Cornell University

"I would found an institution where any person can find instruction in any study." – Ezra Cornell, 1868

Competing Ferroic Orders

The magnetoelectric effect

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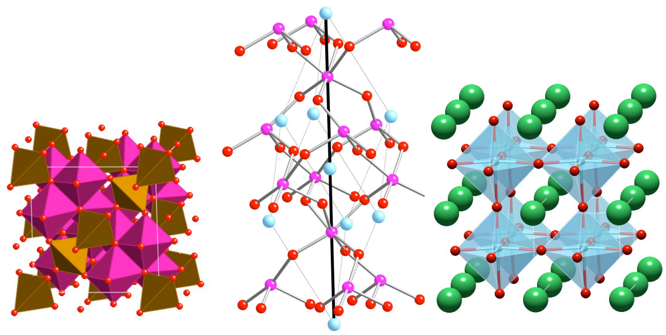


Basic Training in Condensed Matter Theory 2009

Module Outline (Extremely tentative)

1. Overview and Background
   - Ferro ordering, the magnetoelectric effect
   - Complex oxides basics: Types of insulators (i.e., ZSA classifications), Coordination chemistry
2. Structure and Ferroelectricity
   - Basics of space groups
   - Soft mode theory, lattice dynamics, group theoretic methods
   - Competing lattice instabilities
   - microscopic mechanisms, improper FE
   - Modern theory of polarization (Berry Phase)
3. Magnetism
   - Basics, exchange interactions, superexchange, Dzyaloshinskii-Moria
   - How spins couple to the lattice! Phenomenology and microscopics (spin-phonon, spin-lattice, etc)
   - Competing magnetic orders
4. Lets start putting things together
   - Phase competition: magnetic and polar orders and colossal magnetoelectric responses
   - Magnetic order induced ferroelectricity
   - Ferroelectric induced ferromagnetism, switching magnetism 180° with an electric field aren't these forbidden by some symmetry? NO!)
5. Finish up loose ends and recent papers I wish I understood better
   - Toroidal moments

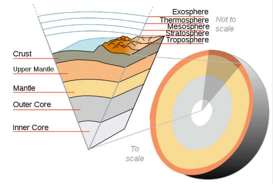
Ab initio

Yes a play on what I do.

➢What does my title mean?

"ferro" derived from the Latin "ferrum"→ Iron

- *Iron is the sixth most abundant element in the Universe*

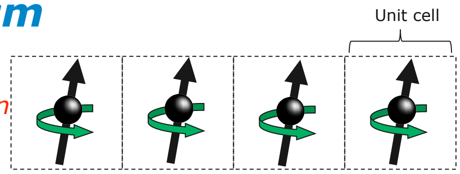


- *While it makes up about 5% of the Earth's crust, the Earth's core is believed to consist largely of an iron-nickel alloy constituting 35% of the mass of the Earth as a whole.*
- *Iron is consequently the most abundant element on Earth, but only the fourth most abundant element in the Earth's crust.*
- *Most of the iron in the crust is found combined with oxygen as iron oxide minerals such as hematite and magnetite.*

http://en.wikipedia.org/wiki/Iron

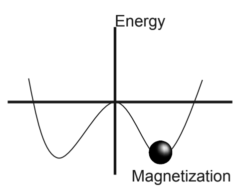
Ferromagnetism

Ordering of spins →
spontaneous magnetization



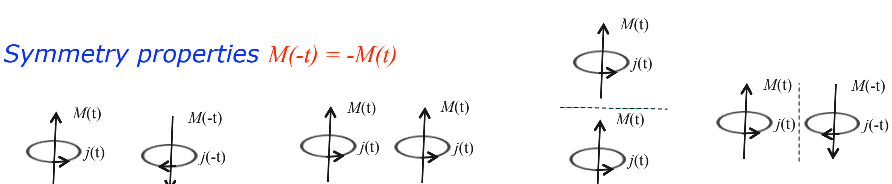
$$M \equiv \sum_i \langle S_i \rangle \neq 0$$

*Spontaneous time-reversal, **R**, symmetry breaking*



$\mathcal{F}(M) = \alpha M^2 + \beta M^4 - M\mathrm{H}$

Symmetry properties $M(-t) = -M(t)$



Time inversion R *t → -t*

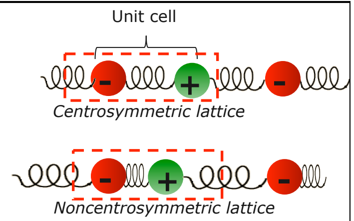
Space inversion I *r → -r*

M and H are Axial vectors

Mirror reflection m

Ferroelectricity

Spontaneous polarization ⇒ Dipole moment per unit volume

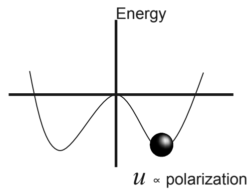


Ordering of polar mode

in many cases, this turns out to be a lattice mode

$$P_\alpha \approx \sum_i Z^*_{\alpha,\beta;i} \langle u_{\beta;i} \rangle \neq 0$$

