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

Plan for Lecture 19:

Review of topics in group theory

Chapters 1-10 in DDJ

1. **General concepts and definitions in group theory**
2. **Representations of groups; great orthogonality theorem**
3. **Point groups; space groups**

9	Wed: 02/01/2017	Chap. 8	Vibrational excitations	#7	02/03/2017
10	Fri: 02/03/2017	Notes	Continuous groups	#8	02/06/2017
11	Mon: 02/06/2017	Notes	Group of three-dimensional rotations	#9	02/08/2017
12	Wed: 02/08/2017	Notes	Continuous groups	#10	02/10/2017
13	Fri: 02/10/2017	Chap. 5	Atomic orbitals	#11	02/13/2017
14	Mon: 02/13/2017	Chap. 6	Direct product groups	#12	02/15/2017
15	Wed: 02/15/2017	Chap. 7	Molecular orbital	#13	02/17/2017
16	Fri: 02/17/2017	Chap. 9	Introduction to Space Groups	#14	02/20/2017
17	Mon: 02/20/2017	Chap. 10	Group theory for the periodic lattice		
18	Wed: 02/22/2017	Chap. 10	Group theory for the periodic lattice		
19	Fri: 02/24/2017	Chap. 1-10	Review -- Distribute take-home exam		
20	Mon: 02/27/2017				Exam
21	Wed: 03/01/2017				Exam
22	Fri: 03/03/2017				Exam Due
	Mon: 03/06/2017		*Spring break - no class*		
	Wed: 03/08/2017		*Spring break - no class*		
	Fri: 03/10/2017		*Spring break - no class*		
	Mon: 03/13/2017		*APS Meeting - no class*		
	Wed: 03/15/2017		*APS Meeting - no class*		
	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017				
24	Wed: 03/22/2017				

Group theory
An abstract algebraic construction in mathematics
Definition of a group:

A group is a collection of "elements" – $A, B, C, \ldots$ and a "multiplication" process. The abstract multiplication $(\cdot)$ pairs two group elements, and associates the "result" with a third element. (For example $(A \cdot B = C)$.) The elements and the multiplication process must have the following properties.

1. The collection of elements is closed under multiplication. That is, if elements A and B are in the group and $A \cdot B = C$, element C must be in the group.
2. One of the members of the group is a "unit element" (E). That is, for any element A of the group, $A \cdot E = E \cdot A = A$.
3. For each element A of the group, there is another element A^{-1} which is its "inverse". That is $A \cdot A^{-1} = A^{-1} \cdot A = E$.
4. The multiplication process is "associative". That is for sequential mulplication of group elements A, B, and C, $(A \cdot B) \cdot C = A \cdot (B \cdot C)$.

Some definitions:

Order of the group ➔ number of elements (members) in the group (positive integer for finite group, ∞ for infinite group)

Subgroup ➔ collection of elements within a group which by themselves form a group

Coset ➔ Given a subgroup $\mathbf{g_i}$ of a group a right coset can be formed by multiply an element of $\mathbf{g}$ with each element of $\mathbf{g_i}$

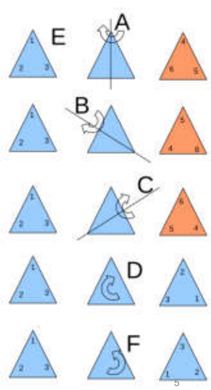
Class ➔members of a group generated by the conjugate construction $\mathcal{C} = X_i^{-1} Y X_i$ where Y is a fixed group element and X_i are all of the elements of the group.

Example of a 6-member group *E,A,B,C,D,F,G*

Group multiplication table

Group of order 6

	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



For our example:

	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

$$A^{-1} = A$$
$$B^{-1} = B$$
$$C^{-1} = C$$
$$D^{-1} = F$$
$$F^{-1} = D$$

Classes:

$$\mathcal{C}_1 = E$$
$$\mathcal{C}_2 = A, B, C$$
$$\mathcal{C}_3 = D, F$$

Representations of a group

A representation of a group is a set of matrices (one for each group element) -- $\Gamma(A), \Gamma(B)...$ that satisfies the multiplication table of the group. The dimension of the matrices is called the dimension of the representation.

