Coupled electricity and magnetism: magnetoelectrics, multiferroics and all that

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- Introduction
- Magnetoelectrics
- Multiferroics; microscopic mechanisms
- Currents, dipoles and monopoles in frustrated systems
- Magnetic textures: domain walls, vortices, skyrmions
- Dynamics; multiferroics as metamaterials
- Conclusions
Degrees of freedom

- Charge ordering $\rho(r)$ (monopole)
- Ferroelectricity P or D (dipole)
- Quadrupole $Q_{\alpha\beta}$
- Spin Magnetic ordering
- Orbital ordering
- Lattice
Maxwell's equations
\[ \nabla \cdot \mathbf{E} = 4\pi \rho_e \]
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ -\nabla \times \mathbf{E} = \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \]
\[ \nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{j}_e \]

Magnetoelectric effect
\[ M_i = \sum \alpha_{ij} E_j + \sum \beta_{ijk} E_j E_k + \ldots \]
\[ P_i = \sum \alpha_{ij} H_j + \sum \beta_{ijk} H_j H_k + \ldots \]
Coupling of electric polarization to magnetism

Time reversal symmetry

\[ \mathbf{P} \rightarrow +\mathbf{P} \quad t \rightarrow -t \]
\[ \mathbf{M} \rightarrow -\mathbf{M} \]

Inversion symmetry

\[ \mathbf{P} \rightarrow -\mathbf{P} \quad \mathbf{r} \rightarrow -\mathbf{r} \]
\[ \mathbf{M} \rightarrow +\mathbf{M} \]

For linear ME effect to exist, both inversion symmetry and time reversal invariance has to be broken

\[ F \propto \alpha HE \]
In Cr$_2$O$_3$ inversion is broken — it is linear magnetoelectric.

In Fe$_2$O$_3$ – inversion is not broken, it is not ME (but it has weak ferromagnetism).
Magnetoelastic coefficient $\alpha_{ij}$ can have both symmetric and antisymmetric parts

**Symmetric:**

$$ \alpha_{ij} = \begin{pmatrix} \alpha_{xx} & 0 & 0 \\ 0 & \alpha_{yy} & 0 \\ 0 & 0 & \alpha_{zz} \end{pmatrix} $$

Then

$$ P_i = \alpha_{ij} H_i ; \quad \text{along main axes} \quad P \parallel H , \quad M \parallel E $$

For antisymmetric tensor $\alpha_{ij}$ one can introduce a dual vector $T_i = \varepsilon_{ijk} \alpha_{jk}$

$T$ is the **toroidal moment** (both $P$ and $T$-odd). Then

$$ P \perp H , \quad M \perp E , $$

$$ P = [T \times H] , \quad M = - [T \times E] $$

For localized spins

$$ T = \sum_i r_i \times S_i $$

For example, toroidal moment exists in a magnetic vortex
MULTIFERROICS

Materials combining ferroelectricity, (ferro)magnetism and (ferro)elasticity

If successful – a lot of possible applications (e.g. electrically controlling magnetic memory, etc)

Field active in 60-th – 70-th, mostly in the Soviet Union

Revival of the interest starting from ~2000

D.Kh. JMMM 306, 1 (2006); Physics (Trends) 2, 20 (2009)
March meetings, # of sessions
(normalized to the peak number in these years)

- Multiferroics
- HTSC (E vortices)
- CMR
**Magnetism:** In principle clear: spins; exchange interaction; partially filled d-shells

**Ferroelectricity:** Microscopic origin much less clear. Many different types, mechanisms → several different mechanism, types of multiferroics

**Type-I multiferroics:** Independent FE and magnetic subsystems
1) Perovskites: either magnetic, or ferroelectric; why?
2) “Geometric” multiferroics ($YMnO_3$)
3) Lone pairs ($Bi; Pb, ….$)
4) FE due to charge ordering

