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Magnetism and Matter

MM-3: Magnetic Interactions

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Conclusion of my lecture

- Competing interactions leads to complex magnetic structures.
- Magnetism is a field with many different types of interactions at different length and energy scales.
- The competition can be altered by temperature and time (non-equilibrium excitations).
- Additional complexity is provided by spatial constrictions.
- The magnetic structures can be very complex and very esthetic.
- Some magnetic structures have strong impact on electron transport properties.

Outline

- Conclusion of my lecture
- Zoo of Interactions
- Reminder Magnetic Interactions
- Examples of Magnetic Phases
  - Collinear ones
  - Non-collinear ones
- Magnetism of single atoms
  - See lecture MM-1
  - Open shell atoms in crystal field
- Dipolar Interaction
- Magnetic anisotropy
  - Phenomenological description of the Anisotropy
  - Quenching of orbital moment
  - Magnetiocrystalline anisotropy
- Heisenberg Model
- Dzyalonshinskii Moriya Interaction

But also Small Things Matter *!*

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"David, I want you tested for steroids."

Zoo of magnetic interactions

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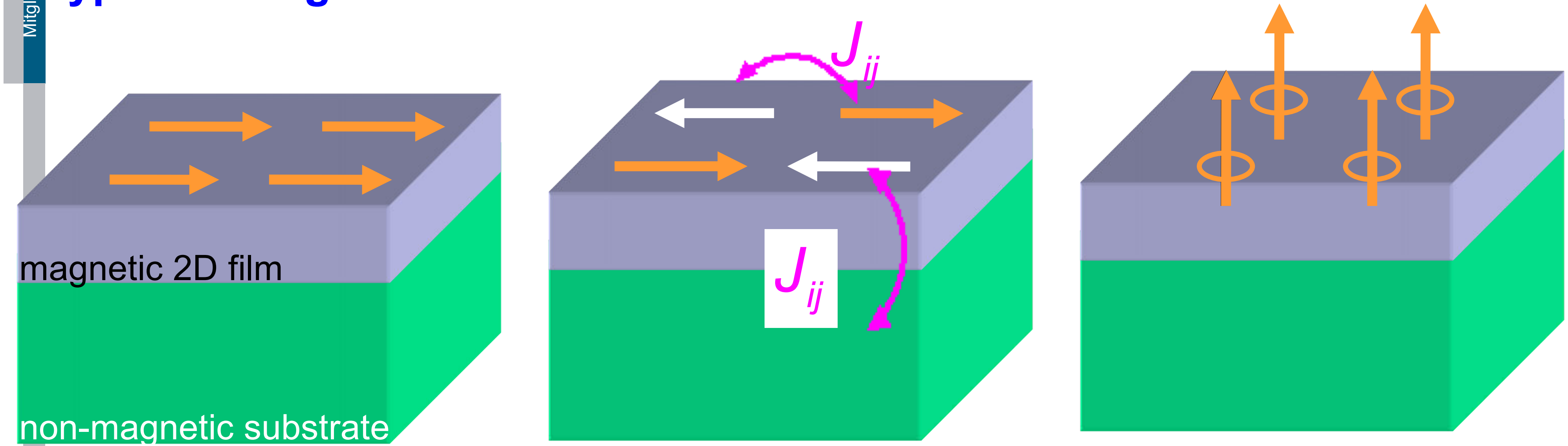
- Dipol interaction
- Nuclear spin - electron spin interaction
- Direct exchange interaction
- Indirect exchange Interaction
- Superexchange Interaction
- Double exchange Interaction
- Kinetic exchange Interaction
- Zener p-d exchange Interaction
- Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction
- Biquadratic exchange Interaction
- Pseudo-dipolar exchange Interaction
- Magnetic anisotropy Interaction
- Dzyaloshinskii-Moriya interaction

1) Reminder Magnetic Interactions

- Magnetism is a field with many different types of interactions at different length and energy scales.

Some Fundamental Interactions

Typical Energies: ≈1 eV | **≈0.2 eV** | **≈0.0005 eV**



Magnetic Moments	Magnetic Order	Magnetic Orientation
Magnetism: Yes or No?	Ferro ⟺ Antiferro	In-plane ⟺ Out-of-plane
Intra-atomic Exchange	**Inter-atomic Exchange**	**Spin-Orbit + Dipole-Dip**
$H = -\frac{1}{2}\sum_i I_i m_i^2$	$H = -\frac{1}{2}\sum_{i,j} J_{i,j}\,\vec{m}_i\vec{m}_j$	$H = \sum_i K_i(\vec{m}_i\,\vec{e}_i)^2 + \sum_{i,j}\frac{1}{r_{i,j}^3}[\cdots]$

Typical Ground State Energies

	E(eV/atom)
Cohesive energy	5.5
Local moment formation	1.0
Alloy formation	0.5
Magnetic order	0.2
Structural relaxation	0.05
Magnetic anisotropy	0.0005

[Of course: Thermal excitation, dynamics,….]

Magnetism on all scales:

What happens to Magnetism on the Way from Large to Small

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macroscopic

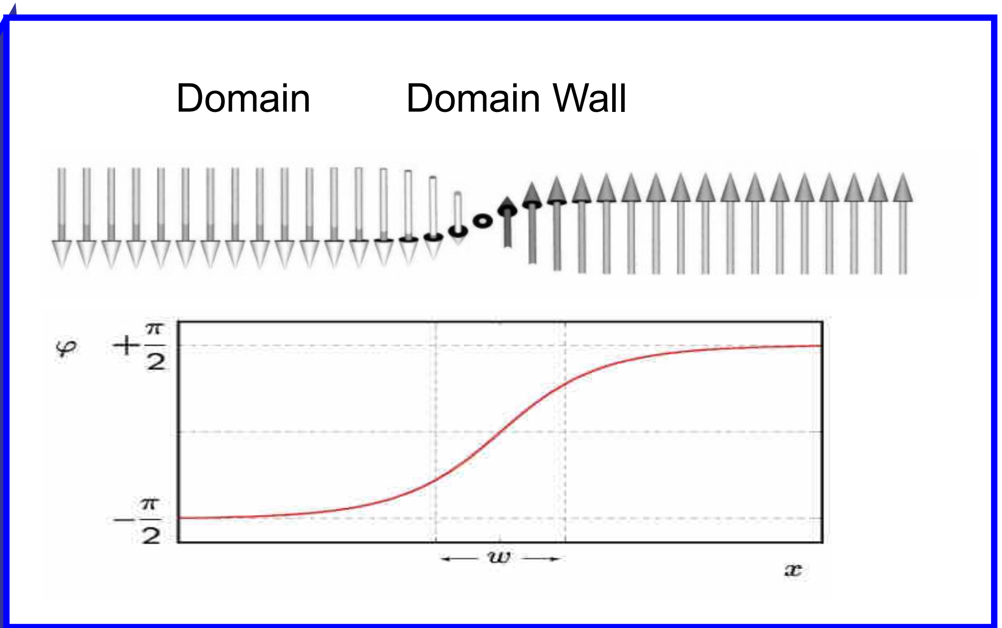
permanent magnets

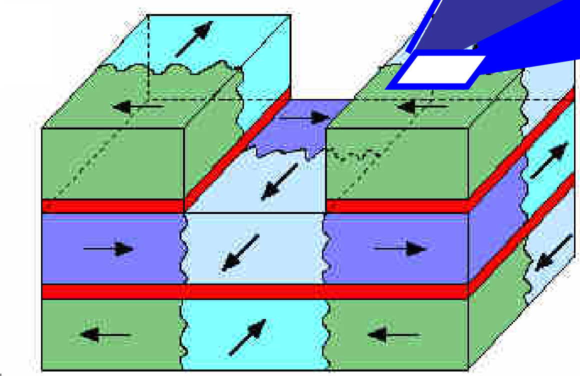
micron particles

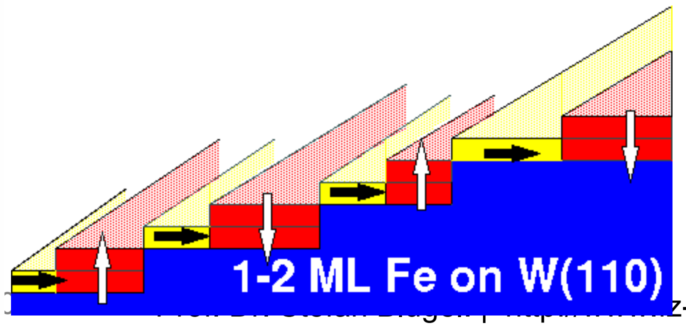
$S=10^{20}$ 10^{10} 10^{8}

com

micrometer s







quantum tunneling,
quantization
quantum interference

"Single Molecule" Magnets

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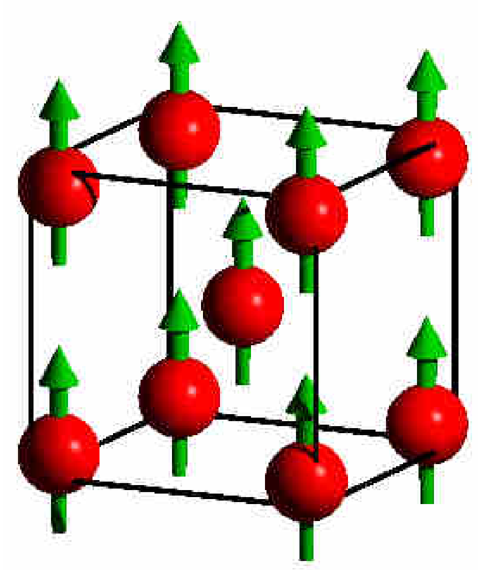
2. Magnetic Phases
2.1 Collinear Magnetic Phases

Bulk Magnetism

ferromagnet



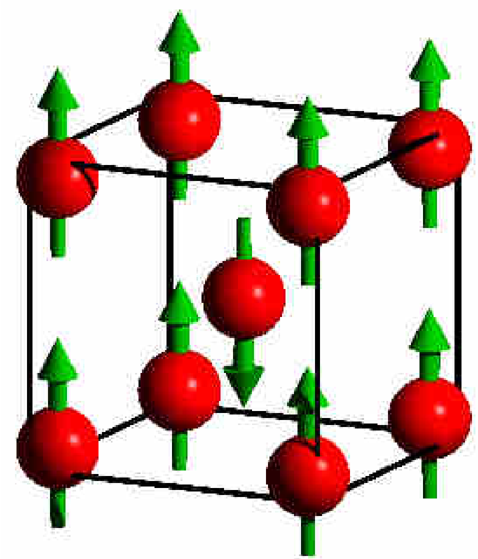
bcc-Fe:

M= 2.12 μ_B

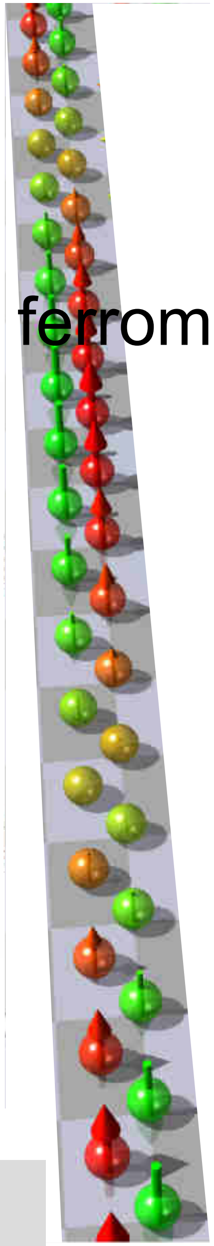
Bulk Magnetism

Spin density wave

antiferromagnet



ferromagnet



bcc-Cr:

M= 0.59 μ_B

Bulk Magnetism

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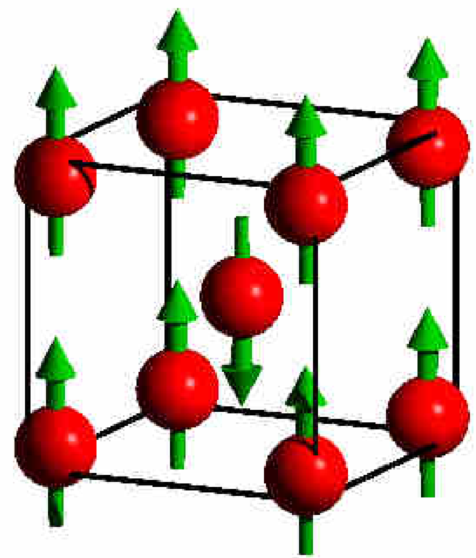
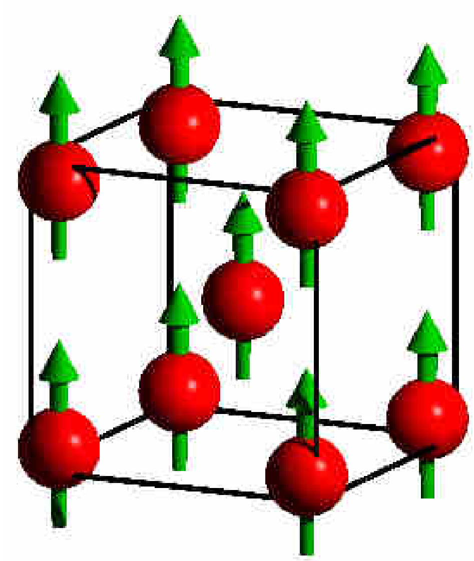
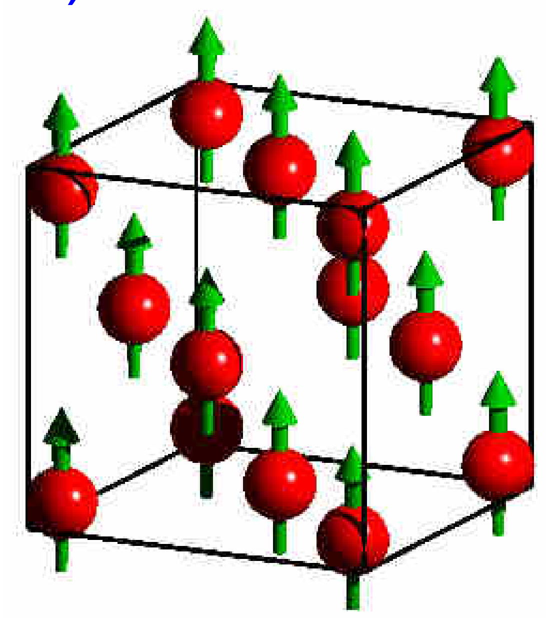
- Itinerant magnets (metals)
- Collinear magnetic structure (quantization axis the same at each atom)







bcc-Cr:

M= $0.59\,\mu_B \times \cos(1-\delta)\frac{\pi}{a}na$

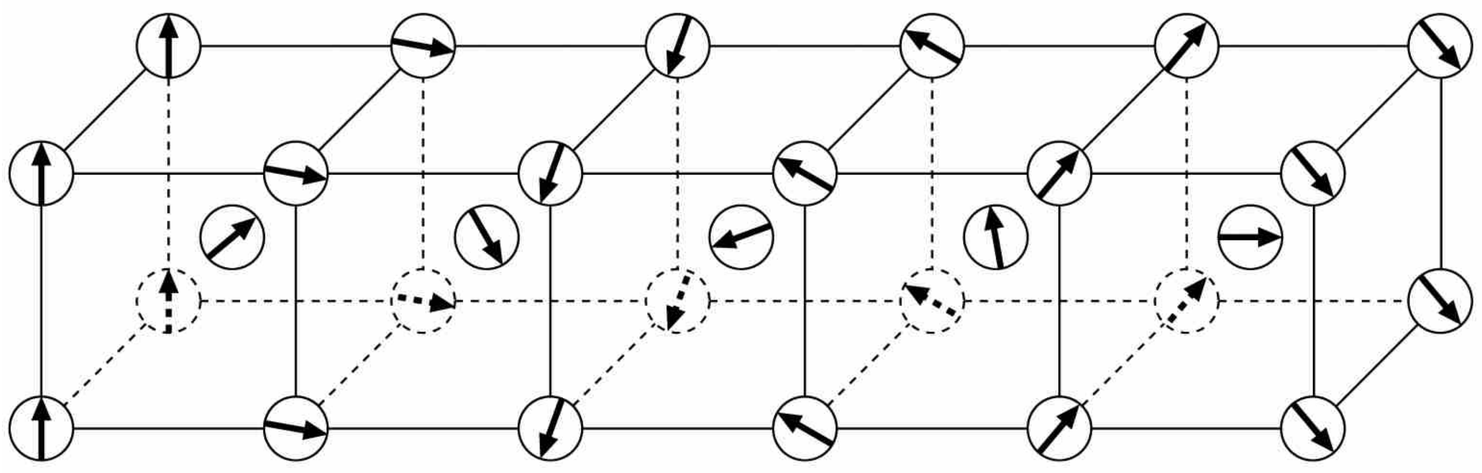
bcc-Fe:

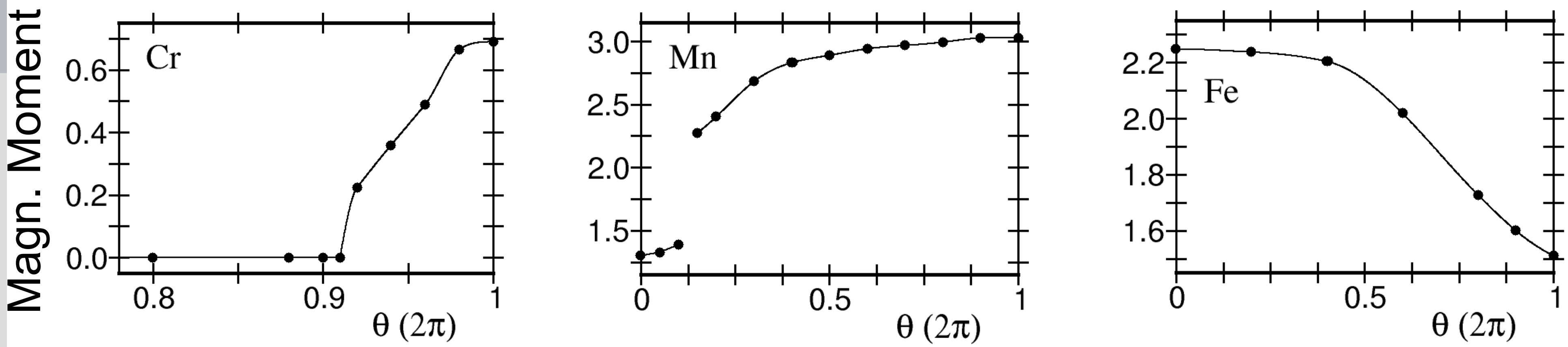
M= $2.12\,\mu_B$

fcc-Ni:

M= $0.55\,\mu_B$

Signature of Itinerant magnetism

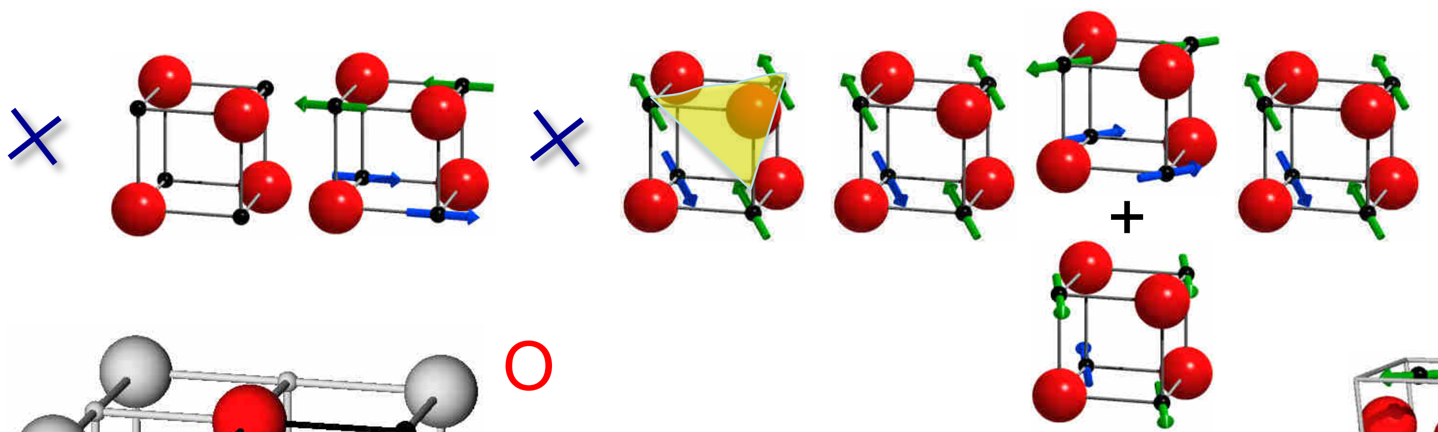


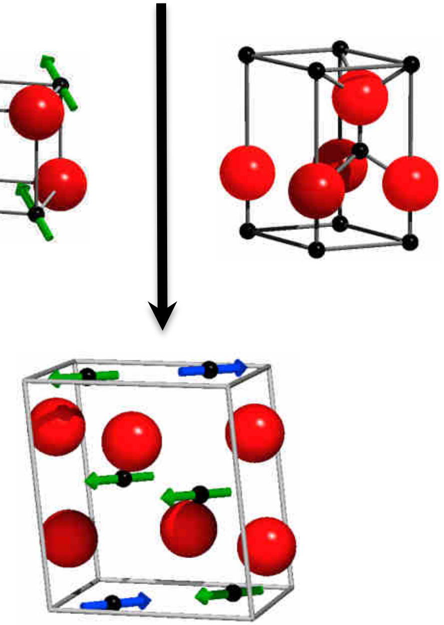


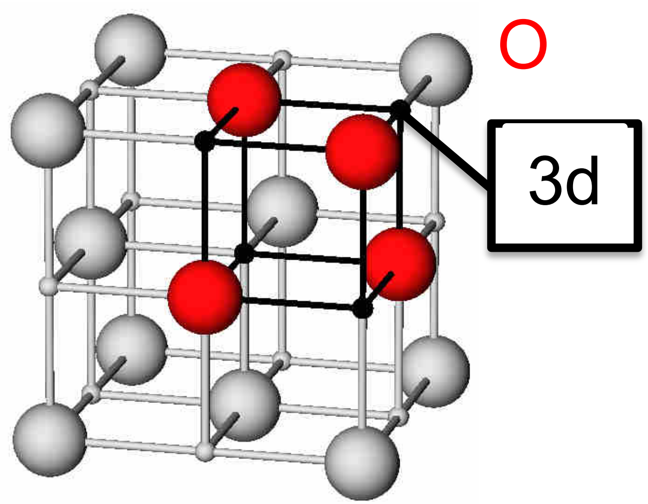
S. Blügel, G. Bihlmayer in: Handbook of Magnetism and Advanced Magnetic Materials (2007)

Example 2:
Transition-metal mono-oxides

ScO TiO VO CrO MnO FeO CoO NiO CuO ZnO





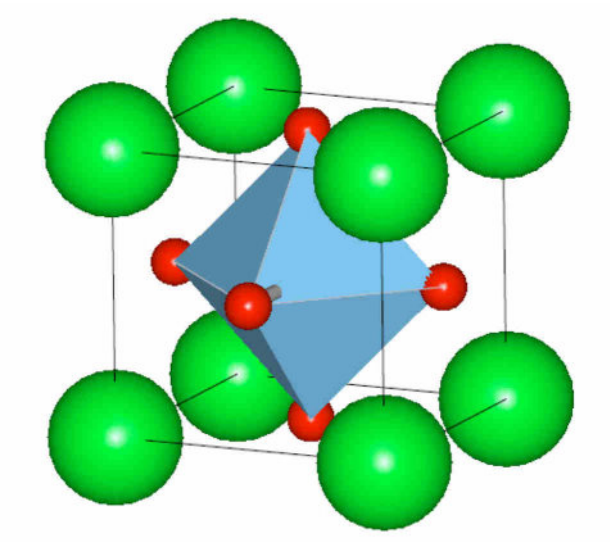


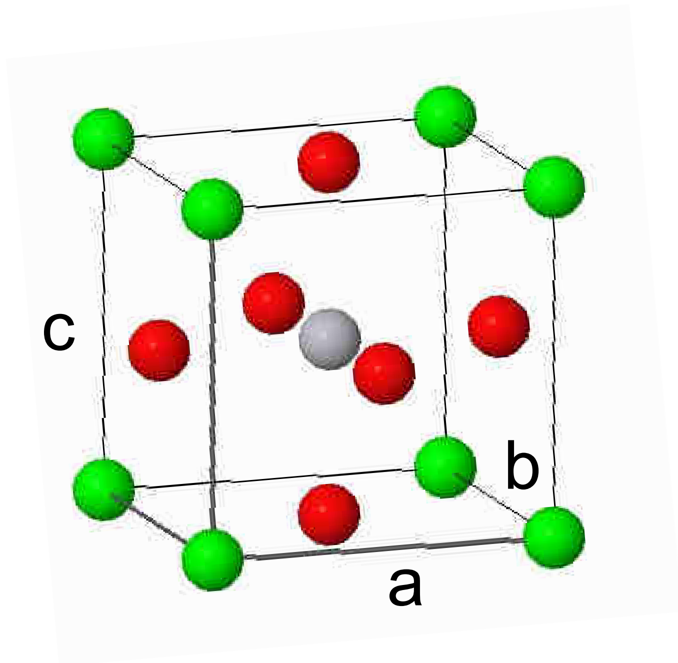
Rock Salt structure

- Question:
  How is such a variety of magnetic configurations realized ?

