

Magnetism

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Optical Condensed Matter Physics

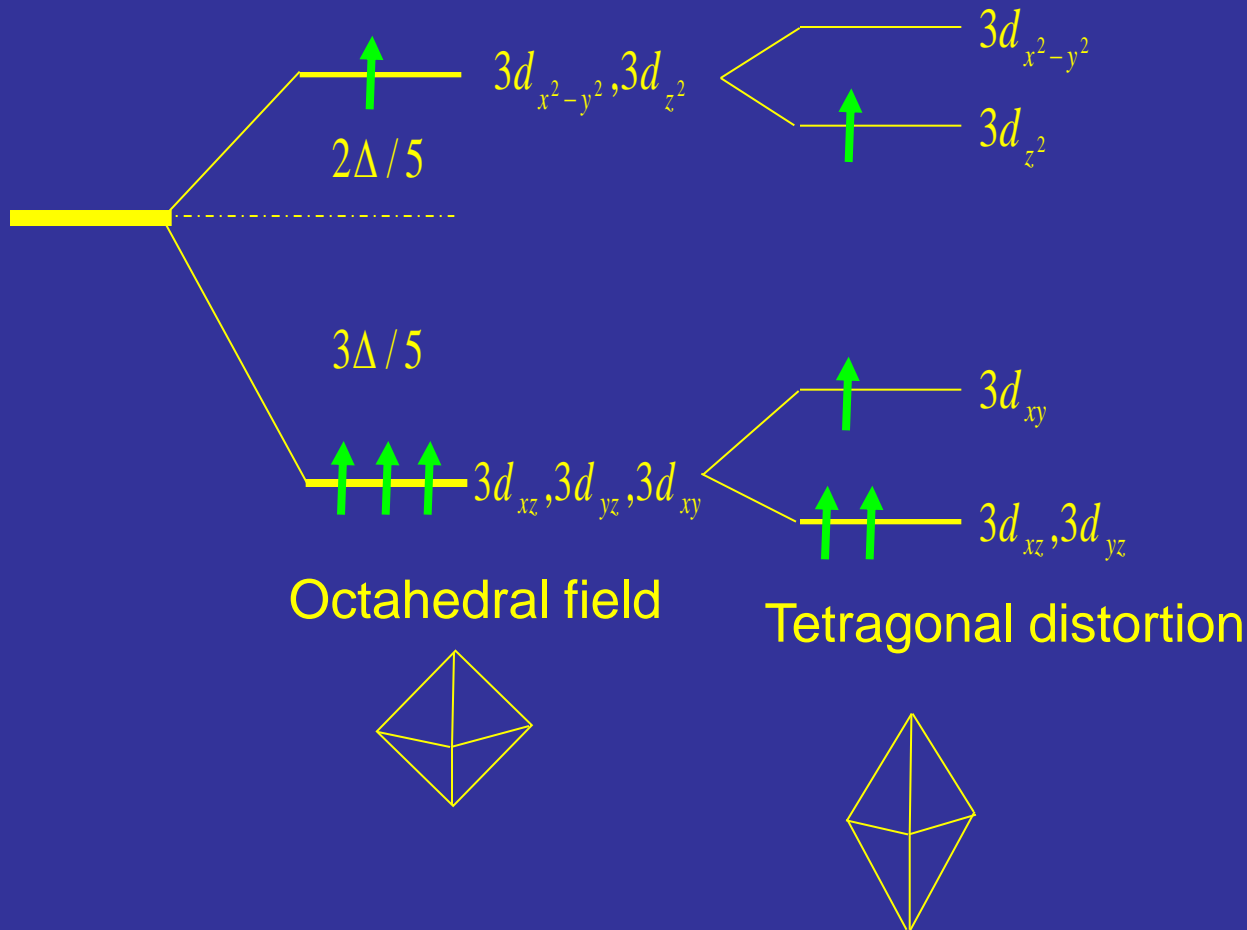
Last time

- Crystal fields
- d,f electrons
- angular momentum quenching
- p-d interactions, splitting of levels
- Spin peierls
- Jahn Teller
- Charge, orbital, spin ordering

Today

Last time	Introduction, environment	Ch.1; 2.1-2.5; 8.9; 3.1
Today	Environment, interactions	3.1; Ch.4; 7.1-7.7