Example:

	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

Identical Representation:

$$\Gamma^1(A)=\Gamma^1(B)=\Gamma^1(C)$$
$$=\Gamma^1(D)=\Gamma^1(E)=\Gamma^1(F)=1$$

Another Representation

$$\Gamma^2(A)=\Gamma^2(B)=\Gamma^2(C)=-1$$
$$\Gamma^2(E)=\Gamma^2(D)=\Gamma^2(F)=1$$

Third Representation

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

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

The great orthogonality theorem on unitary irreducible representations

Notation: $h \equiv$ order of the group

$R \equiv$ element of the group

$\Gamma^i(R)_{\alpha\beta} \equiv$ ith representation of R

$_{\mu\nu\alpha\beta}$ denote matrix indices

$l_i \equiv$ dimension of the representation

$$\sum_R \left(\Gamma^i(R)_{\mu\nu}\right)^* \Gamma^j(R)_{\alpha\beta} = \frac{h}{l_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}$$

Great orthogonality theorem for characters

$$\sum_R \left(\Gamma^i(R)_{\mu\nu}\right)^* \Gamma^j(R)_{\alpha\beta} = \frac{h}{l_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}$$

Let $\mu = \nu$ and $\alpha = \beta$ and perform summations

$$\sum_{R\mu\alpha} \left(\Gamma^i(R)_{\mu\mu}\right)^* \Gamma^j(R)_{\alpha\alpha} = \frac{h}{l_i}\delta_{ij}\sum_{\mu\alpha}\delta_{\mu\alpha}\delta_{\mu\alpha}$$

$$\sum_R \left(\chi^i(R)\right)^* \chi^j(R) = h\delta_{ij}$$

In terms of classes $\mathcal{C}$, each with $N_{\mathcal{C}}$ elements:

$$\sum_{\mathcal{C}} N_{\mathcal{C}} \left(\chi^i(\mathcal{C})\right)^* \chi^j(\mathcal{C}) = h\delta_{ij}$$

Character table for *P(3):*

$$\Gamma^1(A) = \Gamma^1(B) = \Gamma^1(C) = \Gamma^1(D) = \Gamma^1(E) = \Gamma^1(F) = 1$$

$$\Gamma^2(A) = \Gamma^2(B) = \Gamma^2(C) = -1 \quad \Gamma^2(E) = \Gamma^2(D) = \Gamma^2(F) = 1$$

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

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

Classes: $\mathcal{C}_1 = E \quad \mathcal{C}_2 = A, B, C \quad \mathcal{C}_3 = D, F$

	$\mathcal{C}_1$	$3\mathcal{C}_2$	$2\mathcal{C}_3$
χ^1	1	1	1
χ^2	1	-1	1
χ^3	2	0	-1

The characters χ^i behave as a vector space with the dimension equal to the number of classes.

➔The number of characters=the number of classes

Second character identity:

$$\sum_i \left(\chi^i(\mathcal{C}_k)\right)^* \chi^i(\mathcal{C}_l) = \frac{h}{N_{\mathcal{C}_k}}\delta_{kl}$$

Example of H_2O

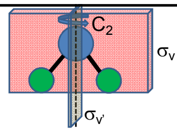
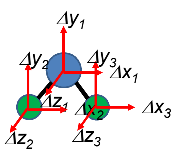


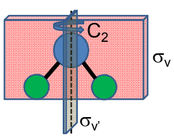
Table 3.14: Character Table for Group C_{2v}

C_{2v} (2mm)			E	C_2	σ_v	σ_v'
x^2, y^2, z^2	z	A_1	1	1	1	1
xy	R_z	A_2	1	1	−1	−1
xz	R_y, x	B_1	1	−1	1	−1
yz	R_x, y	B_2	1	−1	−1	1

"Standard" notation for representations of C_{2v}

Symmetry analysis





$$R \begin{bmatrix} \Delta x_1 \\ \Delta y_1 \\ \Delta z_1 \\ \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \\ \Delta x_3 \\ \Delta y_3 \\ \Delta z_3 \end{bmatrix}$$

$$E \begin{bmatrix} \Delta x_1 \\ \Delta y_1 \\ \Delta z_1 \\ \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \\ \Delta x_3 \\ \Delta y_3 \\ \Delta z_3 \end{bmatrix} = \begin{bmatrix} 1&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&1 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta y_1 \\ \Delta z_1 \\ \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \\ \Delta x_3 \\ \Delta y_3 \\ \Delta z_3 \end{bmatrix}$$

$\chi(E)=9$

$$C_2 \begin{bmatrix} \Delta x_1 \\ \Delta y_1 \\ \Delta z_1 \\ \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \\ \Delta x_3 \\ \Delta y_3 \\ \Delta z_3 \end{bmatrix} = \begin{bmatrix} -1&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0 \\ 0&0&-1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&-1&0&0 \\ 0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&-1 \\ 0&0&0&-1&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&-1&0&0&0 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta y_1 \\ \Delta z_1 \\ \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \\ \Delta x_3 \\ \Delta y_3 \\ \Delta z_3 \end{bmatrix}$$

