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

Plan for Lecture 29:

Time reversal symmetry and Magnetic groups
Chap. 16 in DDJ

1. **Effects of magnetic configurations on point groups and space groups**
2. **Examples of magnetic point groups**

Note: These slides contain materials from an electronic version of the Dresselhaus textbook.

23	Mon: 03/20/2017	Chap. 7.7	Jahn-Teller Effect	#15	03/24/2017
24	Wed: 03/22/2017	Chap. 7.7	Jahn-Teller Effect		
25	Fri: 03/24/2017		Spin 1/2	#16	03/27/2017
26	Mon: 03/27/2017		Dirac equation for H-like atoms	#17	03/29/2017
27	Wed: 03/29/2017	Chap. 14	Angular momenta	#18	03/31/2017
28	Fri: 03/31/2017	Chap. 16	Time reversal symmetry	#19	04/07/2017
29	Mon: 04/03/2017	Chap. 16	Magnetic point groups		
30	Wed: 04/05/2017				
31	Fri: 04/07/2017				
32	Mon: 04/10/2017				
33	Wed: 04/12/2017				
	Fri: 04/14/2017		*Good Friday Holiday -- no class*		
34	Mon: 04/17/2017				
35	Wed: 04/19/2017				
36	Fri: 04/21/2017				
	Mon: 04/24/2017		Presentations I		
	Wed: 04/26/2017		Presentations II		

Topic for presentation

Presentation ideas

1. Digest the content of a literature paper which involves aspects of group theory and present the theory and results.
2. Find a particular molecule or crystal and analyze its group theoretic aspects
   a. Band structure analysis; find at least 3 special k-points or directions, analyzing their groups and compatibility relationships
   b. Point group analysis, finding selection rules for various transitions between representations
   c. Vibrational mode analysis

Group theory describing magnetic configurations

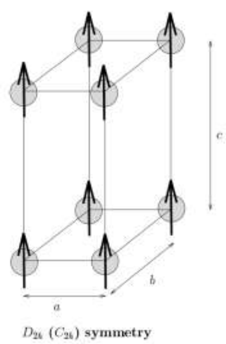


Figure 22.3: Magnetic spin arrangement in $D_{2h}(C_{2h})$ for an orthorhombic ferromagnetic system.

When is magnetic ordering important?

$$H = H_0 + H_M$$

Effective magnetic model (Heisenberg):

$$H_M = -J\sum_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

What does time reversal symmetry have to do with magnetic configurations?

- Time reversal symmetry does not effect charge density
- Time reversal symmetry does effect internal spin so that the effects of the *T* operator on the group operations must be taken into account

For the purpose of analyzing magnetic groups, it is convenient to distinguish two kinds of elements:

$\{A_i\}$ and $\{M_k\}$ where $M_k \equiv TA_k$

Note that $\{M_k\}$ are "antioperators"

In general, we can describe the group as $G = \{\{A_i\},\{M_k\}\}$

Note that:

$$A_i A_{i'} = A_{i''}$$
$$M_k M_{k'} = A_{i''}$$
$$A_i M_k = M_{k'}$$
$$M_k A_i = M_{k''}$$

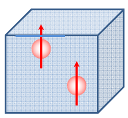
Properties of a point group $G = \{\{A_i\},\{M_k\}\}$

Possibility #1: $\{M_k\}$ is the null set $\Rightarrow$ 32 "ordinary" point groups

Possibility #2: $\{M_i\} \equiv \{TA_i\}$ $\Rightarrow$ direct product of T with 32 original point groups

Possibility #3: $\{M_k\} \neq \{TA_i\}$ $\Rightarrow$ 58 new magnetic point groups

Example #1:



$\{A_i\} = E, i$

T is not a symmetry element for this ferromagnetic configuration

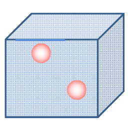
Properties of a point group $G = \{\{A_i\},\{M_k\}\}$

Possibility #1: $\{M_k\}$ is the null set $\Rightarrow$ 32 "ordinary" point groups

Possibility #2: $\{M_i\} \equiv \{TA_i\}$ $\Rightarrow$ direct product of T with 32 original point groups

Possibility #3: $\{M_k\} \neq \{TA_i\}$ $\Rightarrow$ 58 new magnetic point groups