Jahn Teller distortion



Mn³⁺ : 3d⁴

Energy gain due to lowering e_g orbital

Cost: elastic energy

Strong e-p coupling

Does not work for Mn⁴⁺

Jahn Teller effect

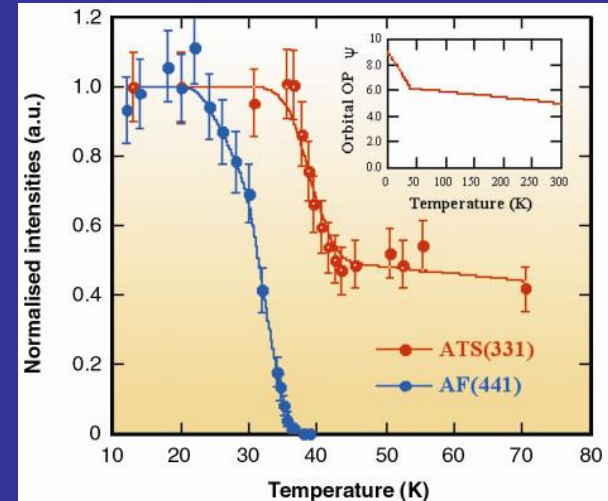
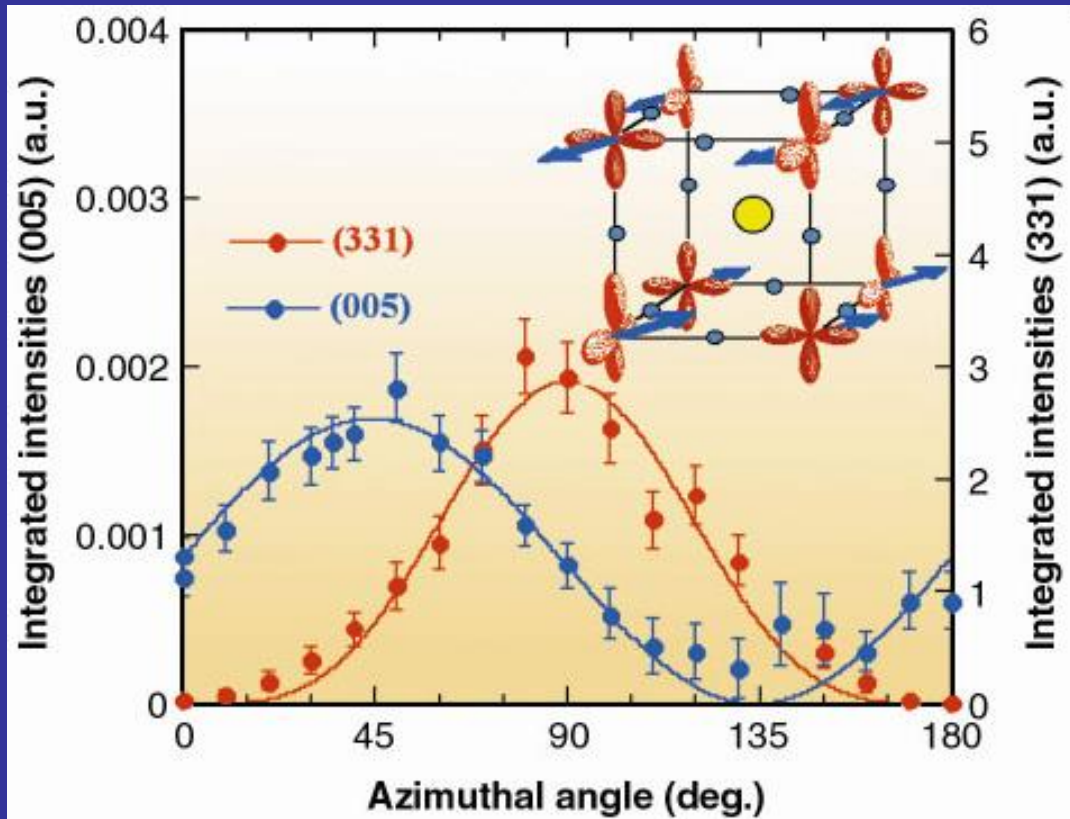
- Dynamic
Fluctuations x,y,z distortions (e.g. cubic perovskites)
- Cooperative
Lattice mediated

LaMnO₃ : T > 800 K Cubic, below that tetragonal

KCuF₃ : Orbital ordering (z²-x² and z²-y² orbitals)

Spin and Orbital ordering

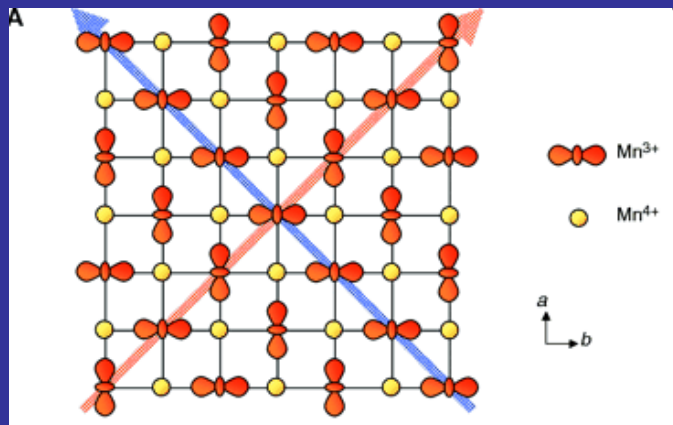
KCuF₃ : Orbital ordering (z^2-x^2 and z^2-y^2 orbitals)



Murakami et al. PRL 1998

Charge and Orbital order

Charge, Orbital, Spin order in $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$



folk.uio.no/ravi

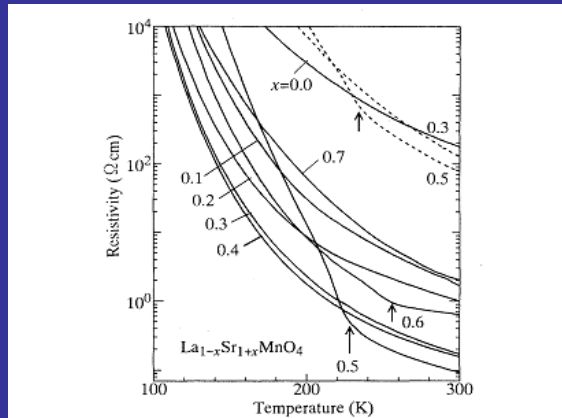


FIG. 1. Temperature dependence of resistivity (ρ) for single crystals of $\text{La}_{1-x}\text{Sr}_{1+x}\text{MnO}_4$ with various hole concentrations (x). Solid and broken curves stand for the in-plane (ρ_{ab}) and the out-of-plane (ρ_c) components, respectively. A steep increase in ρ is observed at a specific temperature (T_V) for $x=0.5$ and 0.6 , as indicated by upward arrows.