**Type-II multiferroics:** FE due to magnetic ordering
1) MF due to exchange striction
2) Spiral MF
3) Electronic mechanism
<table>
<thead>
<tr>
<th>material</th>
<th>$T_{FE}$ (K)</th>
<th>$T_{M}$ (K)</th>
<th>$P$ ($\mu$C cm$^{-2}$)</th>
</tr>
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<tr>
<td>BiFeO$_3$</td>
<td>1103</td>
<td>643</td>
<td>60 - 90</td>
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<tr>
<td>YMnO$_3$</td>
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<td>76</td>
<td>5.5</td>
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<td>HoMnO$_3$</td>
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<td>TbMnO$_3$</td>
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<td>41</td>
<td>0.06</td>
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<tr>
<td>TbMn$_2$O$_5$</td>
<td>38</td>
<td>43</td>
<td>0.04</td>
</tr>
<tr>
<td>Ni$_3$V$_2$O$_8$</td>
<td>6.3</td>
<td>9.1</td>
<td>0.01</td>
</tr>
</tbody>
</table>
**Type-I multiferroics:** Independent ferroelectricity and magnetism

- **Perovskites:** $d^0$ vs $d^n$

  Empirical rule: FE for perovskites with empty d-shell (BaTiO$_3$, PbZrO$_3$; KNbO$_3$) contain Ti$^{4+}$, Zr$^{4+}$; Nb$^{5+}$, Ta$^{5+}$; Mo$^{6+}$, W$^{6+}$, etc.

  Magnetism – partially filled d-shells, $d^n$, $n>0$

  **Why such mutual exclusion?**

  Not quite clear. Important what is the mechanism of FE in perovskites like BaTiO$_3$

  Classically: polarization catastrophe; Clausius-Mossotti relations, etc.

  Real microscopic reason: **chemical bonds**
Ti$^{4+}$: establishes \textit{covalent bond} with oxygens (which “donate” back the electrons), using empty d-levels

Better to have one strong bond with one oxygen that two weak ones with oxygens on the left and on the right

Two possible reasons:

d$^0$ configurations: only bonding orbitals are occupied

Other localized d-electrons break \textit{singlet} chemical bond by Hund’s rule pair-breaking (a la pair-breaking of Cooper pairs by magnetic impurities)
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\begin{center}
\begin{tikzpicture}
\draw[pink] (-1,0) -- (1,0) + (0,0.5) node[anchor=west] {O};
\draw[red] (0,0) -- (2,0) + (0,0.5) node[anchor=west] {Ti};
\draw[gray] (2,0) -- (4,0) + (0,0.5) node[anchor=west] {O};
\end{tikzpicture}
\end{center}

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“Geometric” multiferroics: hexagonal manganites RMnO$_3$

YMnO$_3$: $T_{FE}$~900 K; $T_N$~70 K

The origin (T. Palstra, N. Spaldin): tilting of MnO$_5$ trigonal bipiramids – a la tilting of MO$_6$ octahedra in the usual perovskites leading to orthorombic distortion.

In perovskites one AMO$_3$ one A-O distance becomes short, but no total dipole moment – dipole moments of neighbouring cells compensate.

In YMnO$_3$ – total dipole moment, between Y and O; Mn plays no role!
Crystal structure of YMnO$_3$

Ferroelectric distortion

Displacements from: centrosymmetric high temp to ferroelectric room temp

Van Aken, Palstra, Filipetti, Spaldin, Nature Materials 2004

B. Van Aken, A. Meetsma, T. Palstra
Lone pairs and ferroelectricity

$\text{Bi}^{3+}; \text{Pb}^{2+}$. Classically – large polarizability. Microscopically – easy orientation of the lone pairs

Many nonmagnetic ferroelectrics with $\text{Bi}^{3+}; \text{Pb}^{2+}$. – e.g. PZT $[\text{Pb(ZrTi)}\text{O}_3]$

Some magnetic:

Aurivillius phases: good ferroelectrics, layered systems with perovskite slabs/$\text{Bi}_2\text{O}_2$ layers ($\text{SrBi}_2\text{Nb}_2\text{O}_9; \text{SrBi}_4\text{Ti}_4\text{O}_{15}$, etc). Exist with magnetic ions, but not really studied.