Spontaneous space-inversion, ,I, symmetry breaking

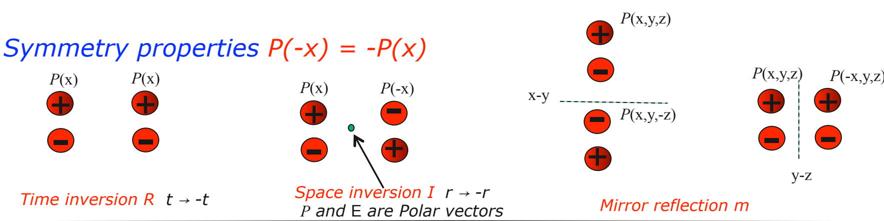


$\mathcal{F}(u) = \alpha\, u^2 + \beta\, u^4 - Z^* u \cdot E$

or

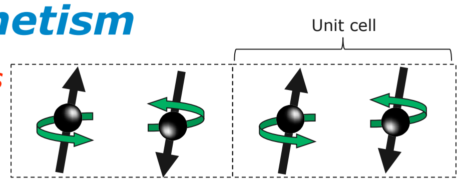
$\mathcal{F}(P) = \alpha P^2 + \beta P^4 - PE$

Symmetry properties P(-x) = -P(x)



AntiFerromagnetism

q≠ 0, Ordering of spins



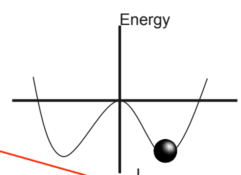
$$M \equiv \sum_i \langle S_i \rangle = 0$$

e.g., two sublattice spin system

$$L = S_1 - S_2$$

Symmetry properties

$L(-t) = -L(t)\ ;\ L(-x) = \pm L(x)$



$\mathcal{F}(M) = \alpha L^2 + \beta L^4 - L H_q$

*Does the AFM ordering of spins spontaneously break time-reversal, **R**, symmetry breaking ?*

First, what does the question mean?

Does the point group of the space group contain R?

Depends on details of crystallographic structure!

Cant ignore structure!! i.e., LATTICE + BASIS (don't just pick your favorite sublattice and ignore the rest!!!)

AntiFerromagnetism

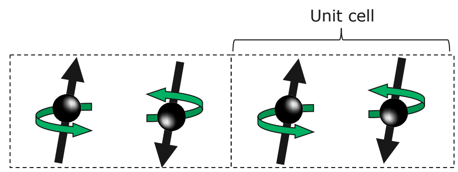
*Does the AFM ordering of spins spontaneously break time-reversal, **R**, symmetry breaking ?*

Symmetry properties *L(-t) = -L(t) ; L(-x) = ± L(x)*

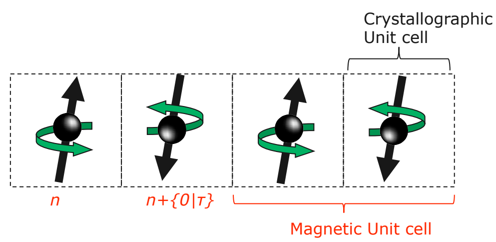
e.g., two sublattice spin system (in the ordered phase)

$$L = S_1 - S_2$$

Example 1: two spins sit in the same unit cell in the paramagnetic phase, Yes! R is not a symmetry element.



Example 2: two spins sit in different unit cells in the paramagnetic phase, No! the space group contains {R|τ} ⇒ the point group, τ→ 0 contains {R|0}.



Ab initio

Yes a play on what I do.

➢What does my title mean?