Moritomo et al. PRB 1995

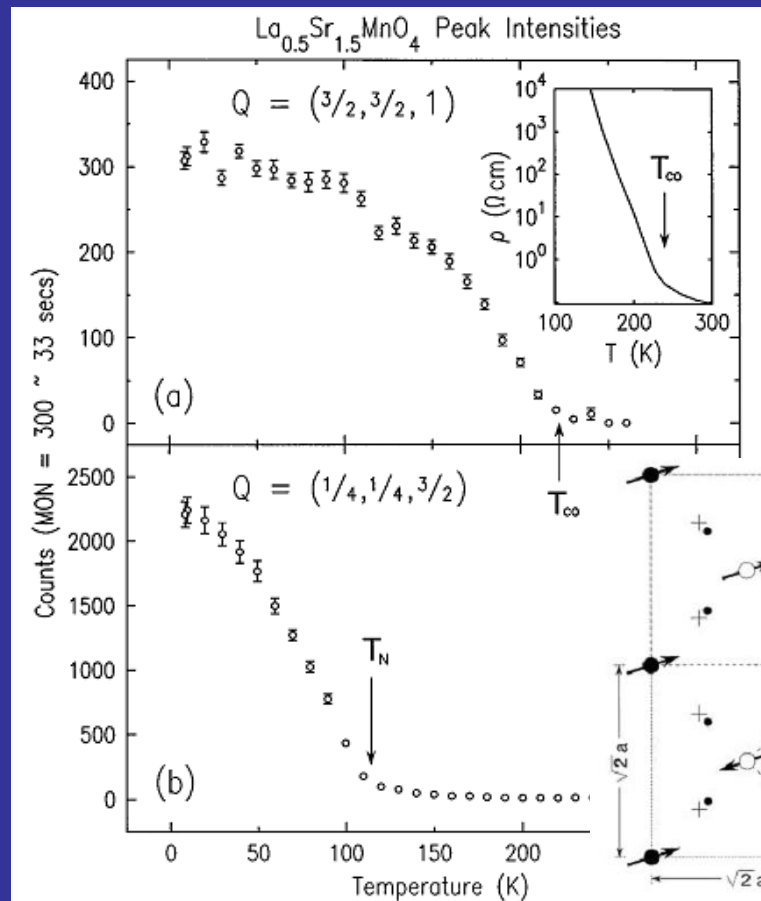


FIG. 4. Temperature dependence of the (a) charge and (b) magnetic order. Inset in (a): Resistivity vs T .

Sternlieb et al. PRL 1996

Mn^{3+} : $3d^4$ ($t_{2g}^3 e_g^1$, $S=2$)

Mn^{4+} : $3d^5$ (t_{2g}^3 , $S=3/2$)

Interactions

Interactions

- Dipole – Dipole
- Direct exchange (H_2 molecule)
- Indirect exchange
- Double exchange
- Anisotropic exchange
- Rudeman Kittel Kasuya Yoshida (RKKY)
- Stoner (“spontaneous Pauli”)

- Ch. 4 & 7.2,7.3,7.7

Dipole-dipole interaction

Dipole-dipole interaction is an anisotropic interaction

$$E = \frac{\mu_0}{4\pi} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \vec{e}_{12})(\vec{\mu}_2 \cdot \vec{e}_{12})}{r_{12}^3}$$

$$E \approx 10^{-23} \text{ J} \sim 1 \text{ K} \text{ for } r = 2 \text{ \AA} \text{ and } \mu = \mu_B$$

In real materials: $T_c \sim 10^2 - 10^3 \text{ K} !!$

→ Dipole-dipole interaction hardly ever dominates

Reminder H_2 molecule

- LCAO gives wrong solution (e.g. triplet ground state)
- Correlated picture (Heitler-London approach) is better
 - Starting point: two electron orbitals $|\phi_a(1)\phi_b(2)\rangle$ and $|\phi_a(2)\phi_b(1)\rangle$

– Wavefunctions

$$\Psi_S = \frac{1}{\sqrt{2}} [\phi_a(1)\phi_b(2) + \phi_a(2)\phi_b(1)]\chi_S$$

$$\Psi_T = \frac{1}{\sqrt{2}} [\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)]\chi_T$$

– Spin parts:

$$\chi_S = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\chi_T = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases}$$

H_2 molecule

- Singlet ground state
- Exchange energy: Pauli + Coulomb

$$H = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + V_H(1) + V_H(2) + V_C(1,2)$$

$$V_C(1,2) = \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|R_1 - R_2|} - \frac{e^2}{|r_1 - R_2|} - \frac{e^2}{|r_2 - R_1|}$$

$$E_s - E_t = 2 \langle \phi_a(1)\phi_b(2) | V_C | \phi_a(2)\phi_b(1) \rangle$$

$$H = -2J \vec{S}_1 \cdot \vec{S}_2 = \begin{cases} -2J \cdot -\frac{3}{4} = \frac{3}{2}J & \text{for the spin singlet} \\ -2J \cdot \frac{1}{4} = -\frac{1}{2}J & \text{for the spin triplet} \end{cases}$$