$\text{PbVO}_3$ – a novel compound. Distortion so strong that probably impossible to reverse polarization – i.e. it is probably not ferroelectric, but rather pyroelectric
Ferroelectricity due to charge ordering

Bond- versus site-centred ordering and possible ferroelectricity in manganites

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Published online: 21 November 2004; doi: 10.1038/nmat1236

Transition metal oxides with a perovskite-type structure constitute a large group of compounds with interesting properties. Among them are materials such as the prototypical ferroelectric system BaTiO$_3$, colossal magnetoresistance manganites and the high-T$_c$ superconductors. Hundreds of these compounds are magnetic, and hundreds of others are ferroelectric, but these properties very seldom coexist. Compounds with an interdependence of magnetism and ferroelectricity could be very useful; they would open up a plethora of new applications, such as switching of magnetic memory elements by electric fields. Here, we report on a possible way to avoid this incompatibility, and show that in charge-ordered and orbital ordered perovskites it is possible to make use of the coupling between magnetic and charge ordering to obtain ferroelectric magnets. In particular, in manganites that are less than half doped there is a type of charge ordering that is intermediate between site-centred and bond-centred. Such a state breaks inversion symmetry and is predicted to be magnetic and ferroelectric.

Perovskites consist of corner-sharing O$_6$ octahedra with a transition metal ion in the centre. Almost all the ferroelectric perovskites contain non-magnetic transition metal ions with an empty d-shell (d$^0$ configuration); for example Ti$^+$, Nb$^{5+}$ and W$^{6+}$. Apparently the presence of the d$^0$ plays an important role in formation of a ferroelectric state. In all of these systems ferroelectricity originates from a shift of the transition metal ion from the centre of the O$_6$ octahedron. This way a stronger covalent bond with one (or three) instead of six weaker bonds with neighbouring oxygen atoms is formed.

The problem of why magnetism and ferroelectricity seem to avoid each other is a long-standing one. One of the clues lies in the tetragonal distortion which is present in all ferroelectric perovskites. This is due to the tetragonal distortion in the perovskite structure, which is due to the Jahn-Teller (JT) effect. The JT effect is a result of the strong electron-lattice coupling, which leads to a distortion of the lattice to relieve the electronic instability. The JT effect is strong in materials with a low symmetry, such as the manganites. This is the reason why the manganites are often used as a model system for studying the interplay between magnetism and ferroelectricity.

In conclusion, we have demonstrated a possible way to avoid the incompatibility between magnetism and ferroelectricity in perovskites. This approach could lead to the development of new materials with novel properties.
- Charge density waves:
  - manganites
  - magnetite Fe₃O₄ (Verwey transition at 118K)

- Bond-centered charge density waves vs site centered charge density waves,

![Diagram showing SCDW and BCDW](image)

**SCDW**

**BCDW (Jener polarons)**

(Daoud-Aladine et al., PRL 2002)

**Id:**

![Diagram showing CO and Peierls state](image)

**CO**

**Peierls state**
Systems with ferroelectricity due to charge ordering

Some quasi-one-dimensional organic materials (Nad’, Brazovskii & Monceau; Tokura)

**Fe3O4**: ferroelectric below Verwey transition at 119 K! Also ferrimagnetic with large magnetization and high Tc

**LuFe2O4**?

**RNiO3**?
**Type-II multiferroics**: Ferroelectricity due to magnetic ordering

- Magnetostriiction mechanism
Ca₃Co₂₋ₓMnₓO₆

Mn⁴⁺  Co²⁺

Spiral mechanism (cycloidal spiral)

\[ P = c(Q \times e), \quad e \sim S_1 \times S_2 \]

\[ P_{ij} = c' r_{ij} \times (S_i \times S_j) \]

(Mostovoy)

(Katsura, Nagaosa and Balatsky)
Magnetic ordering in TbMnO$_3$

$28K < T < 41K$

Sinusoidal SDW spins along b axis

$T < 28K$

Helicoidal SDW spins rotating in bc plane

M. Kenzelmann et al (2005)
Ferroelectricity in a proper screw

Sometimes also proper screw structures can give ferroelectricity.
They should not have 2-fold rotation axis perpendicular to the helix.