Example 3: Perovskites ABO_3

Crystal Structures and Chemical Bonds in TMO





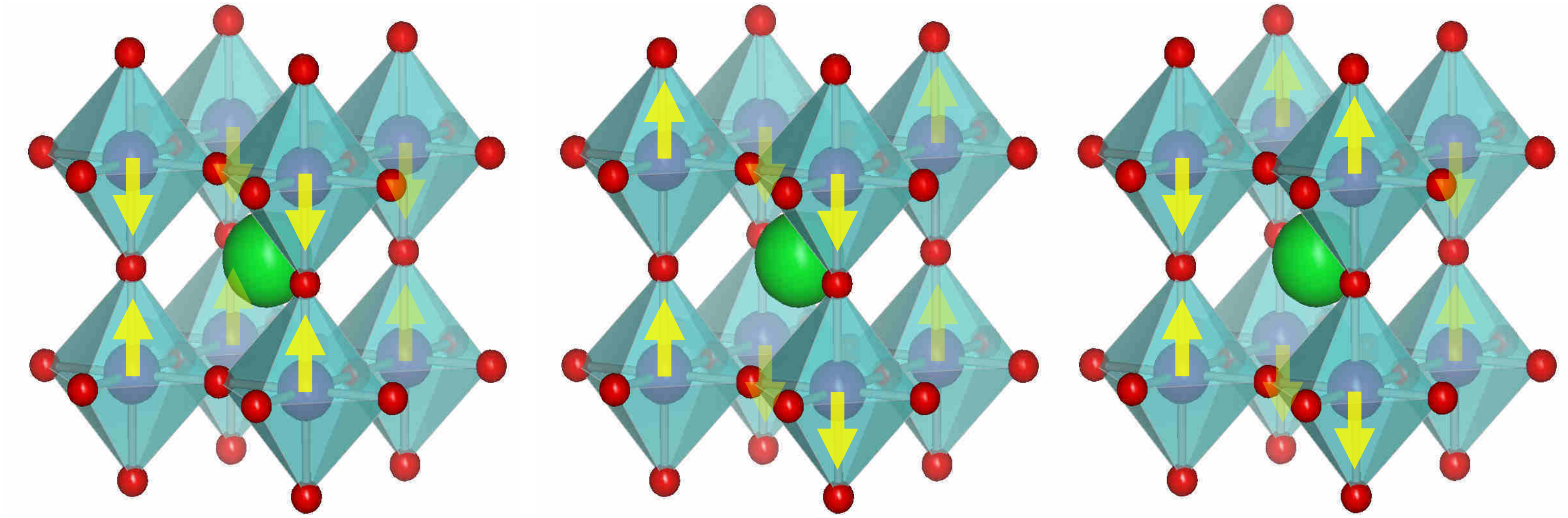
ABO_3

^

TM-ion

a=b=c

Example 3: Perovskites $[La_{1-x}Sr_x]MnO_3$



AFM-A-type AFM-C-type AFM-G-type

- Remark 2:

Novel Physical Properties Originate from Variety of Antiferromagnetic Configurations

- Colossal magnetoresistance
- Half-metallicity

Spin spiral Canted antiferromagnetic

2. Magnetic Phases
2.2 Non-Collinear Magnetic Phases

Non-collinear Magnetism

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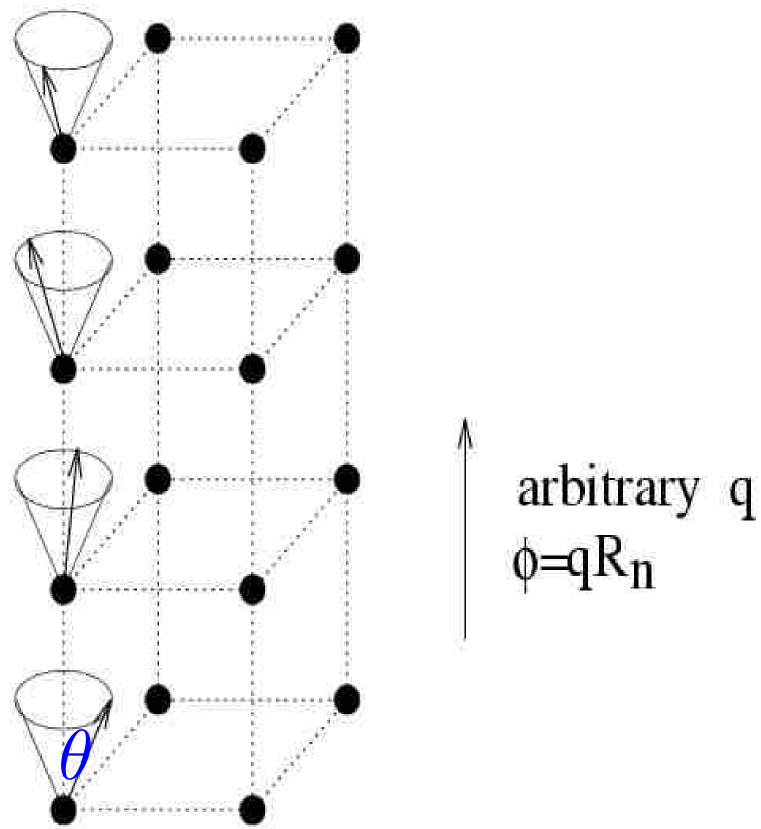
Incomensurate Spin Spiral



Spin-spiral is characterized by

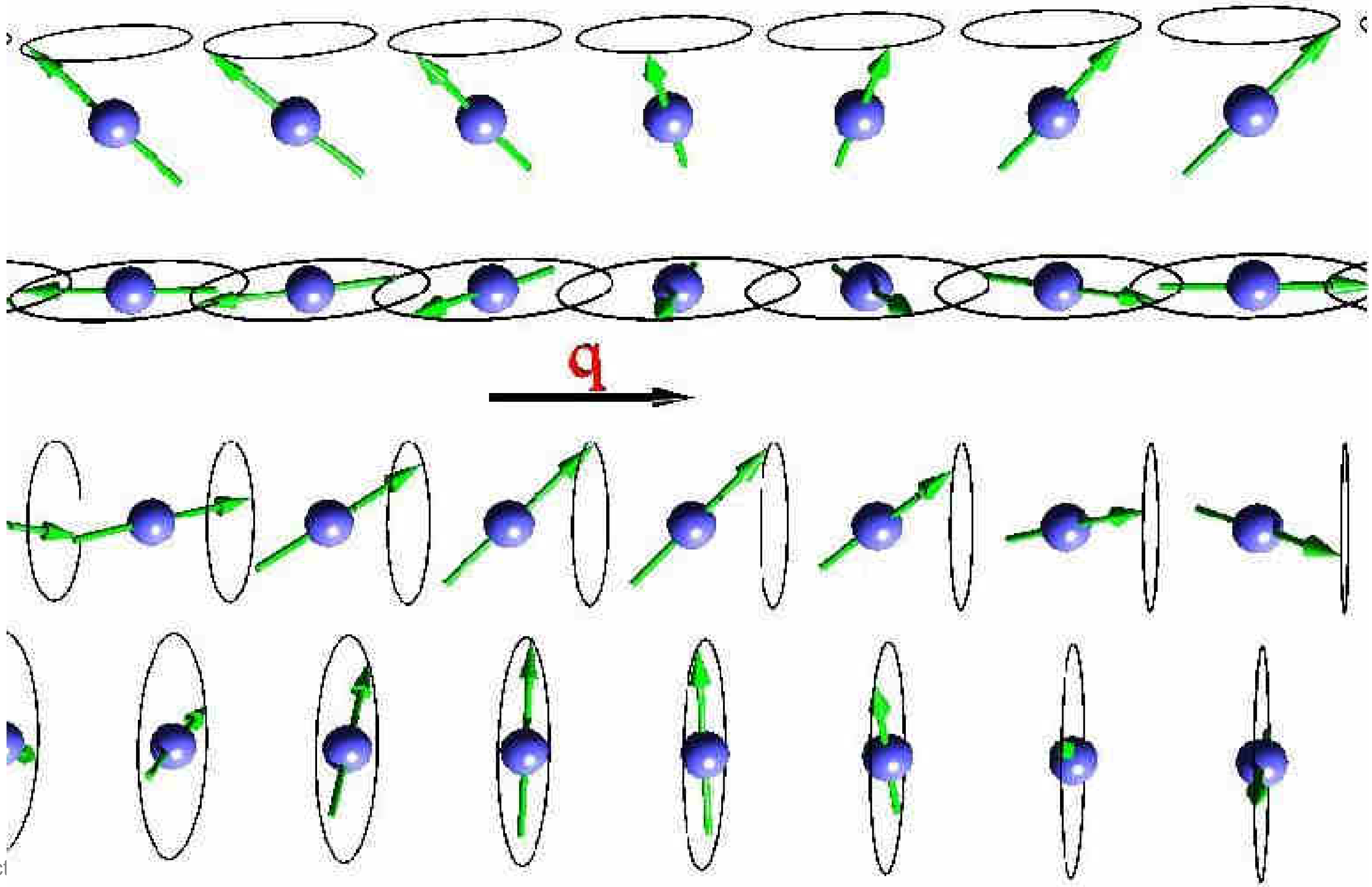
- Wave vector
- Rotation axis
- Cone angle

$$\vec{M}^n = M \begin{Bmatrix} \sin\theta \cos \vec{q}\vec{R}^n \\ \sin\theta \sin \vec{q}\vec{R}^n \\ \cos\theta \end{Bmatrix}$$

cone angle (θ) — wave vector ($\vec{q}$)