Exchange interaction

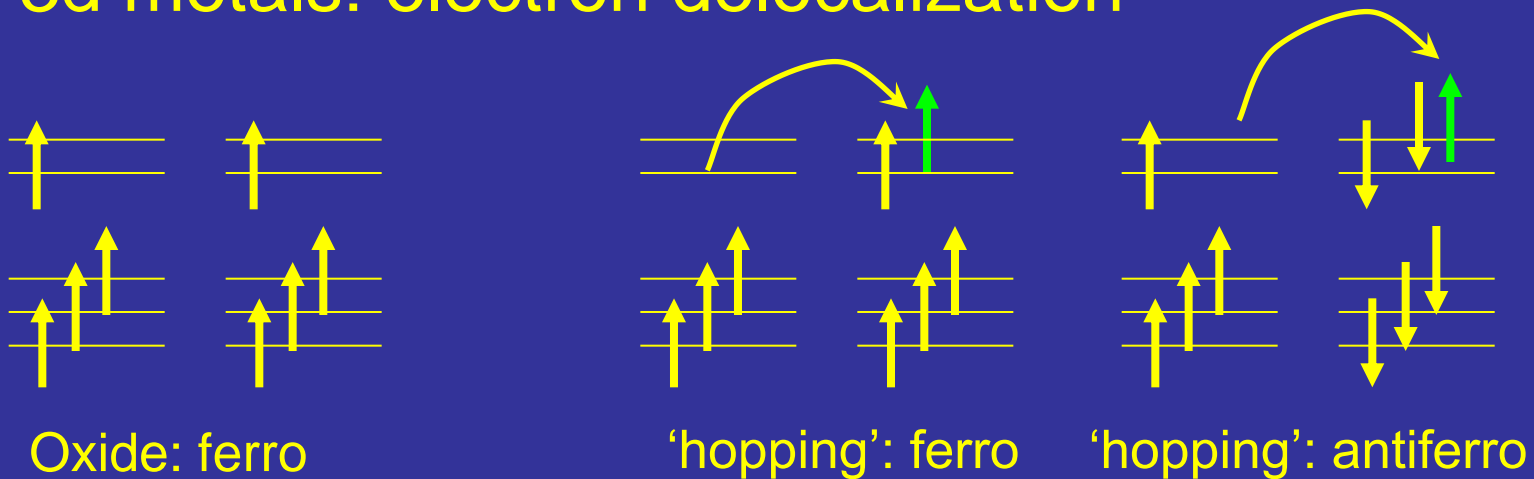
- Heisenberg Hamiltonian

$$H = -2 \cdot \sum'_{i,j} J_{i,j} S_i \cdot S_j$$

- $J > 0$: Ferro
- $J < 0$: Antiferro

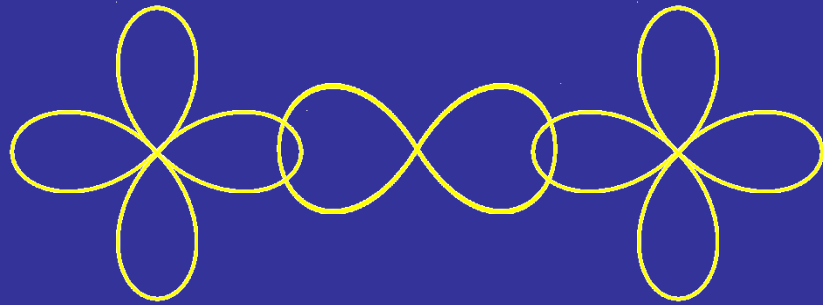
Direct exchange

- Need direct wave function overlap
 - Often ferromagnetic
 - Small in 4f, 5f elements
 - Can be important in 3d oxides (but see indirect!)
 - In 3d metals: electron delocalization

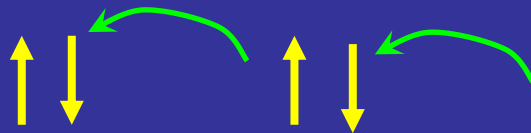


- Relatively small
- Depends on orbital occupation and geometry

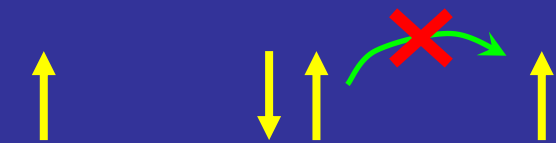
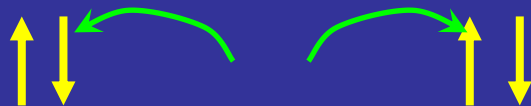
Indirect exchange



Ground state antiferro



'2*hopping'