Special class of systems: ferroaxial crystals (L.Chapon, P.Radaelli).
Crystals with inversion symmetry but existing in two inequivalent modifications, which are mirror image of one another.

Characterised by pseudovector (axial vector) \( \mathbf{A} \).
Proper screw may be characterised by chirality \( \kappa = r_{12} [\mathbf{S}_1 \times \mathbf{S}_2] \).
Then one can have polarization \( \mathbf{P} = \kappa \mathbf{A} \) (or have invariant \( (\kappa \mathbf{A} \mathbf{P}) \)).

Examples: \( \text{AgCrO}_2, \text{CaMn}_7\text{O}_{12}, \text{RbFe(MoO}_4\text{)}_2 \)
Electronic Orbital Currents and Polarization in frustrated Mott Insulators

L.N. Bulaevskii, C.D. Batista, M. Mostovoy and D. Khomskii

\[ H = - \sum_{ij\sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + \frac{U}{2} \sum_i (n_i - 1)^2, \]

Standard paradigm: for U>>t and one electron per site electrons are localized on sites. All charge degrees of freedom are frozen out; only spin degrees of freedom remain in the ground and lowest excited states

\[ H_s = \frac{4t^2}{U} (\vec{S}_1 \cdot \vec{S}_2 - 1/4). \]
Not the full truth!

For certain spin configurations there exist in the ground state of strong Mott insulators **spontaneous electric currents** (and corresponding orbital moments)!

For some other spin textures there may exist a **spontaneous charge redistribution**, so that $<n_i>$ is not 1! This, in particular, can lead to the appearance of a spontaneous **electric polarization** (a purely **electronic mechanism of multiferroic behaviour**)

These phenomena, in particular, appear in frustrated systems, with **scalar chirality** playing important role
Spin systems: often complicated spin structures, especially in frustrated systems – e.g. those containing triangles as building blocks

- **Isolated triangles** (trinuclear clusters) - e.g. in some magnetic molecules (V15, …)
- Solids with isolated triangles (La$_4$Cu$_3$MoO$_{12}$)
- Triangular lattices
- Kagome
- Pyrochlore
Triangular lattices:

$Na_xCoO_2, LiVO_2, CuFeO_2, LiNiO_2, NiGa_2S_4, \ldots$
Kagome:

\[ \text{ZnCu}_3(\text{OH})_6\text{Cl}_2 \ (\text{herbertsmithite}) \]
The Cathedral San Giusto, Trieste, 6-14 century
The B-site pyrochlore lattice: geometrically frustrated for AF

Spinels, pyrochlores:
Often complicated ground states; sometimes $\langle \vec{S}_i \rangle = 0$ spin liquids

Some structures, besides $\langle \vec{S}_i \rangle$, are characterized by:

Vector chirality

$$\begin{bmatrix} \vec{S}_i \times \vec{S}_j \end{bmatrix}$$

Scalar chirality

$$\chi_{123} = \vec{S}_1 \left[ \vec{S}_2 \times \vec{S}_3 \right]$$

- solid angle

$\chi$ may be + or - :
But what is the scalar chirality physically?
What does it couple to?
How to measure it?

Breaks time-reversal-invariance $T$ and inversion $P$ - like currents!

$\chi_{123} \neq 0$ means spontaneous circular electric current $j_{123} \neq 0$ and orbital moment $L_{123} \neq 0$

$L_{123} \propto j_{123} \propto \chi_{123}$

Couples to magnetic field:
$-\vec{L} \vec{H} \sim -\chi H$
Spin current operator and scalar spin chirality

- Current operator for Hubbard Hamiltonian on bond $ij$:

$$\vec{I}_{ij} = \frac{i e t_{ij} \vec{r}_{ij}}{\hbar r_{ij}} \sum_{\sigma} \left( c_{i\sigma}^+ c_{j\sigma} - c_{j\sigma}^+ c_{i\sigma} \right).$$

- Projected current operator: odd # of spin operators, scalar in spin space. For smallest loop, triangle,

$$\vec{I}_{S,12}(3) = \frac{\vec{r}_{ij}}{r_{ij}} \frac{24 e t_{12} t_{23} t_{31}}{\hbar U^2} [\vec{S}_1 \times \vec{S}_2] \vec{S}_3.$$ 

