ell,m}(\theta,\phi) = C P_\ell^m(\theta)\ \mathrm{e}^{\mathrm{i}m\phi}$$



First determine the characters of their representation in O

Rotation of angle α around *z*

$$D^{(\ell)}(\alpha) = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\ell\alpha} & & & \mathcal{O} \\ & \mathrm{e}^{-\mathrm{i}(\ell-1)\alpha} & & \\ & & \ddots & \\ \mathcal{O} & & & \mathrm{e}^{\mathrm{i}\ell\alpha} \end{pmatrix} \Rightarrow \chi^{(\ell)}(\alpha) = \frac{\sin[(\ell+\frac{1}{2})\alpha]}{\sin[\alpha/2]}$$

Inversion

$$\chi^{(\ell)}(i) = \sum_{m=-\ell}^{m=\ell} (-1)^\ell = (-1)^\ell(2\ell+1)\,,$$

Decomposition of a reducible representation

We deduce the character table for the various harmonics

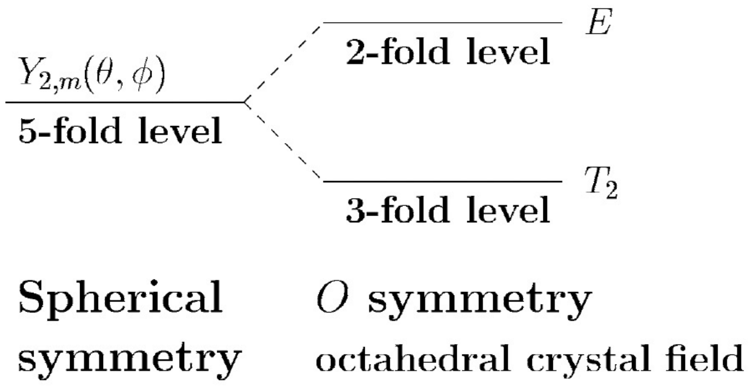
	O	E	$8C_3$	$3C_2 = 3C_4^2$	$6C_2'$	$6C_4$
Γ_1	A_1	1	1	1	1	1
Γ_2	A_2	1	1	1	-1	-1
Γ_{12}	E	2	-1	2	0	0
$\Gamma_{15'}$	T_1	3	0	-1	-1	1
$\Gamma_{25'}$	T_2	3	0	-1	1	-1
$\Gamma_{\ell=0}$	A_1	1	1	1	1	1
$\Gamma_{\ell=1}$	T_1	3	0	-1	1	-1
$\Gamma_{\ell=2}$	$E + T_2$	5	-1	1	1	-1
$\Gamma_{\ell=3}$	$A_2 + T_1 + T_2$	7	1	-1	-1	-1
$\Gamma_{\ell=4}$	$A_1 + E + T_1 + T_2$	9	0	1	1	1
$\Gamma_{\ell=5}$	$E + 2T_1 + T_2$	11	-1	-1	-1	1

Decomposition formula

$$\chi(\mathcal{C}_k) = \sum_{\Gamma_i} a_i \chi^{(\Gamma_i)}(\mathcal{C}_k)$$

$$a_j = \frac{1}{h} \sum_k N_k \left[\chi^{(\Gamma_j)}(\mathcal{C}_k)\right]^* \chi(\mathcal{C}_k)$$

For instance, for l=2



Invariant theory and basis functions

We have talked a lot about how symmetry operations can be represented by matrices
Now, let us determine the functions that remain invariant under these operations

Associated with each irreducible representation, these "basis functions" can be used to generate the matrices that represent the symmetry elements of a particular irreducible representation.