Def: Linear magnetoelectric effect

Landau and Lifshitz, "Electrodynamics of continuous media"
Dzyaloshinskii, JETP 1957; Astrov JETP 1960 -> Cr_2O_3
Hans Schmid, Geneva; Smolenskii USSR

Requirements: 1) broken space-inversion symmetry
2) broken time-reversal symmetry

$$\mathcal{F} = \mathcal{F}_0 + P_s E + M_s H + \epsilon E^2 + \mu H^2 + \gamma E H$$

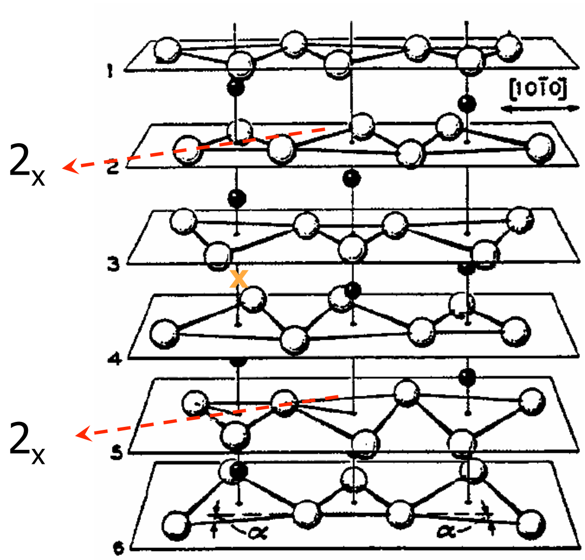
$$P = \frac{\partial \mathcal{F}}{\partial E}|_{E=0} = P_s + \gamma H$$

$$M = \frac{\partial \mathcal{F}}{\partial H}|_{H=0} = M_s + \gamma E$$

γ ≡ linear magnetoelectric coefficient

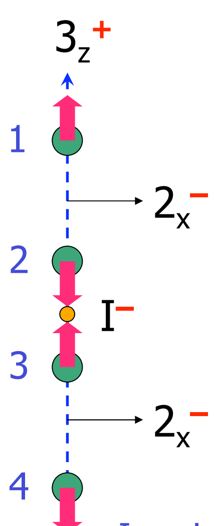
From Max Mostovoy

Crystal structure of Cr_2O_3



From Max Mostovoy

Cr_2O_3



AFM order parameter T_N = 306K

$$\mathbf{L} = \mathbf{M}_1 - \mathbf{M}_2 + \mathbf{M}_3 - \mathbf{M}_4 \qquad L_z \neq 0$$

symmetries of paramagnetic phase

	I	2_x	3_z
L_z	−	+	+
E_z	−	−	+
H_z	+	−	+

point group

$\bar{3}m$

$1,\ 3(2_\perp),\ \pm 3_z$

$\bar{1},\ 3(m_\perp),\ \pm \bar{3}_z$

Invariants:

$$\lambda L_z E_z H_z = \alpha_\parallel E_z H_z$$

$$L_z\left(E_x H_x + E_y H_y\right)$$

$$\alpha_\parallel, \alpha_\perp \propto L_z$$

From Max Mostovoy

Cr_2O_3

magnetic point group $\bar{3}'m'$

Symmetries of low-T phase: $1,\ 3(2_\perp),\ \pm 3_z,\ \bar{1}',\ 3(m'_\perp),\ \pm \bar{3}'_z$

	I'	2_x	3_z
$\begin{pmatrix} E_x \\ E_y \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$R_{2\pi/3}$
E_z	-1	-1	$+1$
$\begin{pmatrix} H_x \\ H_y \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$R_{2\pi/3}$
H_z	-1	-1	$+1$

Inversion combined with time reversal

$I' = IT$

120°-rotation

$$R_{2\pi/3} = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$$

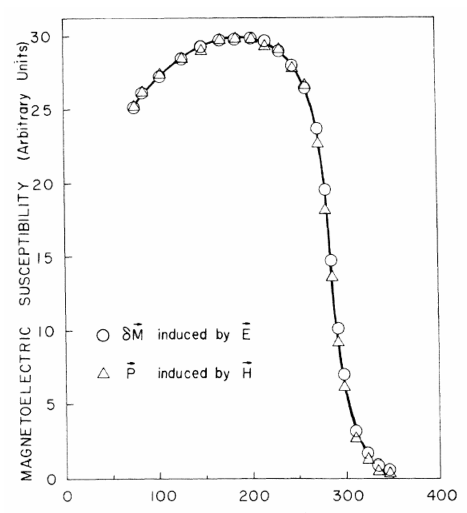
Invariants: $F_{\rm me} = -\alpha_{\parallel} E_z H_z - \alpha_{\perp}\left(E_x H_x + E_y H_y\right)$

From Max Mostovoy

Linear magnetoelectric effect

Cr_2O_3

*I. E. Dzyaloshinskii JETP **10** 628 (1959),*
*D. N. Astrov, JETP **11** 708 (1960)*



$$P = \chi_e E + \alpha H$$

$$M = \alpha E + \chi_m H$$

*G.T. Rado PRL **13** 335 (1964)*

Next time

ME revisited, and basic oxide physics

- ME effect revisited: Toroidal moments
- Complex oxides basics: Types of insulators (i.e., ZSA classifications), Coordination chemistry