- Current via bond 23

$$I_{S,23} = I_{S,23}(1) + I_{S,23}(4).$$

- On bipartite nn lattice $I_S$ is absent.
Spin-dependent electronic polarization

Charge operator on site $i$:

$$Q_i = e \sum_{\sigma} c_{i\sigma}^+ c_{i\sigma}.$$

Projected charge operator

$$n_{S,i} = Pe^S n_i e^{-S} P,$$

$$\langle n_1 \rangle = 1 + \delta n_1 = 1 - 8 \left( \frac{t}{U} \right)^3 \left[ S_1 (S_2 + S_3) - 2 S_2 S_3 \right].$$

Polarization on triangle

$$\vec{P}_{123} = e \sum_{i=1,2,3} n_{S,i} \vec{r}_i,$$

$$\sum_i n_{S,i} = 3.$$

Charge on site $i$ is sum over triangles at site $i$. 
Electronic polarization on triangle

\[ \langle n_1 \rangle = 1 + \delta n_1 = 1 - 8 \left( \frac{t}{U} \right)^3 [S_1(S_2 + S_3) - 2S_2S_3] \]

or

Purely electronic mechanism of multiferroic behavior!
Diamond chain (azurite $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$)

- Spin singlet

Saw-tooth (or delta-) chain

- Will develop S-CDW

Net polarization
Figure 1. (a) Structure of euchroite, (b) schematic view of the delta chain.
ESR: magnetic field (-HM) causes transitions

\[ |1/2, \chi\rangle \rightarrow |-1/2, \chi\rangle, \text{ or } |-1/2, \chi\rangle \rightarrow |1/2, \chi\rangle \]

Here: electric field (-Ed) has nondiagonal matrix elements in \( \chi \):

\[ \langle \chi = + |d| \chi = - \rangle \neq 0 \]

\[ S^z, + \leftrightarrow S^z, - \]

-- ESR caused by electric field E!
Chirality as a qubit?

Triangle: S=1/2, chirality (or pseudosin T) = ½

Can one use chirality instead of spin for quantum computation etc, as a qubit instead of spin?

We can control it by magnetic field (chirality = current = orbital moment ) and by electric field


Magnetoelectrics as methamaterials

(systems with negative refraction index)
Multiferroics as metamaterials

LHM: negative $\varepsilon(\omega) < 0$ and $\mu(\omega) < 0$

Maxwell Eqs: $\nabla \times \vec{E} = \frac{i\omega}{c} \vec{B}$
$\nabla \times \vec{H} = -\frac{i\omega}{c} \vec{D}$

$\nabla \cdot \vec{D} = 0$  $\nabla \cdot \vec{B} = 0$  $\vec{D} = \varepsilon(\omega)\vec{E}$,  $\vec{B} = \mu(\omega)\vec{H}$,

$n^2 = \varepsilon\mu > 0$

Vectors $\vec{k}$, $\vec{E}$, $\vec{H}$

form a left-handed orthogonal set (LHM) (V. Veselago, 1967).
Monopoles and dipoles in spin ice

Pyrochlore: Two interpenetrating metal sublattices

\[ \text{Ho}_2 \text{Ti}_2 \text{O}_7 \]
pyrochlore $R_2Ti_2O_7$ \cdot geometrical spin frustration

$R=\text{Ho}$
Ferromagnetic interaction, Ising spin (spin ice)

$R=\text{Gd}$
Antiferromagnetic interaction, Heisenberg spin

$2\text{in} 2\text{out}$

$H \parallel [001]$, $>H_c$

$H=0$
Excitations creating magnetic monopole (Castelnovo, Moessner and Sondhi)

\[ H = 0 \]

\[ H \parallel [111] > H_c \]

\[ H \parallel [001] > H_c \]

M J P Gingras Science 2009;326:375-376
2-in/2-out: net magnetic charge inside tetrahedron zero

3-in/1-out: net magnetic charge inside tetrahedron ≠ 0
- monopole or antimonopole
$H \parallel [111], > H_c$