Vector of a representation Γ_n

$$\hat{P}_R|\Gamma_n\alpha\rangle = \sum_j D^{(\Gamma_n)}(R)_{j\alpha}|\Gamma_n j\rangle$$

Operator for symmetry R

Matrix represention of R in Γ_n

The basis vectors $|\Gamma_n j\rangle$ form an orthonormal basis

Therefore $D^{(\Gamma_n)}(R)_{j\alpha} = \langle\Gamma_n j|\hat{P}_R|\Gamma_n\alpha\rangle$

Invariant theory and basis functions

Let's go back to our D_3 group

$\hat{P}_R$	x'	y'	z'
$E = E$	x	y	z
$C_3 = F$	$\frac{1}{2}(-x+\sqrt{3}y)$	$\frac{1}{2}(-y-\sqrt{3}x)$	z
$C_3^{-1} = D$	$\frac{1}{2}(-x-\sqrt{3}y)$	$\frac{1}{2}(-y+\sqrt{3}x)$	z
$C_{2(1)} = A$	$-x$	y	$-z$
$C_{2(2)} = B$	$\frac{1}{2}(x-\sqrt{3}y)$	$\frac{1}{2}(-y-\sqrt{3}x)$	$-z$
$C_{2(3)} = C$	$\frac{1}{2}(x+\sqrt{3}y)$	$\frac{1}{2}(-y+\sqrt{3}x)$	$-z$

class $\rightarrow$ IR $\downarrow$	$\mathcal{C}_1$ $\chi(E)$	$3\mathcal{C}_2$ $\chi(A,B,C)$	$2\mathcal{C}_3$ $\chi(D,F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Invariant theory and basis functions

Let's go back to our D_3 group

$\hat{P}_R$	x'^2	y'^2	z'^2
$E = E$	x^2	y^2	z^2
$C_3 = F$	$\frac{1}{4}(x^2 + 3y^2 - 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 + 2\sqrt{3}xy)$	z^2
$C_3^{-1} = D$	$\frac{1}{4}(x^2 + 3y^2 + 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 - 2\sqrt{3}xy)$	z^2
$C_{2(1)} = A$	x^2	y^2	z^2
$C_{2(2)} = B$	$\frac{1}{4}(x^2 + 3y^2 - 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 + 2\sqrt{3}xy)$	z^2
$C_{2(3)} = C$	$\frac{1}{4}(x^2 + 3y^2 + 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 - 2\sqrt{3}xy)$	z^2

class → IR ↓	$\mathcal{C}_1$ $\chi(E)$	$3\mathcal{C}_2$ $\chi(A, B, C)$	$2\mathcal{C}_3$ $\chi(D, F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Invariant theory and basis functions

Let's go back to our D_3 group

$\hat{P}_R$	x'^2	y'^2	z'^2
$E = E$	x^2	y^2	z^2
$C_3 = F$	$\frac{1}{4}(x^2 + 3y^2 - 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 + 2\sqrt{3}xy)$	z^2
$C_3^{-1} = D$	$\frac{1}{4}(x^2 + 3y^2 + 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 - 2\sqrt{3}xy)$	z^2
$C_{2(1)} = A$	x^2	y^2	z^2
$C_{2(2)} = B$	$\frac{1}{4}(x^2 + 3y^2 - 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 + 2\sqrt{3}xy)$	z^2
$C_{2(3)} = C$	$\frac{1}{4}(x^2 + 3y^2 + 2\sqrt{3}xy)$	$\frac{1}{4}(y^2 + 3x^2 - 2\sqrt{3}xy)$	z^2

$$\begin{cases} D(xy) = \frac{1}{4}\left(-2xy - \sqrt{3}[x^2 - y^2]\right) \\ D(x^2 - y^2) = -\frac{1}{4}\left(2[x^2 - y^2] - 4\sqrt{3}xy\right) \\ D(xz) = \left(-\frac{x}{2} - \frac{\sqrt{3}}{2}y\right) z \, , \\ D(yz) = \left(-\frac{y}{2} + \frac{\sqrt{3}}{2}x\right) z \, . \end{cases}$$

Invariant theory and basis functions

So, in summary

$D_3(32)$			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	-1
$\left.\begin{array}{l}(xz, yz)\\(x^2-y^2, xy)\end{array}\right\}$	$\left.\begin{array}{l}(x, y)\\(R_x, R_y)\end{array}\right\}$	E	2	-1	0