This particular example:
helical coned spin spiral $\vec{q} \parallel \hat{z}$

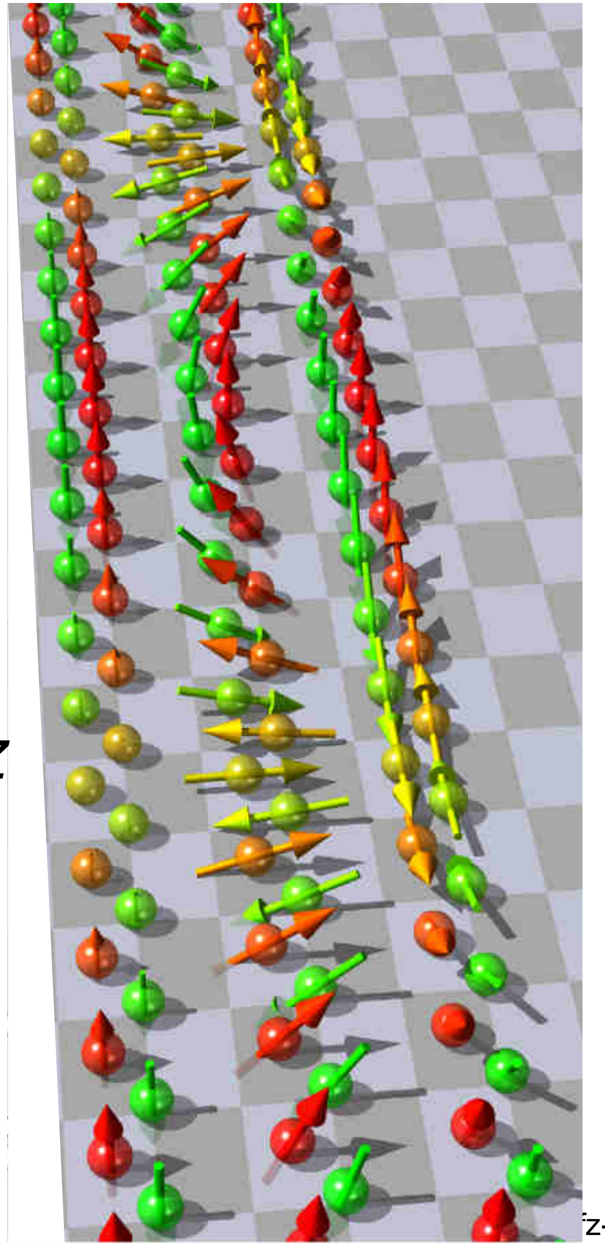
Flat Spiral and Spiral with cones



Non-collinear Magnetism

spin-density
wave

helical spin spiral $\vec{q} \parallel \hat{z}$



cycloidal spin
spiral $\vec{q} \perp \hat{z}$

fz-juelich.de/pgi/Bluegel_S

Example 4: 4f-Helimagnets

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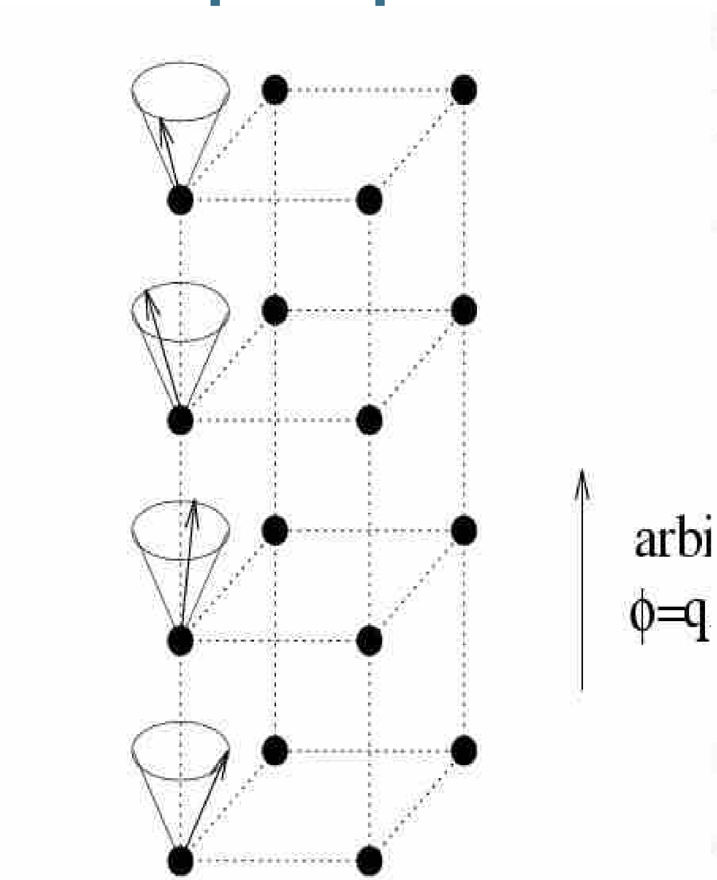
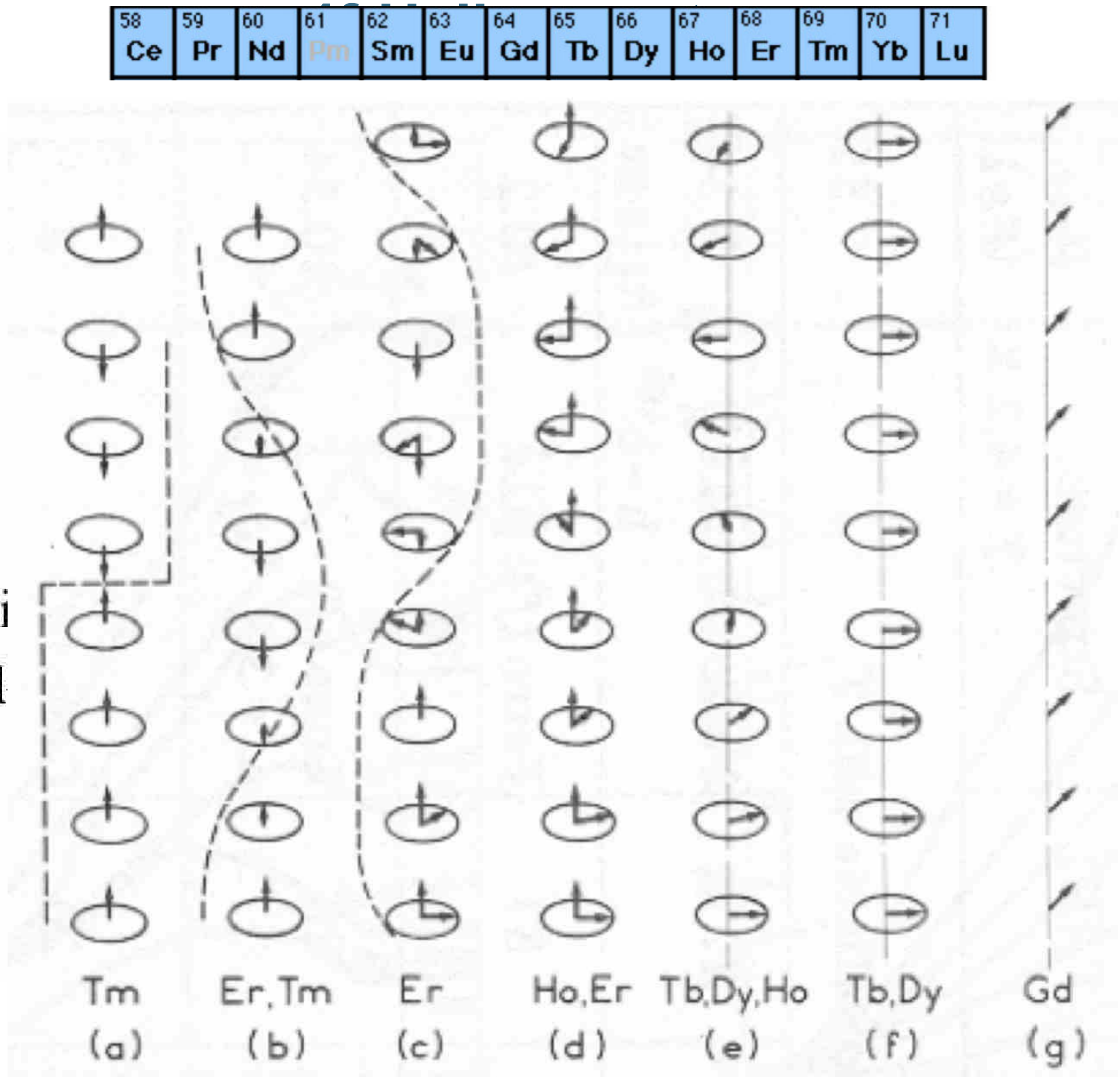
Incomensurate Spin Spiral





Example 6: Orthorombic $RMnO_3$

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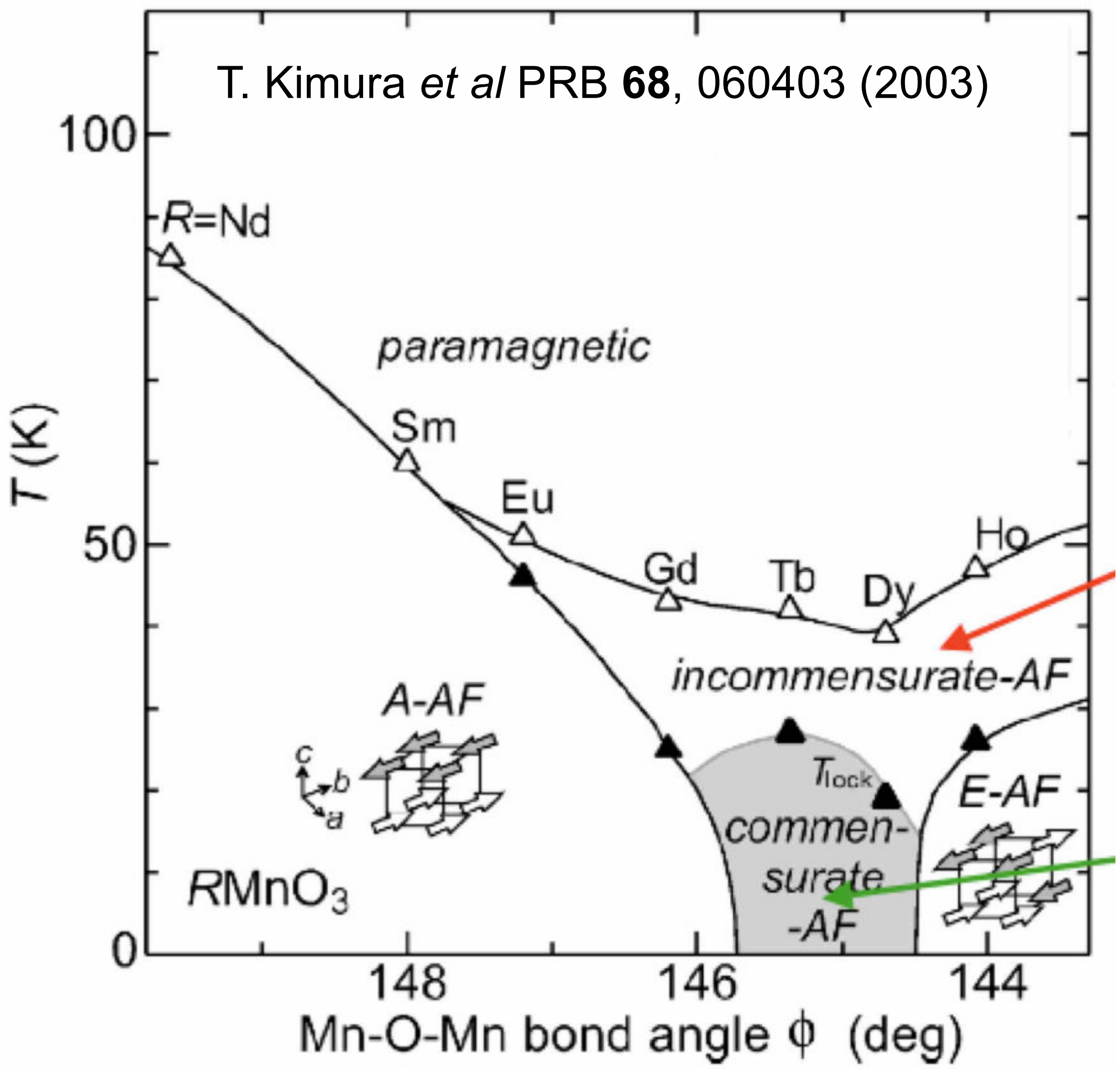
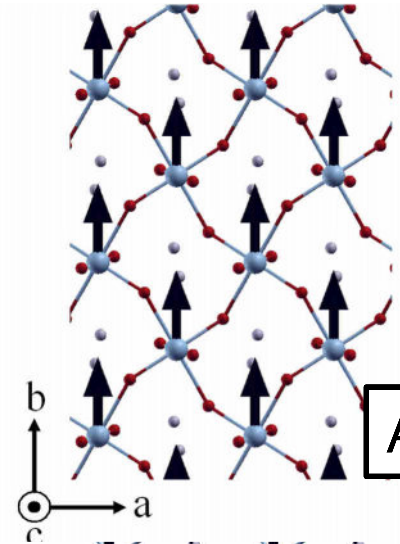
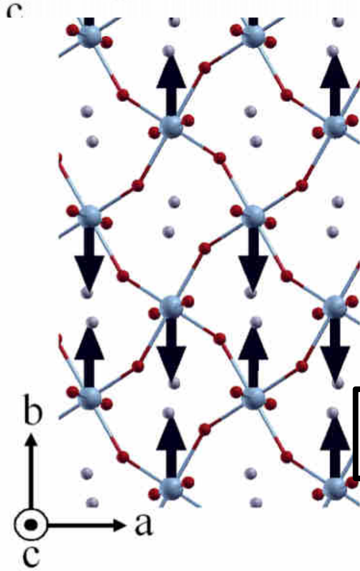
R=Rare Earth