Monopoles/antimonopoles at every tetrahedron, staggered
Fig. 1. Phase diagram of Dy$_2$Ti$_2$O$_7$ in a [111] magnetic field, determined by magnetization and specific heat measurements. The dashed line
Dipoles on tetrahedra:

4-in or 4-out: \( d=0 \)

2-in/2-out (spin ice): \( d=0 \)

3-in/1-out or 1-in/3-out (monopoles/antimonopoles): \( d \neq 0 \)

\[
\langle n_1 \rangle = 1 + \delta n_1 = 1 - 8 \left( \frac{t}{U} \right)^3 \left[ S_1 (S_2 + S_3) - 2S_2 S_3 \right]
\]

For 4-in state: from the condition \( S_1 + S_2 + S_3 + S_4 = 0 \) \( \delta n_1 = 0 \). Change of \( S_1 \rightarrow -S_1 \) (3-in/1-out, monopole) gives nonzero charge redistribution and \( d \neq 0 \).

Charge redistribution and dipoles are even functions of \( S \); inversion of all spins does not change direction of a dipole: Direction of dipoles on monopoles and antimonopoles is the same: e.g. from the center of tetrahedron to a “special” spin.
In strong field $\mathbf{H} \parallel [111]$ there is a staggered $\mu/\bar{\mu}$, and simultaneously staggered dipoles – i.e. it is an **antiferroelectric**

Estimates: $\varepsilon = dE = eu(Å)E(V/cm)$

for $u \approx 0.01Å$ and $E \approx 10^5 V/cm$  $\varepsilon \approx 10^{-5} eV \approx 0.1K$
Dipoles on monopoles, possible consequences:

● “Electric” activity of monopoles; contribution to dielectric constant $\varepsilon(\omega)$

● External **electric** field:
  Decreases excitation energy of certain monopoles
  $\omega = \omega_0 - dE$
  Crude estimate: in the field $E \sim 10^5$ V/cm energy shift $\sim 0.1$ K

● Inhomogeneous electric field (tip): will attract some monopoles/dipoles and repel other

● In the magnetic field $H \parallel [001]$ $E$ will promote monopoles, and decrease magnetization $M$, and decrease $T_c$

● In the field $H \parallel [111]$ – staggered Ising-like dipoles; in $E_\perp$?
Inhomogeneous electric field
Electric dipoles at domain walls

Was already observed for Neel domain walls in ferromagnets (cf. spiral multiferroics):

Bloch domain wall: 

Neel domain wall:

Cut tip
Fig. 2 The effect of electric field in the vicinity of electrode (1) on magnetic domain wall (2) in the films of ferrite garnets: a) initial state b) at the voltage of +1500 V applied
Spiral structures in metal monolayers

Chiral magnetic order at surfaces driven by inversion asymmetry

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Atomic-Scale Spin Spiral with a Unique Rotational Sense: Mn Monolayer on W(001)

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(Received 15 April 2008; published 7 July 2008)

Using spin-polarized scanning tunneling microscopy we show that the magnetic order of 1 monolayer Mn on W(001) is a spin spiral propagating along ⟨110⟩ crystallographic directions. The spiral arises on the atomic scale with a period of about 2.2 nm, equivalent to only 10 atomic rows. Ab initio calculations identify the spin spiral as a left-handed cycloid stabilized by the Dzyaloshinskii-Moriya interaction, imposed by spin-orbit coupling, in the presence of softened ferromagnetic exchange coupling. Monte Carlo simulations explain the formation of a nanoscale labyrinth pattern, originating from the coexistence of the two possible rotational domains, that is intrinsic to the system.
rotation direction of spin spiral

6 out of 6 independent islands: same rotational sense → DM-driven spin spiral
Cycloidal SDW

\[ \mathbf{M} = A_1 \mathbf{e}_1 \cos Qx + A_2 \mathbf{e}_2 \sin Qx + A_3 \mathbf{e}_3 \]

\[ \mathbf{P} \propto [\mathbf{e}_3 \times \mathbf{Q}] \]