Projection operators

We define the projection operator acting on a basis $\hat{P}_{k\ell}^{(\Gamma_n)}|\Gamma_n \ell\rangle \equiv |\Gamma_n k\rangle$

Explicitly
$$\hat{P}_{k\ell}^{(\Gamma_n)} = \frac{\ell_n}{h} \sum_R D^{(\Gamma_n)}(R)^*_{k\ell} \hat{P}_R$$

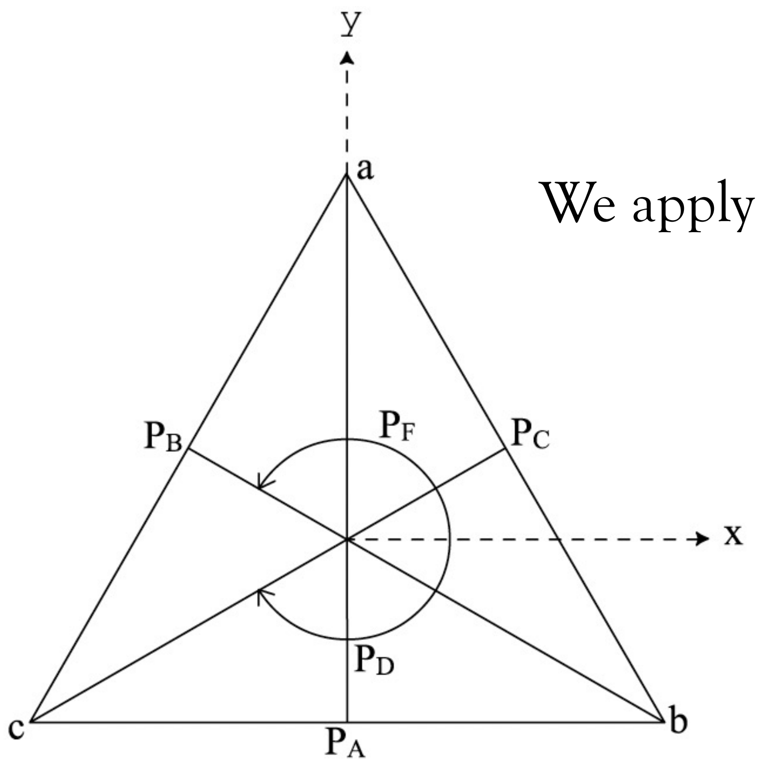
Therefore, for a general function
$$F = \sum_{\Gamma_{n'}} \sum_{j'} f_{j'}^{(\Gamma_{n'})} |\Gamma_{n'} j'\rangle$$

The projection operation yields $\hat{P}_{kk}^{(\Gamma_n)} F = f_k^{(\Gamma_n)} |\Gamma_n k\rangle$

This procedure allows us to expression a general function in the basis of invariants

Projection operators

Back to our favorite D_3



We apply the projection procedure on ψ_a=a, ψ_b=b, ψ_c=c

$$\hat{P}^{(\Gamma_n)}a = \frac{\ell_n}{h}\sum_R \chi^{(\Gamma_n)}(R)^*\hat{P}_R a = f^{(\Gamma_n)}|\Gamma_n\rangle$$

$$\hat{P}^{(\Gamma_1)}a = \hat{P}^{(\Gamma_1)}b = \hat{P}^{(\Gamma_1)}c = \frac{1}{3}(a+b+c)$$

$$\hat{P}^{(\Gamma_{1'})}a = \hat{P}^{(\Gamma_{1'})}b = \hat{P}^{(\Gamma_{1'})}c = 0$$

For the 2d representation, we rather start with a trial function

$$|\Gamma_2\alpha\rangle = a + \omega b + \omega^2 c\,,\ \omega = \mathrm{e}^{2\pi\mathrm{i}/3}$$

Which yields $|\Gamma_2\alpha\rangle = a + \omega b + \omega^2 c\,, \quad |\Gamma_2\beta\rangle = a + \omega^2 b + \omega c\,.$