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu





AFM-A



AFM-E

Example 7: finite temperature magnetism

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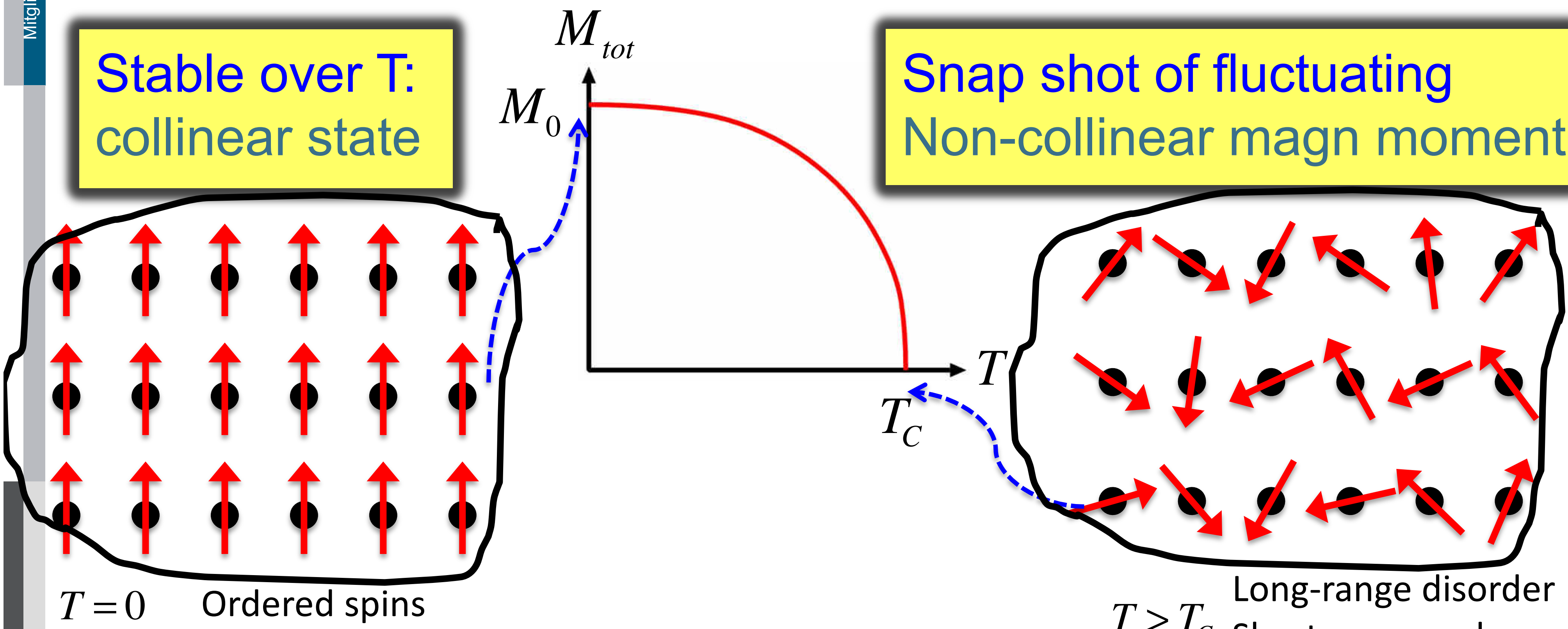
Spontaneous magnetization: $\vec{M}(B_{\rm ext},T) = \frac{1}{V} < \sum_i \vec{m}_i(B_{\rm ext}) >$

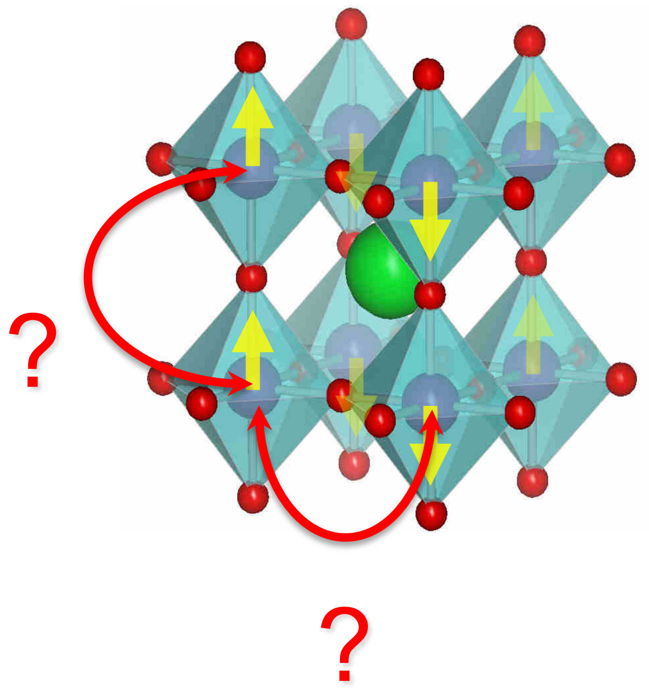
Stable over T:
collinear state

Snap shot of fluctuating
Non-collinear magn moment



magnetic interactions known
➔ one can determine T_C

Aim the lecture: understanding exchange Interactions



Exchange Interactions

Origin of Exchange Interaction

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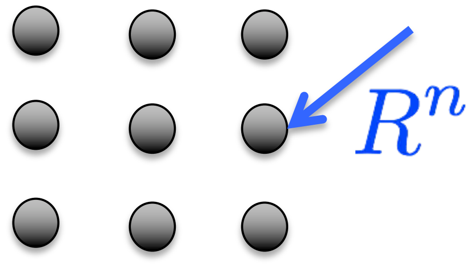
- Hamiltonian

$$H = \sum_i \left\{ \frac{p_i^2}{2m} - \sum_n \frac{Z^n}{|r_i - R^n|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|} \right\}$$

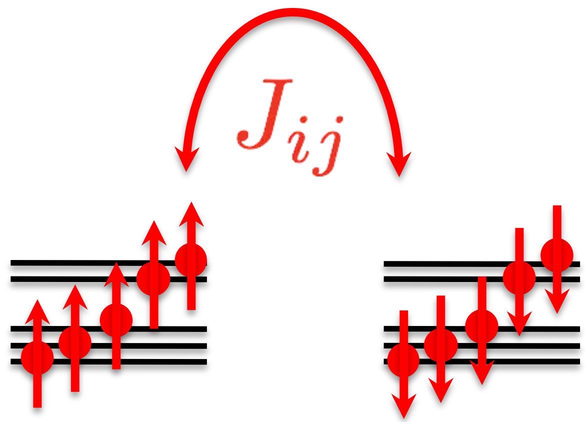


- Surprise ! Hamiltonian not explicit spin dependent:

$$[H, S^2] = 0 \quad \wedge \quad [H, S_z] = 0$$

- Effective Spin-Hamiltonian

$$H_{2\text{-spin}} = \sum_{i,j} J_{ij} \, \mathbf{S}_i \cdot \mathbf{S}_j$$

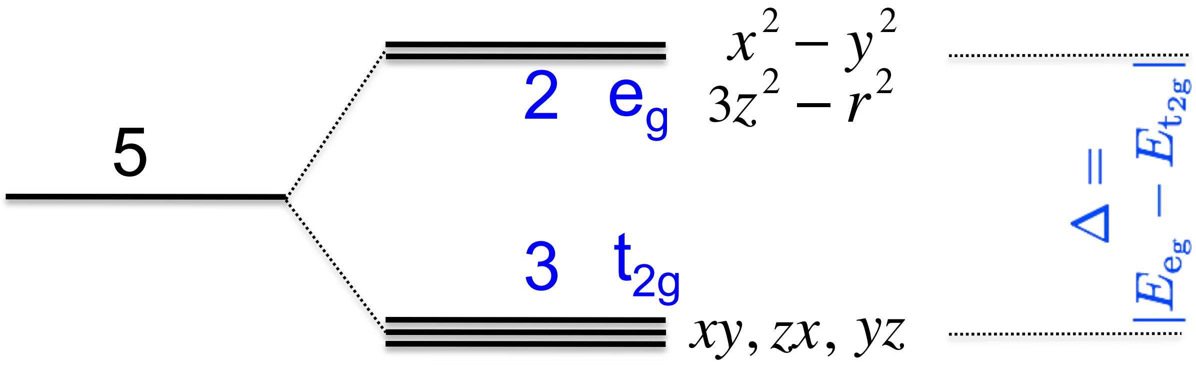


1. Magnetism of single atoms

➡ Discussed in lecture MM-1

Open shell atom in crystal field

See for more information: Crystal Field Theory



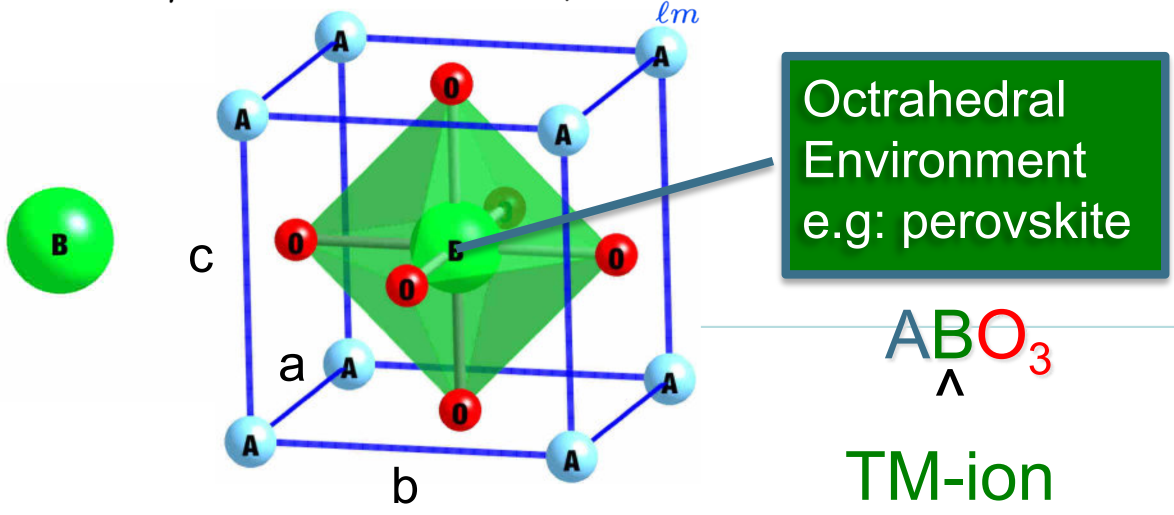
$$\Delta = |E_{e_g} - E_{t_{2g}}|$$

Free atom

$$V_o(r) = -\frac{Z}{r}$$

Cubic a=b=c

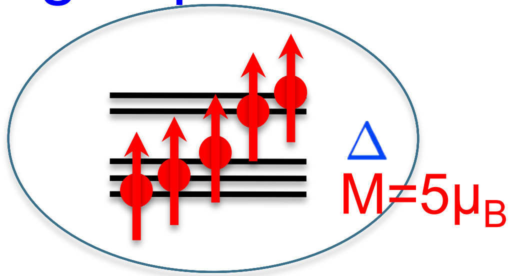
$$V(\vec{r}) = -\frac{Z}{r} + \sum_{\ell m} V_{\ell m}(r)\mathcal{Y}_{\ell m}(\hat{r})$$