Example #2:



$\{A_i\} = E, i$

$\{M_i\} = T, Ti$

(non-magnetic crystal)

Properties of a point group $G = \{\{A_i\},\{M_k\}\}$

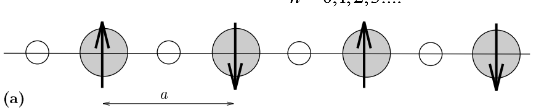
Possibility #1: $\{M_k\}$ is the null set $\Rightarrow$ 32 "ordinary" point groups

Possibility #2: $\{M_i\} \equiv \{TA_i\}$ $\Rightarrow$ direct product of T with 32 original point groups

Possibility #3: $\{M_k\} \neq \{TA_i\}$ $\Rightarrow$ 58 new magnetic point groups

Example #2: (space group) $\{A_n\} = [E|2na]$ $\{M_n\} = [T|(2n+1)a]$

$n = 0,1,2,3....$



(a)

Properties of a point group $G = \{\{A_i\},\{M_k\}\}$

Possibility #1: $\{M_k\}$ is the null set $\Rightarrow$ 32 "ordinary" point groups

Possibility #2: $\{M_i\} \equiv \{TA_i\}$ $\Rightarrow$ direct product of T with 32 original point groups

Possibility #3: $\{M_k\} \neq \{TA_i\}$ $\Rightarrow$ 58 new magnetic point groups

Define $G' = \{\{A_i\},\{A_k\}\}$ where $\{A_i\}$ and $\{A_k\}$ have distinct elements

Magnetic group can be formed from $G = \{\{A_i\},\{TA_k\}\}$

Additional properties:

$H \equiv \{A_i\}$ forms an invariant subgroup of G

$\{TA_k\}$ is a coset of H and therefore has the same order as H

$A_k^n \neq E$ for n odd

Example of possibility #3:

C_{2h} with elements $\{E, C_2, \sigma_h, i\} \equiv G'$

Choose $H = \{E, C_2\}$

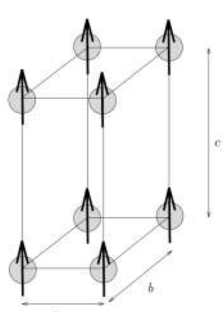
Then $\{TA_k\} = \{T\sigma_h, Ti\}$ — $C_{2h}(C_2)$

or Choose $H = \{E, i\}$

Then $\{TA_k\} = \{T\sigma_h, TC_2\}$ — $C_{2h}(C_i)$

or Choose $H = \{E, \sigma_h\}$

Then $\{TA_k\} = \{TC_2, Ti\}$ — $C_{2h}(C_{1h})$



D_{2h} (C_{2h}) symmetry

$$H = \{E, C_{2z}, \sigma_z, i\}$$

$$\{TA_k\} = \{TC_{2x}, TC_{2y}, T\sigma_x, T\sigma_y\}$$

Figure 22.3: Magnetic spin arrangement in $D_{2h}(C_{2h})$ for an orthorhombic ferromagnetic system.

Note that $\sigma_z = iC_{2z}$

Example of #3

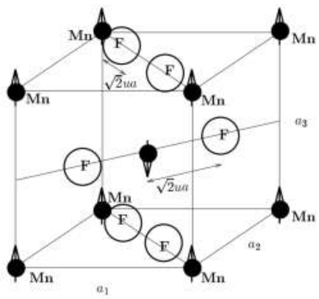


Figure 22.4: The common antiferromagnets MnF_2, FeF_2 and CoF_2 crystallize in the rutile structure with $|a_1| = |a_2| = a$; $|a_3| = c$; $c \neq a$. The diagram shows the magnetic point group D_{4h} (D_{2d}) which describes the antiferromagnetic spin alignment.