Katsura, Nagaosa and Balatsky, 2005
Mostovoy 2006
Simple explanation: at the surface there is a drop of a potential (work function, double layer)
I.e. there is an electric field $E$, or polarization $P$ perpendicular to the surface
By the relation

$$\overline{P} \propto [e_3 \times Q]$$

there will appear magnetic spiral with certain sense of rotation, determined by $P$
Electric dipole carried by the usual spin wave


**FIG. 5:** How polarization emerges in a spin wave (magnon). (a) The classical picture of a spin wave in a ferromagnet: the spin (red arrow) precesses about a fixed axis (blue). The deviation is measured by the black arrows. (b) According to Eq. (1), as a spin-wave packet propagates along \( \vec{Q} \), it will also carry an electric dipole moment. (Illustration: Alan Stonebraker)
Monopoles in magnetoelectrics?

ARTICLE
Received 20 May 2014 | Accepted 24 Jul 2014 | Published 1 Sep 2014

Magnetic monopoles and unusual dynamics of magnetoelectrics

D.I. Khomskii

NATURE COMMUNICATIONS | 5:4793 | DOI: 10.1038/ncomms5793 | www.nature.com/naturecommunications
Magnetic monopoles in topological insulators

Charge close to a surface of ME material: \[ M_i = \alpha_{ij} E_j \]
Charge inside of ME material: \( M_i = \alpha_{ij} E_j \), \( H = 4\pi M \)

Let \( \alpha_{ij} = \alpha \delta_{ij} \), diagonal: magnetic field outside of the charge looks like a field of a magnetic monopole \( \mu = 4\pi \alpha e \)

Moving electron moving monopole.

Electron in a magnetic field: force \( F = \mu H = 4\pi \alpha e H \)

(But one can also consider it as an action of the electric field created in magnetoelectric material on the electric charge: \( E = 4\pi \alpha H \), \( F = Ee = 4\pi \alpha e H \))
Other possible effects? (how to find, to measure such monopoles)

"Electric Hall effect": if electric charge e moving in $\mathbf{H}$ gives a Hall effect, a monopole moving in electric field will do the same.

But one can also explain this effect as the usual Hall effect in an effective magnetic field $\mathbf{B} \sim \alpha \mathbf{E}$.
Magnetic vortices as magnetoelectrics

Superexchange-Driven Magnetoelectricity in Magnetic Vortices

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FIG. 1 (color online).  (a) A magnetic vortex carrying a monopole moment. The thin solid arrows indicate the spin orientation, while the thick open arrows show the local polarization vector. (b) A magnetic field applied to the vortex shown in (a) induces a net polarization along the field direction. (c) A magnetic vortex with a toroidal moment. (d) A magnetic field applied to (c) induces an electric polarization perpendicular to the field.
Skyrmions in magnetic crystals

“Toroidal” skyrmion

Should give magnetoelectric effect with $\mathbf{P} \perp \mathbf{H}$
Skyrmion lattice (e.g. in MnSi) – C. Pfleiderer, A. Rosch
“Radial” skyrmion

Should give magnetoelastic effect with $\mathbf{P} \parallel \mathbf{H}$
Conclusions

- There is strong interplay of electric and magnetic properties in solids, having different forms.
- These are: magnetoelectrics; multiferroics.
- Multiferroics can be metamaterials at certain frequencies.

There should be an electric dipole at each magnetic monopole in spin ice – with different consequences.

Analogy: electrons have electric charge and spin/magnetic dipole. Monopoles in spin ice have magnetic charge and electric dipole.