ABO_3
^
TM-ion

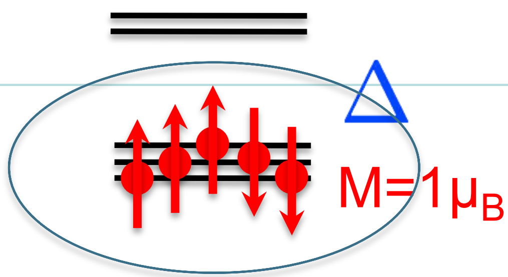
- Δ=small

high-spin state



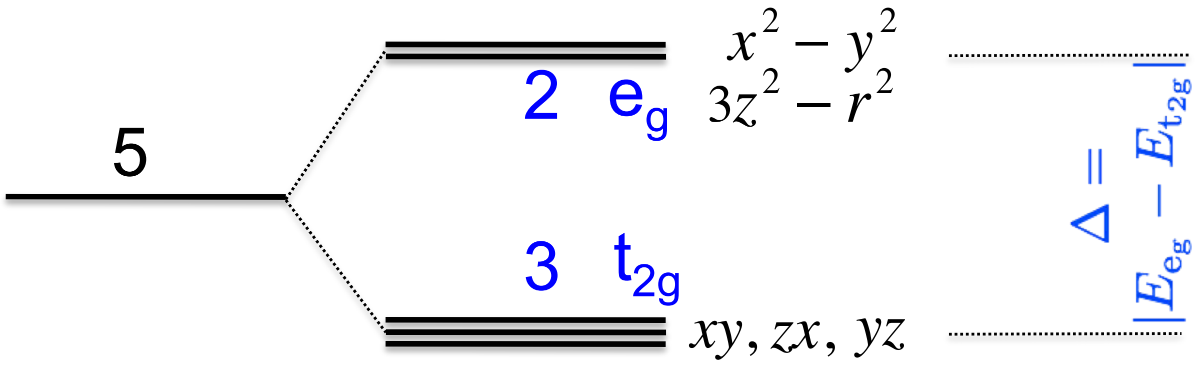
- Δ=large

low-spin state



Open shell atom in crystal field

M. Ležaić A3: Crystal Field Theory and Jahn-Teller Effect



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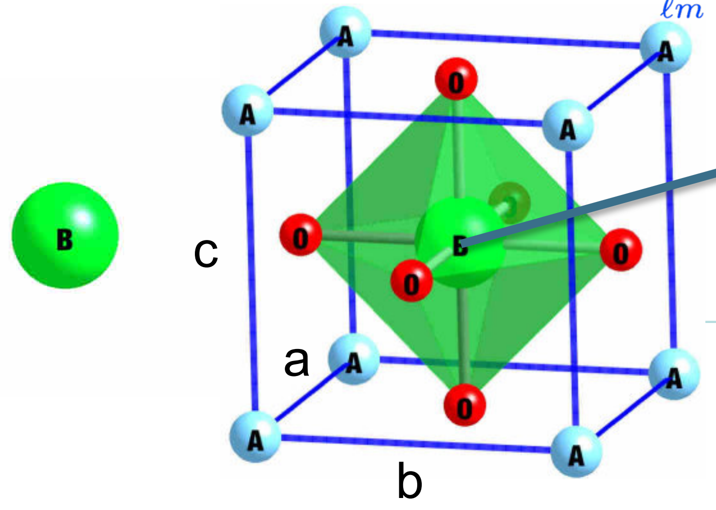
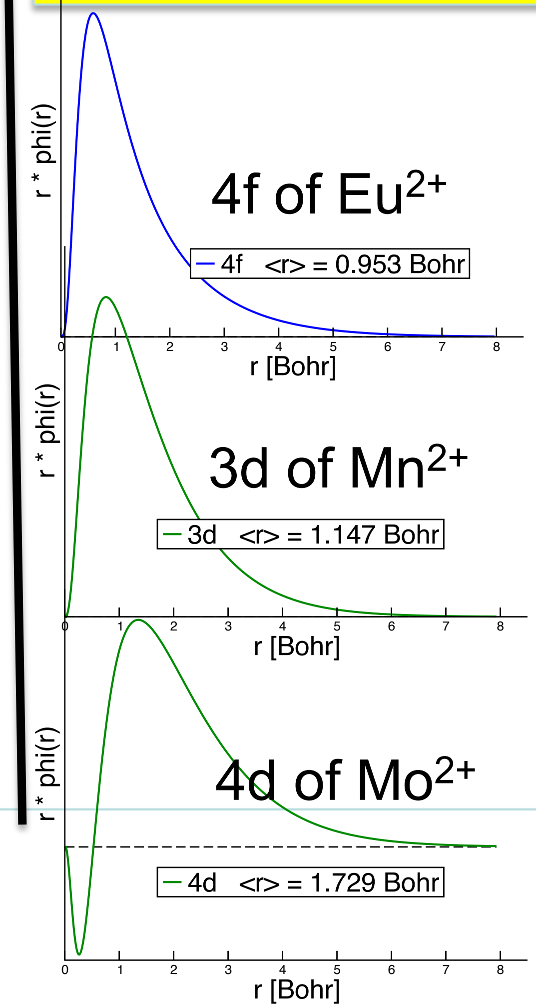


Octrahedral Environment e.g: perovskite

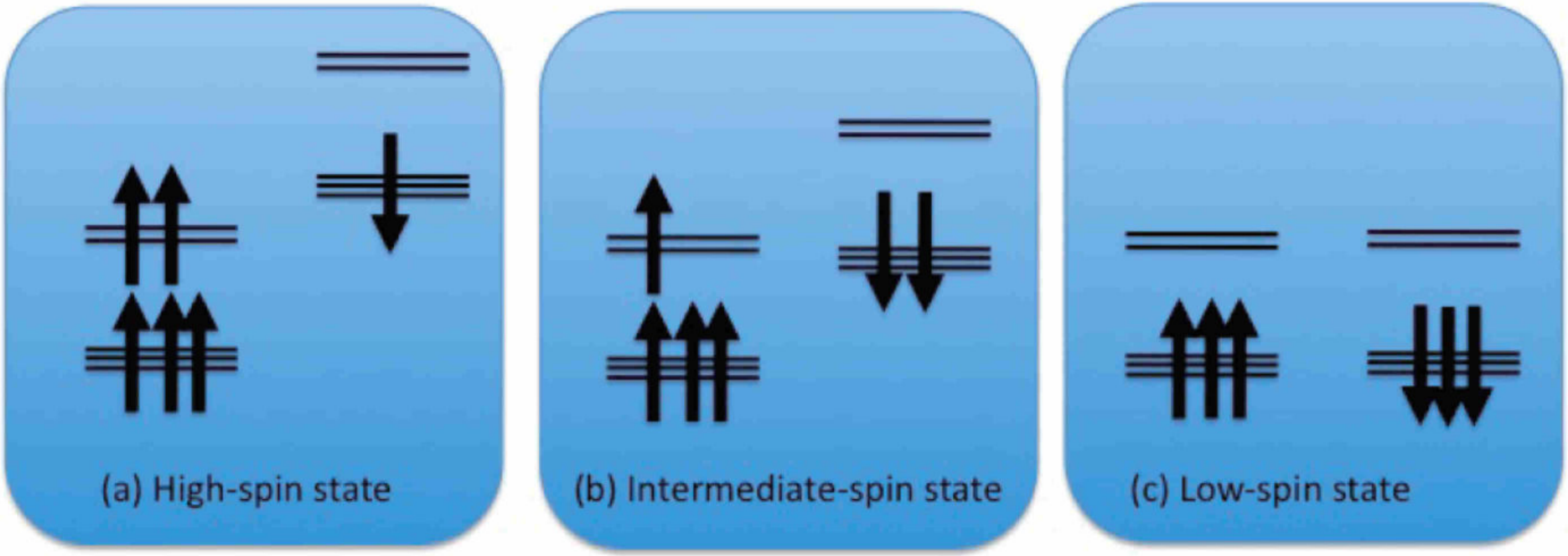
ABO_3

^

TM-ion

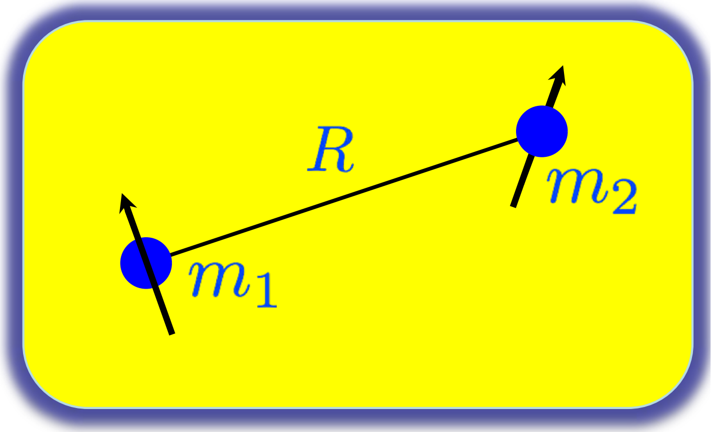


Example: Co^{3+} in cubic crystal



Dipolar Interaction

Energy of a pair of magnetic moments



$$E(\vec{m}_1, \vec{m}_2; \vec{R}) = \frac{\vec{m}_1 \cdot \vec{m}_2 - 3(\vec{m}_1 \cdot \hat{R})(\vec{m}_2 \cdot \hat{R})}{R^3}$$

Energy of magnetic moments on a lattice
(ferromagnetic state, moments along z-direction)

$$E^z_{\mathrm{FM}} = \frac{m_z^2}{R_o^3} \sum_{\vec{a}} \sum_{\vec{n}} \frac{[1 - 3(\hat{R}_z)^2]}{(R^{\vec{n}})^3}.$$

Energy scale: (lattice constant ≈2 Å ≈ 4 a_o; spin S=½; g≈2)

$$\frac{m^2}{R^3} \sim \frac{(g \cdot \mu_{\mathrm{B}} \cdot \frac{1}{2})^2}{(4a_0)^3} = \frac{1}{4^3} \cdot \left(\frac{e\hbar}{2m_e c}\right)^2 \left(\frac{m_e e^2}{\hbar^2}\right)^2 \frac{1}{a_0} = \frac{1}{2 \cdot 4^3} \underbrace{\alpha^2}_{=(1/137)^2} \cdot \underbrace{\frac{e^2}{2a_0}}_{1\,\mathrm{Ry}}$$

$$\frac{m^2}{R^3} \sim \frac{1}{128} \cdot \frac{1}{18769} \mathrm{Ry} \sim 3 \cdot 10^{-6} \mathrm{eV} \approx k_{\mathrm{B}} \times 0.05\,\mathrm{K} \ll k_{\mathrm{B}} T_{\mathrm{C}} \; (T_{\mathrm{C}} \approx 100 \text{ to } 1000\,\mathrm{K}$$