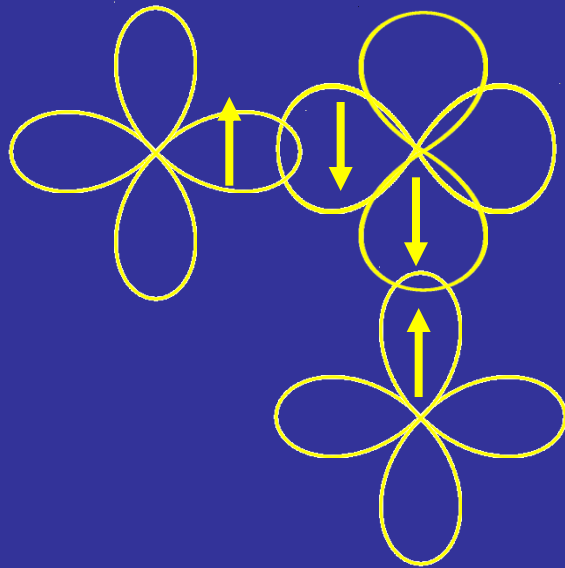
Pauli forbidden

Hopping →
delocalization →
energy gain

Energy: 2 double hops = $(2t)^2$; cost=U
→ $J \sim -4t^2/U$

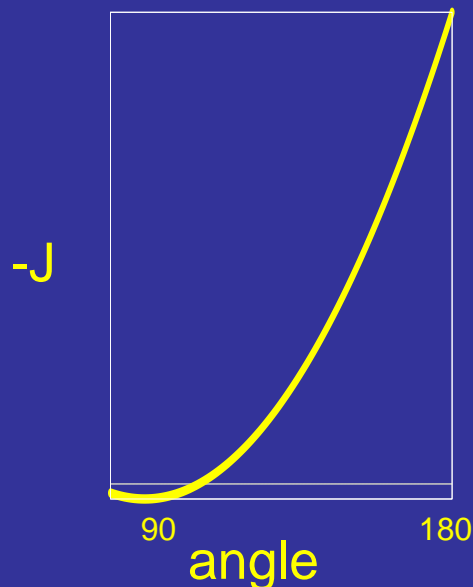
Examples: High T_c 's; MnO; MnF_2

Indirect exchange



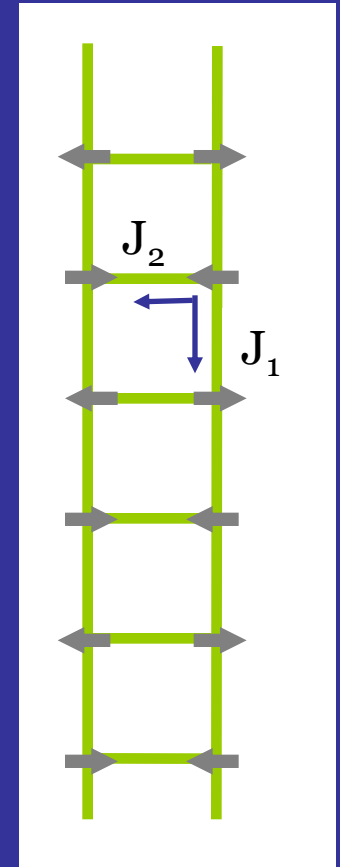
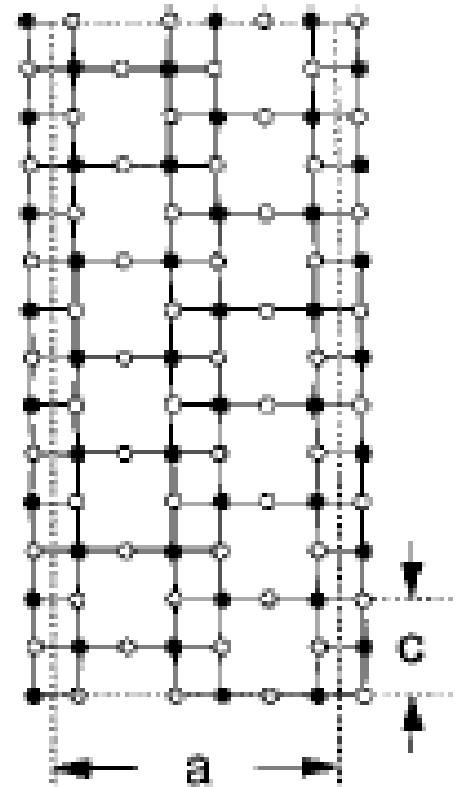
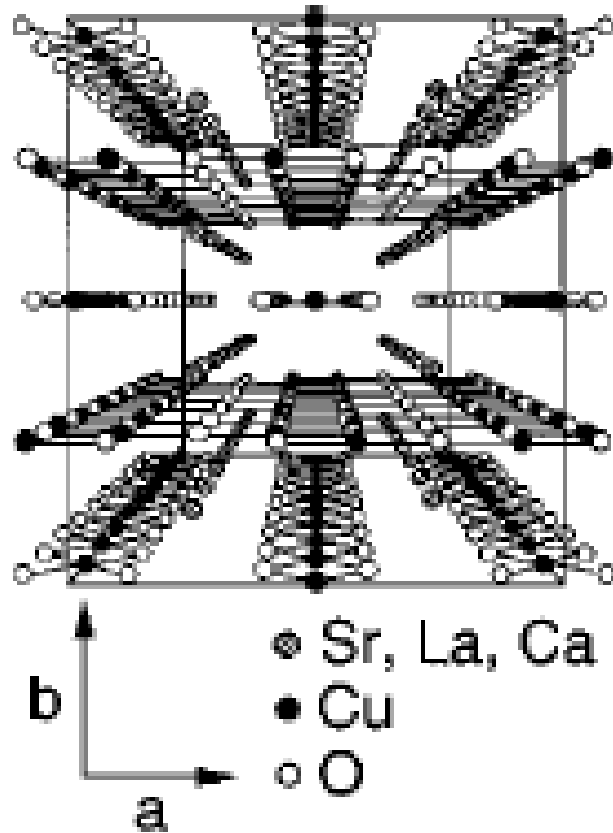
Hopping \rightarrow delocalization \rightarrow energy gain
Energy: $J \sim +4t^2/U$

Examples: High T_c 's; MnO; MnF₂;
telephone number compound



Relatively strong (depends on U)
Usually AF (F when not same 3d, e.g. d^3-d^5)
Strongly dependent on angle of bonding
at 180° strongly AF
at zero weakly F
(goodenough kanamouri rules)