$\chi(C_2)$=-1

Similarly: $\chi(\sigma_v)$=3
$\chi(\sigma_{v'})$=1

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Decomposition of the displacement representation into irreducible representations

$$\chi(R) = \sum_i a_i \chi^i(R)$$

$$a_i = \frac{1}{h}\sum_R \left(\chi^i(R)\right)^* \chi(R)$$

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xy	R_z	A_2	1	1	−1	−1
xz	R_y, x	B_1	1	−1	1	−1
yz	R_x, y	B_2	1	−1	−1	1
$\chi(R)$			9	−1	3	1

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Table 3.14: Character Table for Group C_{2v}

C_{2v} (2mm)			E	C_2	σ_v	σ_v'
x^2, y^2, z^2	z	A_1	1	1	1	1
xy	R_z	A_2	1	1	−1	−1
xz	R_y, x	B_1	1	−1	1	−1
yz	R_x, y	B_2	1	−1	−1	1
$\chi(R)$			9	−1	3	1

$\Rightarrow$ Coordinate representation=$3A_1 + A_2 + 3B_1 + 2B_2$
translations =$A_1 + B_1 + B_2$
rotations =$A_2 + B_1 + B_2$
vibrations =$2A_1 + B_1$

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Some properties of continuous group SO(3)

Taylor expansion:

$$\psi(\phi'-\alpha)=\psi(\phi')-\alpha\frac{\partial\psi(\phi')}{\partial\phi'}+\frac{1}{2}\alpha^2\frac{\partial^2\psi(\phi')}{\partial\phi'^2}+....$$

$$=e^{-\alpha\frac{\partial}{\partial\phi'}}\psi(\phi')$$

$$=R_{-\alpha}\psi(\phi')$$

Generator operator for rotation: $=e^{-\alpha\frac{\partial}{\partial\phi'}}$

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$$O_{-\alpha}=e^{-\alpha\frac{\partial}{\partial\phi}}=e^{-i\alpha L_z/\hbar}$$

More "standard" notation --
operator for counterclockwise
rotation about the $\hat{\mathbf{n}}$ axis by angle α :

$$O_R(\alpha,\ \hat{\mathbf{n}})=e^{-i\alpha\mathbf{L}\cdot\hat{\mathbf{n}}/\hbar}$$

Eigenfunctions of rotation operator

$$O_R(\alpha,\ \hat{\mathbf{n}})=e^{-i\alpha\mathbf{L}\cdot\hat{\mathbf{n}}/\hbar}$$

$$O_R(\alpha,\ \hat{\mathbf{z}})|lm\rangle=e^{-i\alpha L_z/\hbar}|lm\rangle=e^{-i\alpha m}|lm\rangle$$

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Irreducible representations in terms of angular momentum eigenfunctions

$$\chi^l(\alpha)=\sum_{m=-l}^{l}\langle lm|O_R(\alpha,\ \hat{\mathbf{z}})|lm\rangle=\sum_{m=-l}^{l}e^{-i\alpha m}=\frac{\sin\left[\alpha\left(l+\frac{1}{2}\right)\right]}{\sin(\alpha/2)}$$

Note that: $\chi^l(\alpha+2\pi)=(-1)^{2l}\chi^l(\alpha)$

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Group of all unitary matrices of dimension 2 – SU(2)

$$M=\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \quad \text{where } |a|^2+|b|^2=1$$

$$\Rightarrow M=M(\alpha,n)=e^{-i\frac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\left(\tfrac{\alpha}{2}\right)-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\left(\tfrac{\alpha}{2}\right)$$

$$\text{where} \quad \boldsymbol{\sigma}=\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\sigma_x}\hat{\mathbf{x}}+\underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\sigma_y}\hat{\mathbf{y}}+\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\sigma_z}\hat{\mathbf{z}}$$

Group of all unitary matrices of dimension 2 – SU(2) --continued

Note that:

$$e^{-i\frac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}}=1+\left(-i\tfrac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\right)+\frac{1}{2!}\left(-i\tfrac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\right)^2+\frac{1}{3!}\left(-i\tfrac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\right)^3 +\frac{1}{4!}\left(-i\tfrac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\right)^4+\ldots$$

$$\text{since} \quad (\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^2=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$e^{-i\frac{1}{2}\alpha\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\left(1-\frac{1}{2!}\left(\frac{\alpha}{2}\right)^2+\frac{1}{4!}\left(\frac{\alpha}{2}\right)^4-\ldots\right)-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left(\left(\frac{\alpha}{2}\right)-\frac{1}{3!}\left(\frac{\alpha}{2}\right)^3+\ldots\right)$$

$$=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\left(\tfrac{\alpha}{2}\right)-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\left(\tfrac{\alpha}{2}\right)$$