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Magnetic Anisotropy

Rotation of Magnetization

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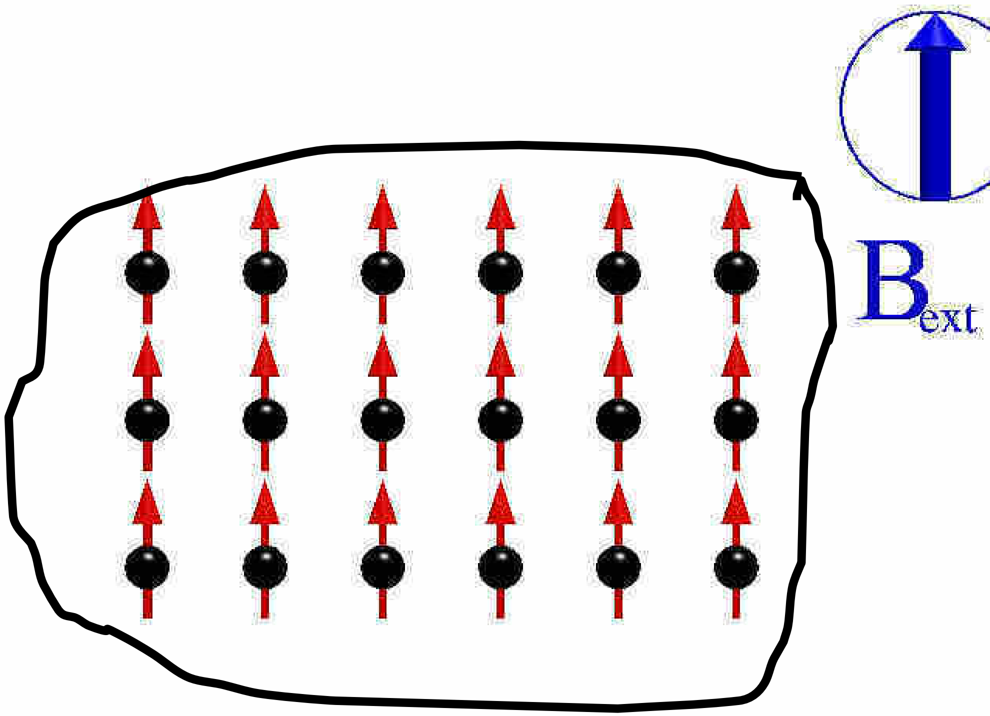
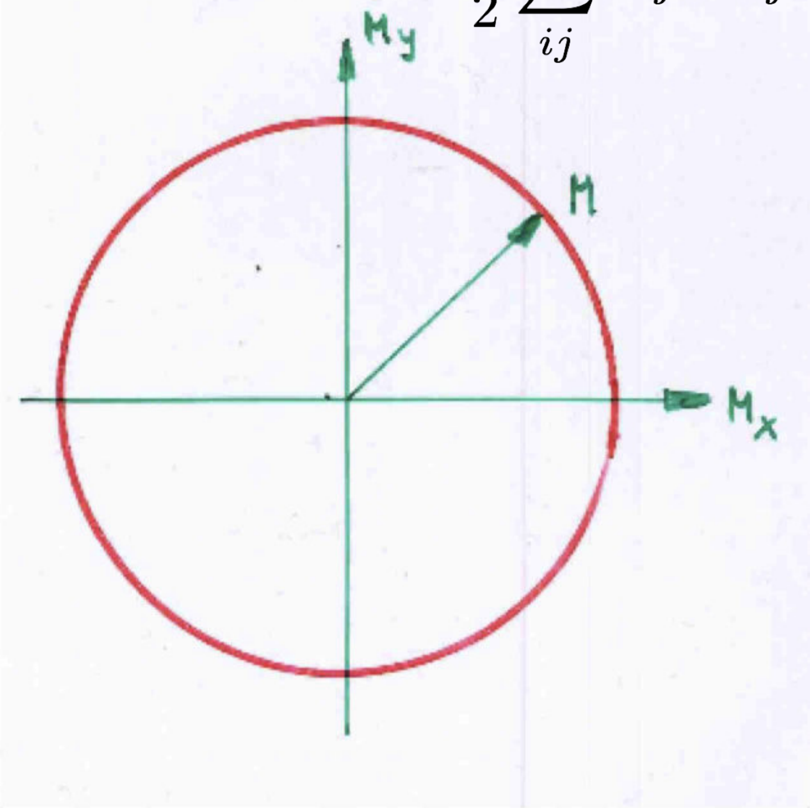
Isotropic: $E(|\vec{M}|)$

(Heisenberg: $H = \frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j$)



Solid



Magnetic anistropy of Energy

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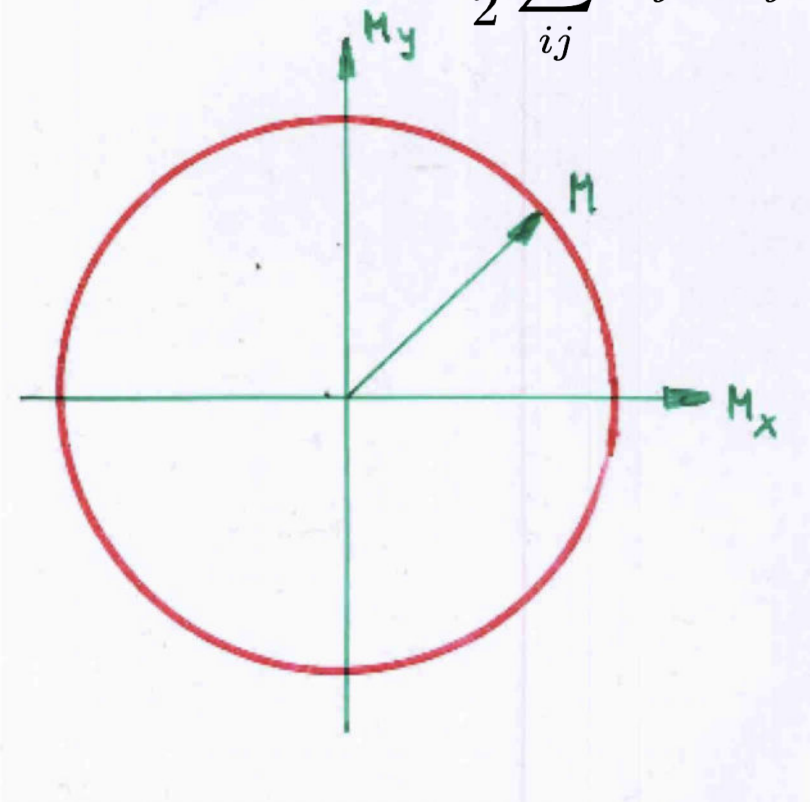
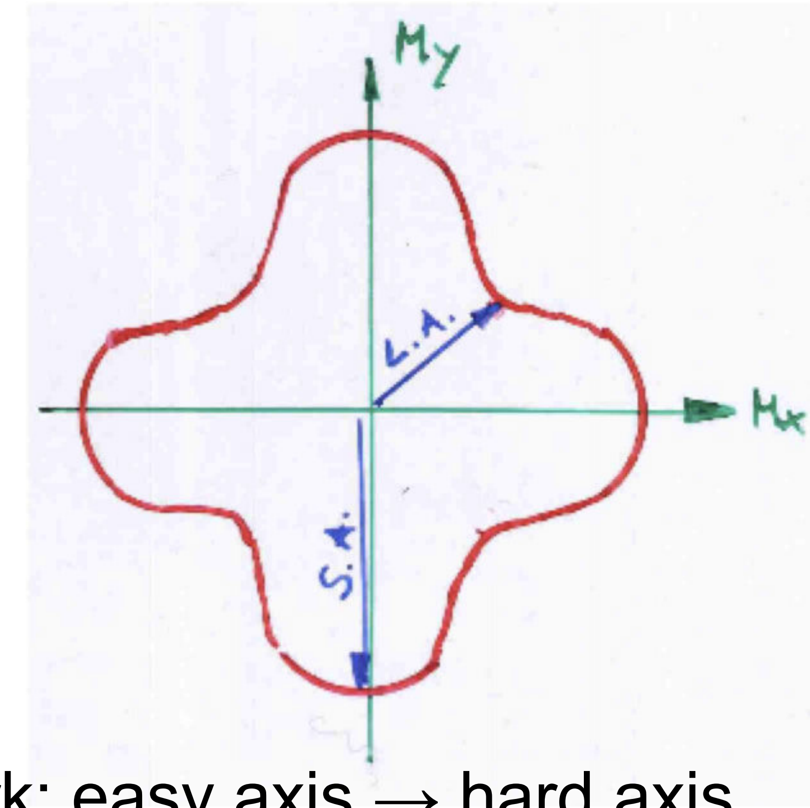
Isotropic: $E(|\vec{M}|)$

(Heisenberg: $H = \frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j$)



Energy anisotropy: $E(|\widehat{M}|)$



Work: easy axis → hard axis

$$W = \int \vec{H} d\vec{M}$$

Phenomenological description

Definition of coordinate system

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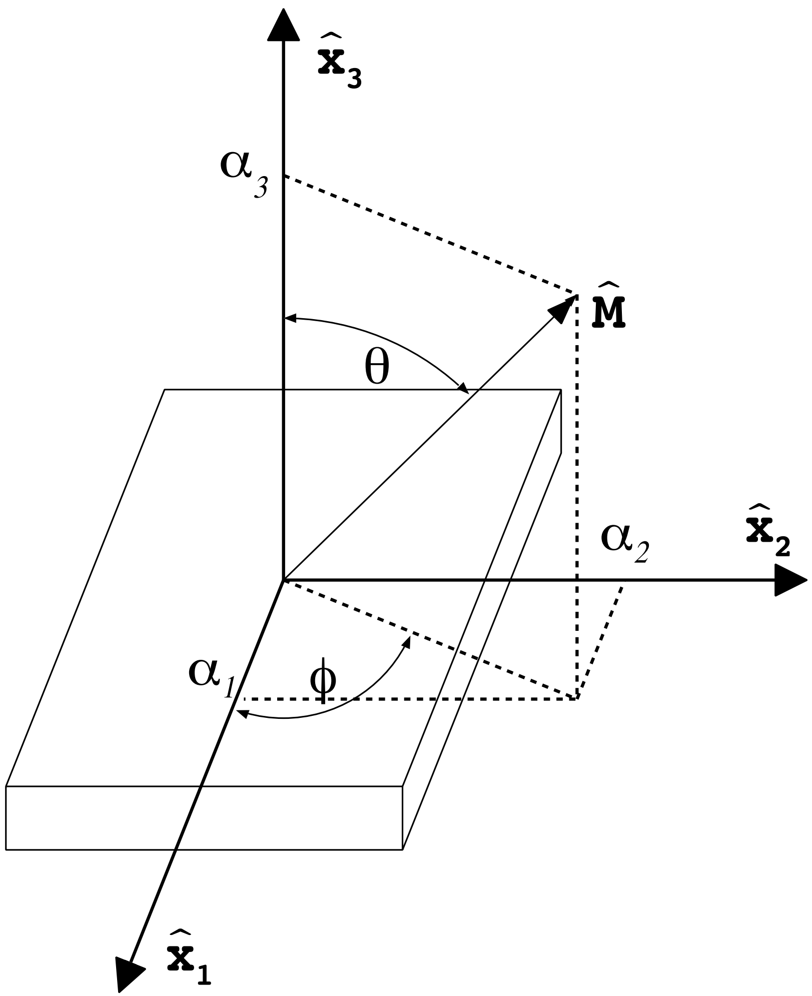

$$\widehat{M} = (\alpha_1, \alpha_2, \alpha_3) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

Phenomenological description of crystal anisotropy

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Power series expansion in the components $\widehat{M} = (\alpha_1, \alpha_2, \alpha_3)$

$$
\begin{aligned}
G_{\mathrm{cryst}}(T, H_M, \widehat{M}) &= b_0(T, H_M) + \sum_i b_i(T, H_M)\alpha_i \\
&+ \sum_{i,j} b_{ij}(T, H_M)\alpha_i\alpha_j + \sum_{i,j,k} b_{ijk}(T, H_M)\alpha_i\alpha_j\alpha_j \\
&+ \text{higher order terms}
\end{aligned}
$$

$\widehat{M}$ is an axial vector (right hand rule!)

$$\widehat{M} \xrightarrow{t \to -t} \widehat{M}' = -\widehat{M} \qquad , \alpha_i \to -\alpha_i$$

$$\Rightarrow b_{2n+1} \text{ axial tensors } \Rightarrow b_{2n+1} := 0 \; \forall n$$

recall:

$$\vec{M} \propto \vec{L} = \vec{r} \times \vec{p}$$

$$\propto \vec{r} \times \frac{d\vec{r}}{dt}$$

Bulk anisotropy cubic systems

Mitglied der Helmholtz Gemeinschaft

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Cubic systems: Fe, Ni, TMO, EuO, Spinel-Ferrites, Magnetite, Garnets

$$G^V_{\text{cryst}} = b_{ij}\alpha_i\alpha_j + b_{ijkl}\alpha_i\alpha_j\alpha_k\alpha_l + b_{ijklmn}\alpha_i\alpha_j\alpha_k\alpha_l\alpha_m\alpha_n$$

Cubic symmetry: $G(\alpha_i) = G(-\alpha_i)$

$$G \sim \alpha_i, \quad \alpha_i\alpha_j \ (i \neq j) \text{ vanish}$$

1. Second order terms:

$$\sum_{ij} b_{ij}\alpha_i\alpha_j = b_{11}(\alpha_1^2 + \alpha_2^2 + \alpha_3^2) = b_{11}$$

isotropic (forget it!)