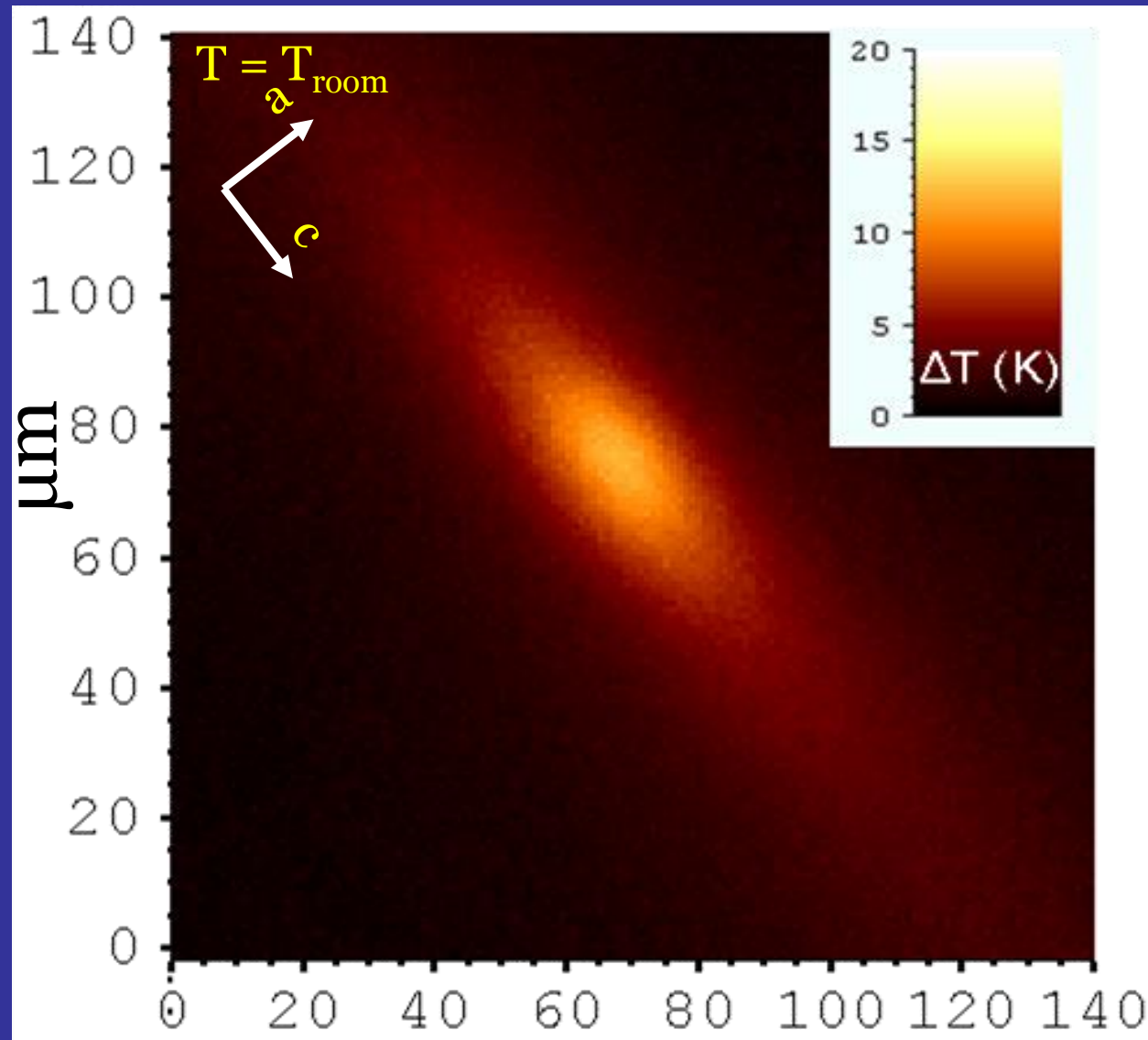
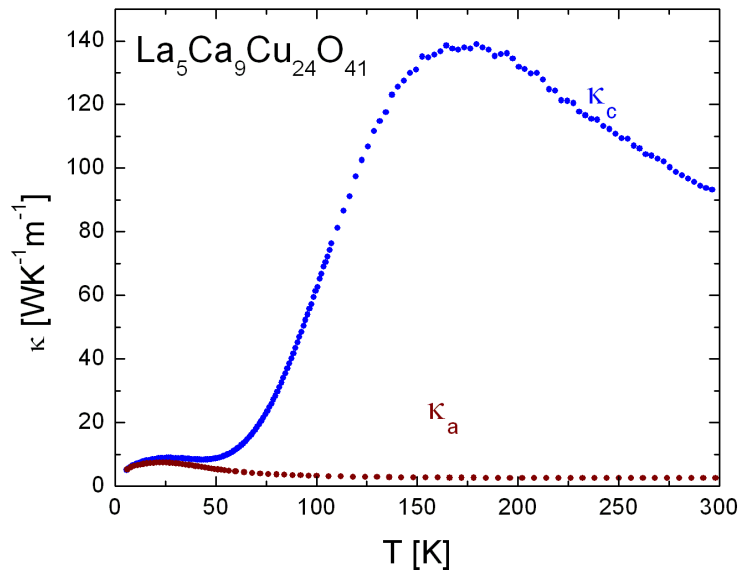
$(\text{Sr,La,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$



$J_1 = 130 \text{ meV}$
 $J_2 = 70 \text{ meV}$
 $\Delta = 32 \text{ meV}$

Eccleston *et al.*, PRL **81**, 1702 (1998)

$La_9Ca_5Cu_{24}O_{41}$



Double exchange

- Mixed valence
- Usually ferro metal
- Relatively strong
- $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($\text{Mn}^{3+}/\text{Mn}^{4+}$)
- Fe_3O_4 (AB_2O_4 , $\text{Fe}^{2+}/\text{Fe}^{3+}$)

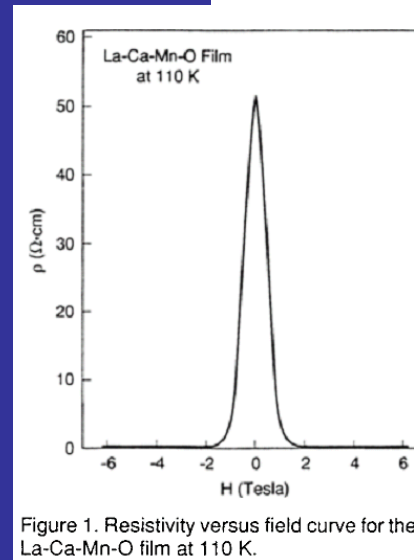
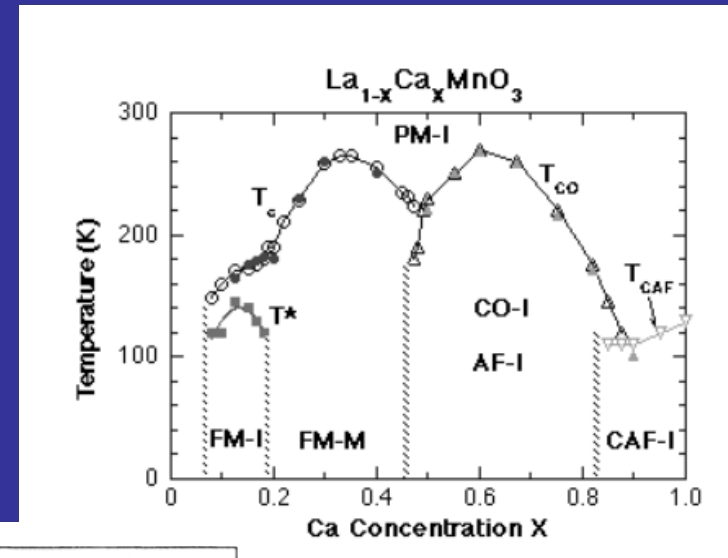
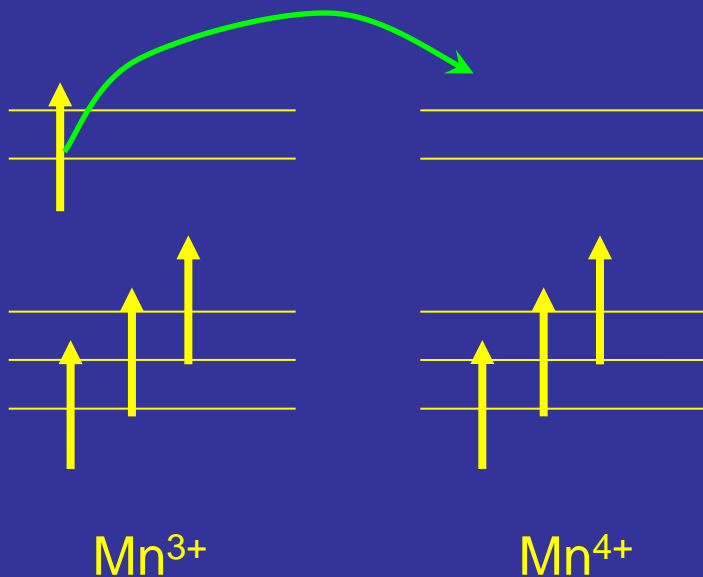