- Ordinary spin waves in ferromagnets should carry dipole moment.
- Different magnetic textures (domain walls, magnetic vortices) can either carry dipole moment, or can be magnetoelectric.
- Electric charges in magnetoelectric should be accompanied by magnetic monopoles.
"The Florida Law of Original Prognostication maps the shifting tide of expectations in materials science."
Ti$^{4+}$: establishes *covalent bond* with oxygens (which “donate” back the electrons), using empty d-levels

![Diagram of Ti-O bonding](image)

Better to have one strong bond with one oxygen that two weak ones with oxygens on the left and on the right

Two possible reasons:

d$^0$ configurations: only bonding orbitals are occupied

![Energy level diagram](image)

Other localized d-electrons break *singlet* chemical bond by Hund’s rule pair-breaking (a la pair-breaking of Cooper pairs by magnetic impurities)
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Phase diagram of manganites near $x=0.5$

Electron density $n_e = 1-x$

- **FM**: ferromagnetic phase
- **G**: antiferromagnetic Neel state
- **A**: F planes coupled AFM
- **C**: F chains coupled AFM
- **CE**: CE-phase
- **120**: Jaffet-Kittel state
- **FE**: Ferroelectric phase
Charge ordering

$2\text{Ni}^{3+} \rightarrow \text{Ni}^{3+\delta} + \text{Ni}^{3-\delta}$ ($\delta = 0.35$)

$\text{Ni}(1) = 1.4(1) \mu_B$

$\text{Ni}(2) = 0.7(1) \mu_B$

neutron diffraction, J.A. Alonso et al.
PRL 82, 3871 (99)
Cycloidal SDW

\[ \mathbf{M} = A_1 \mathbf{e}_1 \cos Qx + A_2 \mathbf{e}_2 \sin Qx + A_3 \mathbf{e}_3 \]

\[ \mathbf{P} \propto [\mathbf{e}_3 \times \mathbf{Q}] \]

Katsura, Nagaosa and Balatsky, 2005
Mostovoy 2006
Effects of Dzyaloshinskii-Moriya interaction

\[ E_{DM} = D_{12} \cdot [S_1 \times S_2] \]

\[ D_{12} \propto \lambda x \times \hat{r}_{12} \]

Weak ferromagnetism

Weak ferroelectricity

Spin systems: often complicated spin structures, especially in \textit{frustrated systems} – e.g. those containing \textit{triangles} as building blocks.

- **Isolated triangles** (trinuclear clusters) - e.g. in some magnetic molecules ($V_{15}$, …)
- Solids with \textit{isolated triangles} ($La_4Cu_3MoO_{12}$)
- Triangular lattices
- **Kagome**
- **Pyrochlore**
Scalar chirality $\chi$ is often invoked in different situations:

- Anyon superconductivity
- Berry-phase mechanism of anomalous Hall effect
- New universality classes of spin-liquids
- Chiral spin glasses

**Chirality in frustrated systems:** Kagome

- a) Uniform chirality ($q=0$)
- b) Staggered chirality ($\sqrt{3} \times \sqrt{3}$)
Boundary and persistent current

Boundary current in gaped 2d insulator

$\chi = \text{const}$
Chirality as a qubit?

Triangle: $S=1/2$, chirality (or pseudosin $T$) = $\frac{1}{2}$

Can one use chirality instead of spin for quantum computation etc, as a qubit instead of spin?

We can control it by magnetic field (chirality = current = orbital moment) and by electric field

Georgeot, Mila, arXiv 26 February 2009
Dipoles are also created by lattice distortions (striction); the expression for polarization/dipole is the same, \( D \sim P \sim S_1(S_2 - S_3) - 2S_2S_3 \) (M. Mostovoy)
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Random ice rule spins (no external magnetic field)
Monopoles/antimonopoles with electric dipoles
In general directions of electric dipoles are “random” – in any of [111] directions
Why NR is interesting: Focusing by a slab.
\[ \omega_\pm^2 = \frac{\omega_0^2 + \Omega^2}{2} \pm \sqrt{\left(\frac{\omega_0^2 - \Omega^2}{2}\right)^2 + 1^2} \approx \begin{cases} \omega_0^2 + \frac{1^2}{\omega_0^2 - \Omega^2} \\ \Omega^2 - \frac{1^2}{\omega_0^2 - \Omega^2} \end{cases} \]

(If \( \omega_0^2 > \Omega^2 \))

For \( \omega \geq \omega_+ \) \( \omega \geq \omega_- \) both \( \varepsilon \times \mu < 0 \), and \( \varepsilon < 0 \)
Monopole with the string!
Visualization of skyrmion crystal

(Y. Tokura et al.)