***$D_{4h}(D_{2h})$* -- continued**

H	***TA_k***
1. $\{E\|0\}$	9. $\{i\|0\}$
2. $\{C_2\|0\}$	10. $\{\sigma_h\|0\} = \{C_2\|0\}\{i\|0\}$
3. $\{C_{2\xi}\|0\}$	11. $\{\sigma_{d\xi}\|0\} = \{C_{2\xi}\|0\}\{i\|0\}$
4. $\{C_{2\nu}\|0\}$	12. $\{\sigma_{d\nu}\|0\} = \{C_{2\nu}\|0\}\{i\|0\}$
5. $\{C_4\|\tau_0\}$	13. $\{S_4^{-1}\|\tau_0\} = \{C_4\|\tau_0\}\{i\|0\}$
6. $\{C_4^{-1}\|\tau_0\}$	14. $\{S_4\|\tau_0\} = \{C_4^{-1}\|\tau_0\}\{i\|0\}$
7. $\{C_{2x}\|\tau_0\}$	15. $\{\sigma_{vx}\|\tau_0\} = \{C_{2x}\|\tau_0\}\{i\|0\}$
8. $\{C_{2y}\|\tau_0\}$	16. $\{\sigma_{vy}\|\tau_0\} = \{C_{2y}\|\tau_0\}\{i\|0\}$

$$\vec{\tau}_0 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$$

Some character table analysis for magnetic groups

PHYSICAL REVIEW VOLUME 127, NUMBER 2 JULY 15, 1962

Symmetry Properties of Wave Functions in Magnetic Crystals*†

J. O. DIMMOCK‡ AND R. G. WHEELER
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(Received February 8, 1962)

The symmetry properties of wave functions in magnetic crystals are discussed in terms of the irreducible representations of magnetic space groups. The specific effects of the magnetic ordering on the crystal eigenstates are found to be of three types: (1) There is a lifting of some eigenfunction degeneracies because the crystal symmetry is reduced in the magnetic state. (2) New Brillouin zone surfaces are introduced if there is a reduction in translational symmetry. (3) The symmetry of the energy band in K space may be reduced. The rutile structure is considered as a specific example, and the space groups of MnF_2 and MnO_2 in their magnetic and nonmagnetic states are obtained. A magnetic structure of MnO_2 where the Mn^{2+} spins point toward the nearest-neighbor oxygens is assumed. The space groups considered are $P4_2/mnm$ (D_{4h}^{14}), $Pnnm$ (D_{2h}^{12}), $I\bar{4}2d$ (D_{2d}^{12}), $P4_2/mnm\ 1'$, $P4_2'/mnm'$, and $I_c\bar{4}2d$. The theory is applied to spin-wave states, and it is found that the structure of the spin-wave energy bands throughout the Brillouin zone may be obtained.

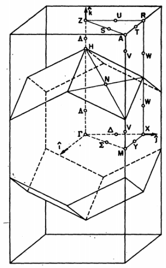

FIG. 5. The Brillouin zones for the simple tetragonal and body-centered tetragonal lattices, with the points and lines of symmetry indicated. The tetragonal prism is the Brillouin zone for the simple lattice defined by the primitive translations $\mathbf{t}_1=a\hat{\imath}$, $\mathbf{t}_2=a\hat{\jmath}$, and $\mathbf{t}_3=c\hat{k}$. The figure enclosed within the prism is the Brillouin zone for the body-centered tetragonal lattice defined by the primitive translations $\mathbf{t}_1+\mathbf{t}_3$, $\mathbf{t}_2-\mathbf{t}_3$, and $\mathbf{t}_1-\mathbf{t}_2$, provided $a>\sqrt{2}c$. For the structures under consideration this requirement is satisfied. The rhombus-shaped plane of which N is the center is the perpendicular bisector of the line ΓA. The point N lies on this line.

TABLE I. Character table for the point $\Gamma(0,0,0)$ of the group $P4_2/mnm$.

	Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
$\{E\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	2	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	−2	−2	−2	−2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	1	1	−1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	1	1	−1	−1	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	1	1	1	1	−2	1	1	1	1	−2	0	0	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\},\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	1	−1	1	−1	0	1	−1	1	−1	0	0	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{0}\}$	1	−1	−1	1	0	1	−1	−1	1	0	0	0	0	0
$\{I\|\mathbf{0}\}$	1	1	1	1	2	−1	−1	−1	−1	−2	2	2	−2	−2
$\{\bar{I}\|\mathbf{0}\}$	1	1	1	1	2	−1	−1	−1	−1	−2	−2	−2	2	2
$\{S_4,S_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	−1	−1	1	1	0	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$\{\bar{S}_4,\bar{S}_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	−1	−1	1	1	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	1	1	−2	−1	−1	−1	−1	2	0	0	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	1	−1	1	−1	0	−1	1	−1	1	0	0	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	−1	−1	1	0	−1	1	1	−1	0	0	0	0	0
Time inv.	a	a	a	a	a	a	a	a	a	a	a	a	a	a