Figure 1. Resistivity versus field curve for the La-Ca-Mn-O film at 110 K.

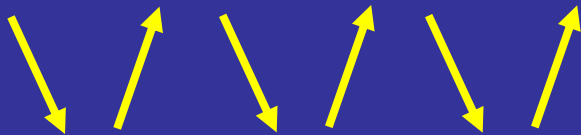
PM-I paramagnetic insulator
 FM-M ferromagnetic metal
 FM-I ferromagnetic insulator
 CO-I charge-ordered insulator
 CAF-I canted antiferromagnetic insulator

Fujishiro and co-workers

CMR in para phase close to T_{curie}

Anisotropic exchange

- Dzyaloshinsky-Moriya interaction
- Mixing in of excited d-states
- LS coupling in excited state
- If spins inversion symm. related then 0
- Form different from Heisenberg: $\vec{D} \cdot \vec{S}_i \times \vec{S}_j$
- Favors perpendicular alignment
- Examples: $\alpha\text{-Fe}_2\text{O}_3$, MnCoO_3
- In AF's leads to net moment \rightarrow weak ferro (canted AF)



Multiferroics

Effects of Dzyaloshinskii–Moriya interaction

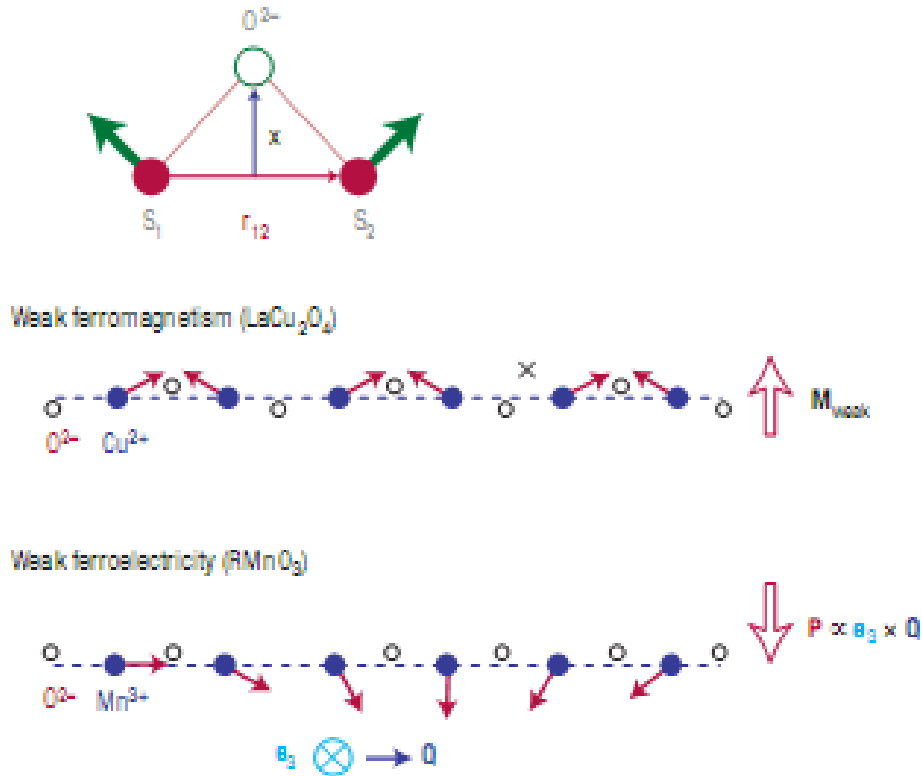
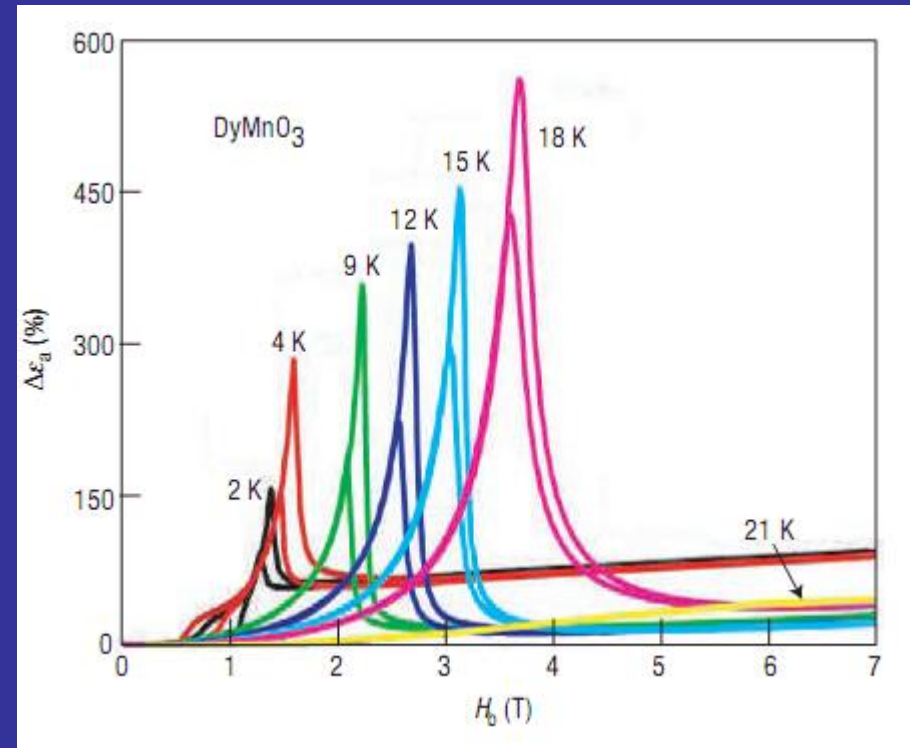


Figure 5 Effects of the antisymmetric Dzyaloshinskii–Moriya interaction. The interaction $H_{DM} = \mathbf{D}_{12} \cdot [\mathbf{S}_1 \times \mathbf{S}_2]$. The Dzyaloshinskii vector \mathbf{D}_{12} is proportional to spin-orbit coupling constant λ , and depends on the position of the oxygen ion (open circle) between two magnetic transition metal ions (filled circles), $\mathbf{D}_{12} \propto \lambda \mathbf{x} \times \mathbf{r}_{12}$. Weak ferromagnetism in antiferromagnets (for example, LaCu_2O_2 layers) results from the alternating Dzyaloshinskii vector, whereas (weak) ferroelectricity can be induced by the exchange striction in a magnetic spiral state, which pushes negative oxygen ions in one direction transverse to the spin chain formed by positive transition metal ions.

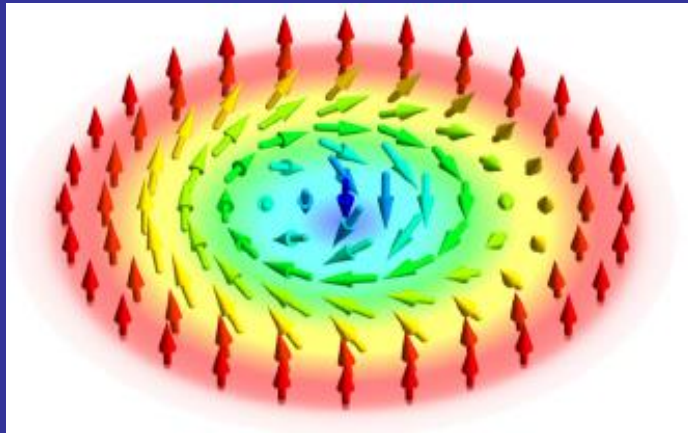


$$\mathbf{P} \propto [(\mathbf{M} \cdot \partial)\mathbf{M} - \mathbf{M}(\partial \cdot \mathbf{M})]$$

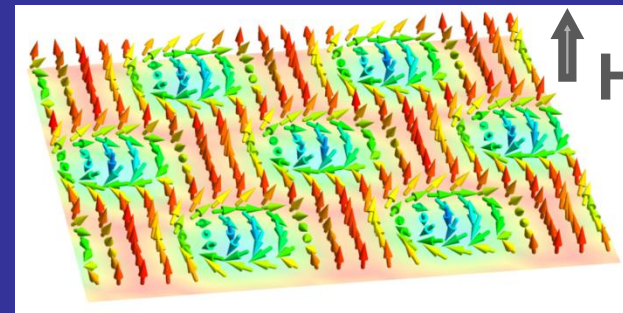
Mostovoy & Cheong

Skyrmions

Bloch skyrmion



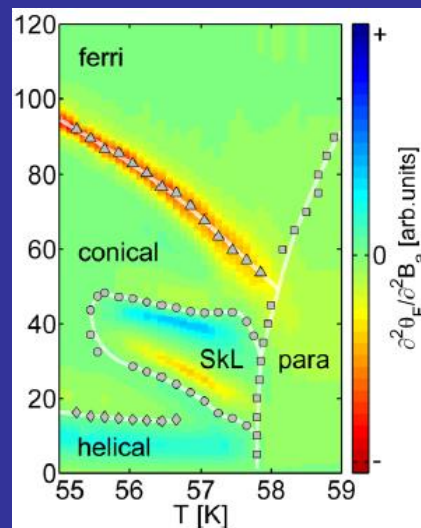
Skyrmion lattice



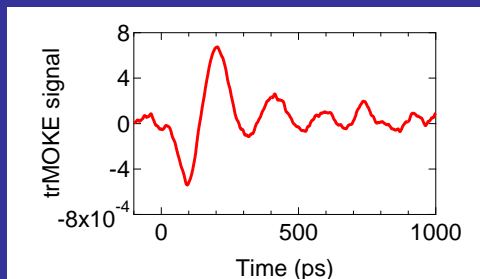
Christoph Schütte and Markus Garst
Phys. Rev. B **90**, 094423 (2014)

Achim Rosch, Nature Nanotechnology **8**, 160–161 (2013)

Phase diagram

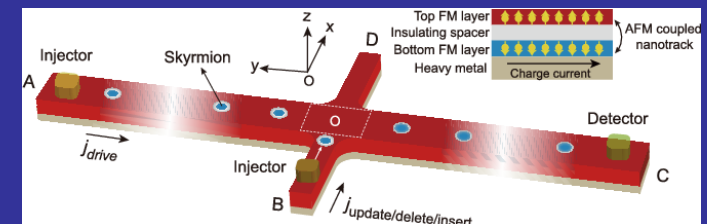


Coherent excitations



P. Padmanabham *et al.*, (2018)

Skyrmion racetrack



Zhu *et al.* (2018)

R. B. Versteeg *et al.*, PRB **94**, 094409 (2016)