TABLE II. Character table for the point $\Lambda(0,0,\gamma)$ of the group $P4_2/mnm$.[a]

	Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_6	Λ_7
$\{E\|\mathbf{0}\}$	1	1	1	1	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	−2	−2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	ω	ω	$-\omega$	$-\omega$	0	$\omega\sqrt{2}$	$-\omega\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	ω	ω	$-\omega$	$-\omega$	0	$-\omega\sqrt{2}$	$\omega\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	1	1	1	1	−2	0	0
$\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0	0	0
$\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	−1	−1	1	0	0	0
Time inv.	a	a	a	a	a	a	a

[a] $\omega=\exp(\frac{1}{2}ic\gamma)$, $0<\gamma<\pi/c$.

TABLE III. Character table for the point $\Delta(0,\beta,0)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	−2
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-\omega$	ω	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	−1	−1	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0
$P4_2/mnm$ time inv.	a	a	a	a	a

[a] $\omega=\exp(\frac{1}{2}ia\beta)$, $0<\beta<\pi/a$.

TABLE XIV. Compatibility tables for the group $P4_2/mnm$.

Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_2	Λ_1	Λ_4	Λ_3	Λ_5	Λ_6	Λ_7	Λ_6	Λ_7
Σ_1	Σ_2	Σ_2	Σ_1	$\Sigma_3+\Sigma_4$	Σ_3	Σ_4	Σ_4	Σ_3	$\Sigma_1+\Sigma_2$	Σ_5	Σ_5	Σ_5	Σ_5
Δ_1	Δ_2	Δ_1	Δ_2	$\Delta_3+\Delta_4$	Δ_3	Δ_4	Δ_3	Δ_4	$\Delta_1+\Delta_2$	Δ_5	Δ_5	Δ_5	Δ_5

Example: MnF_2 and NiF_2

PHYSICAL REVIEW B VOLUME 48, NUMBER 17 1 NOVEMBER 1993-I

Electronic and magnetic structure of MnF_2 and NiF_2

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(Received 20 April 1993; revised manuscript received 6 July 1993)

We present an *ab initio* study of the electronic and magnetic structure of the antiferromagnetic state of MnF_2 and NiF_2. From the band structures of these two compounds we derive densities of states (DOS), electron densities, spin densities, electric-field gradients, and total energies. We use a simple molecular-orbital scheme to interpret the results. The internal coordinate u is determined by total-energy minimization for MnF_2 and agrees well with experiment as well as with the calculated electric-field gradients or the electron densities. Recent spin-dependent x-ray-absorption spectra are interpreted in terms of partial DOS of the unoccupied Mn 4p states.

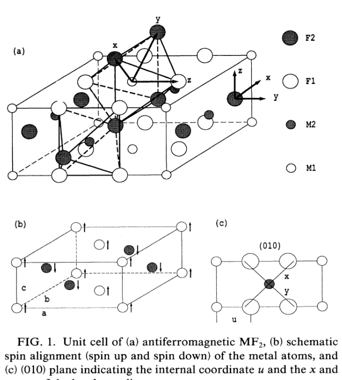

FIG. 1. Unit cell of (a) antiferromagnetic MF_2, (b) schematic spin alignment (spin up and spin down) of the metal atoms, and (c) (010) plane indicating the internal coordinate u and the x and y axes of the local coordinates.

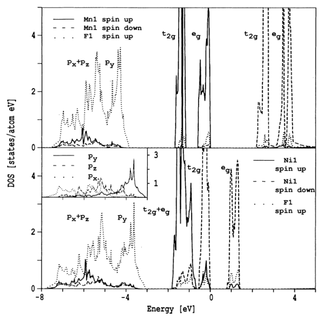

FIG. 4. Spin-projected and symmetry-decomposed densities of states (DOS) of MnF_2 (top panel) and NiF_2 (bottom panel), where the F DOS is further broken up into the *x*, *y*, and *z* components (inset).

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