1. Fourth order terms:

$$\begin{aligned}\sum_{ij} b_{ijkl}\alpha_i\alpha_j\alpha_k\alpha_l &= b_{1111}(\alpha_1^4 + \alpha_2^4 + \alpha_3^4) \\ &+ 6b_{1122}(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2)\end{aligned}$$

$$1^2 = (\alpha_1^2 + \alpha_2^2 + \alpha_3^2)^2 = (\alpha_1^4 + \ldots + \alpha_3^4) + 2(\alpha_1^2\alpha_2^2 \ldots$$

Bulk anisotropy tetragonal systems

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Tetragonal systems: TMPt, $SrCrO_3$, $RECuO_3$, layered sys: BaO/EuO

$$G^V_{\text{cryst}}(\widehat{M}) = K_1(\alpha_1^2+\alpha_2^2) + K_2(\alpha_1^2+\alpha_2^2)^2 + K_3 \ldots$$

$$G^V_{\text{cryst}}(\widehat{M}) = K_1 \sin^2\theta + K_2 \sin^4\theta$$

(cylinder symmetry ≡ uniaxial)

$$+ K_3 \sin^4\theta \cos 4\phi$$

(expresses fourfold symmetry)

For all uniaxial systems (tetra, hex, orthorhombic) polar coordinates

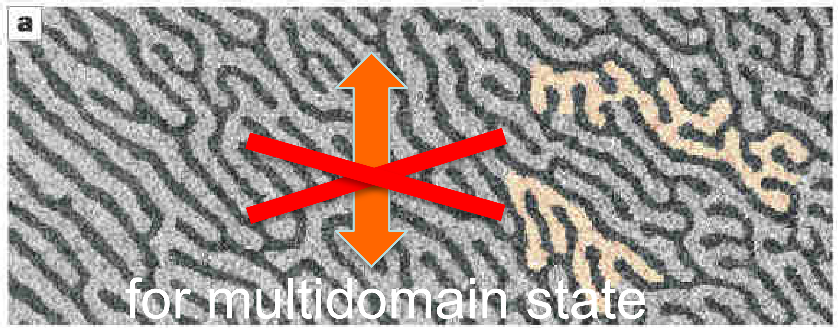
$$M(\widehat{M}) = M_0 + M_1 \sin^2\theta + M_2 \sin^4\theta + M_3 \sin^4\theta \cos 4\phi$$

Description of magnetic anisotropy

Phenomenology

Shape Anisotropy

Magnetocrystalline Aniso



Dipolar Interaction

Spin-Orbit Interaction

Microscopic Theory

Magnetocrystalline Anisotropy

Magnetocrystalline Anisotropy

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Origin : Spin-Orbit interaction − relates spin to dyn'cal degrees of freedom in crystal field

Most important: coupling of spin + orbital motion of same elect.

Spin-Orbit Interaction: $$H_{\rm SO} = \frac{\hbar^2}{2m^2c^2} \sum_i \frac{1}{r}\frac{dV_i}{dr} \vec{L}_i \cdot \vec{S}_i$$

Wavefunction: $$\psi(\vec{r}) \propto R_{n,\ell,\sigma}(r) Y_{\ell m}(\hat{r}) \chi_\sigma$$

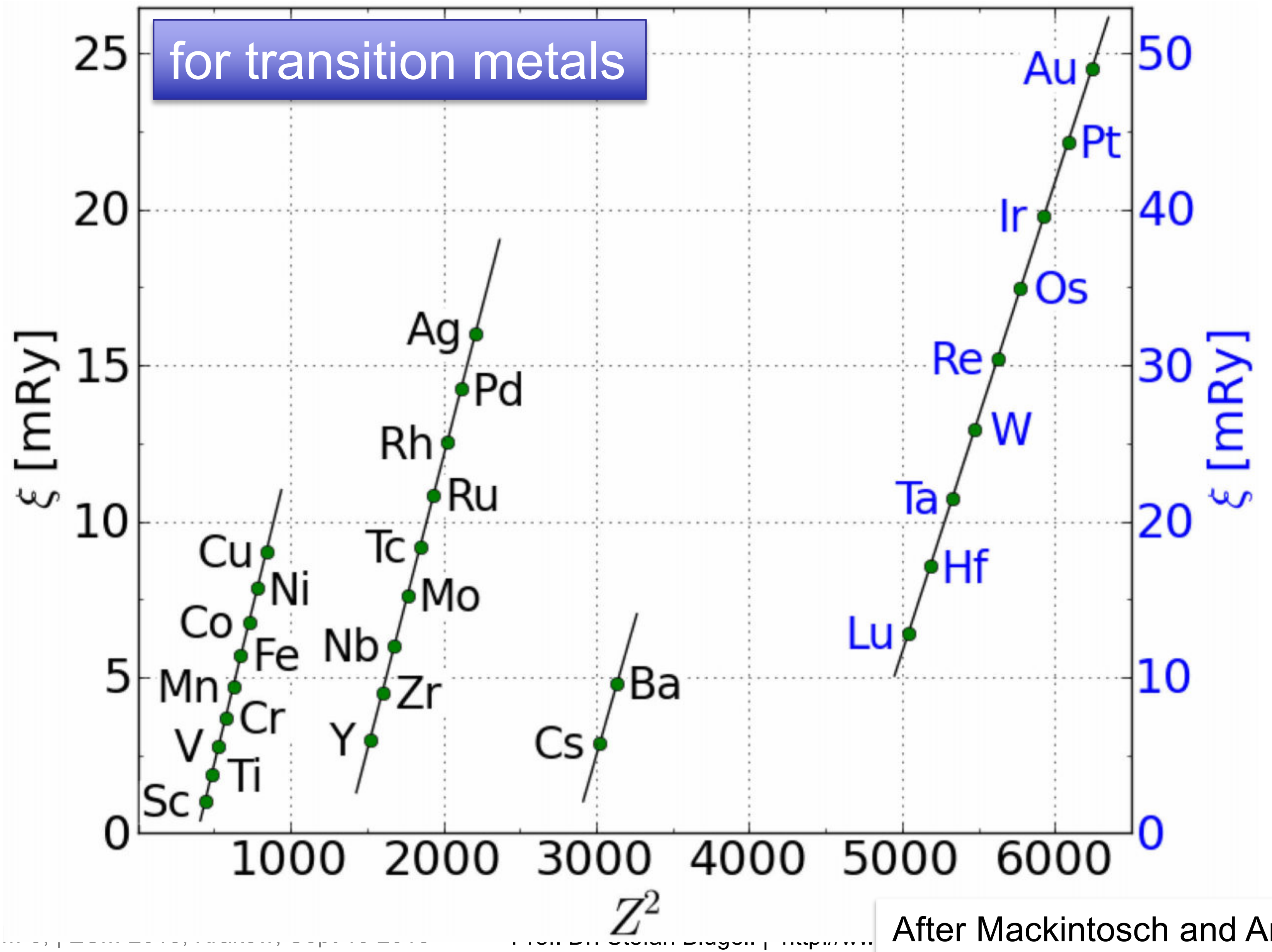
MAE due to MCA: $$E_{\rm MCA} \propto \langle\psi|H_{\rm SO}|\psi\rangle \propto \xi \, \langle Y|\vec{L}|Y\rangle\langle\chi|\vec{S}|\chi\rangle$$

(1st order perturbation)

Spin-Orbit strength: $$\xi_{n,\ell} \approx Z \cdot \left(\frac{Z}{a_{\rm B}}\right)^3 \cdot \frac{1}{n^3 l^2} \approx Z^2$$

(for $V(r) \approx Ze^2/r$)

Spin-Orbit Strength ξ(Z)



After Mackintosch and Andersen

Orbital moment quenching <L>=0

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

For any real wavefunction $|\Psi\rangle \longrightarrow \langle\Psi|L_z|\Psi\rangle$ purely imaginary

but:

L_z is Hermitian $\longrightarrow \langle\Psi|L_z|\Psi\rangle$ purely real

$\downarrow$

$\langle\Psi|L_z|\Psi\rangle$ must vanish!

$$\langle\Psi|L_x|\Psi\rangle = \langle\Psi|L_y|\Psi\rangle = \langle\Psi|L_z|\Psi\rangle = 0$$

For a real Hamiltonian, the non-degenerate states are described with real wavefunctions $|\Psi\rangle$

MAE due to MCA: $E_{\mathrm{MCA}} \propto \xi\langle\vec{L}\rangle\langle\vec{S}\rangle = 0!$

(1st order perturbation)

No MCA in 1st order SOI for orbitally non-degenerate states

Degenerate orbital states: <L>≠0

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Unquenched orbital moment can be expected in the degenerate states: d^1, d^2, *low spin* d^4, d^5 *and high spin* d^6, d^7.

Example doubly degenerate t_{2g} states: $|xz\rangle, |yz\rangle$

Form new complex eigenstates: $|\pm\rangle = 1/\sqrt{2}(|xz\rangle \pm i|yz\rangle)$

Angular momentum operator: $$L_z|\pm\rangle = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)|\pm\rangle$$

$$= \pm\hbar|\pm\rangle$$

Orbital moment: $\langle\pm|L_z|\pm\rangle = 1/2\,\hbar\,(\langle xz|xz\rangle + \langle yz|yz\rangle) \neq 0$

MCA in 1st order SOI possible for orbitally degenerate states

E_{MCA} large because <L> is determined at 1st order perturbation

Example: Spinel-Ferrite (Magnetite)

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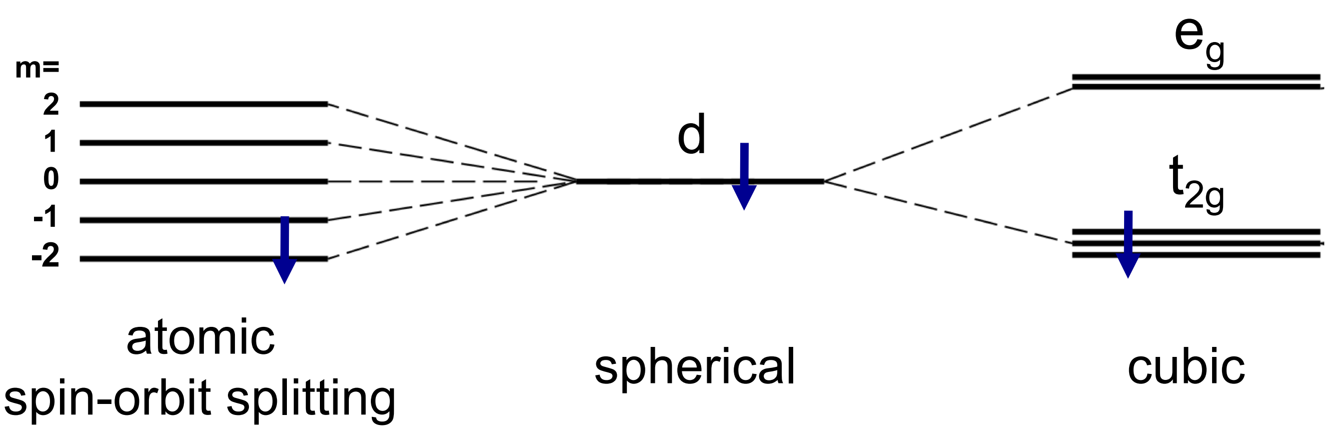
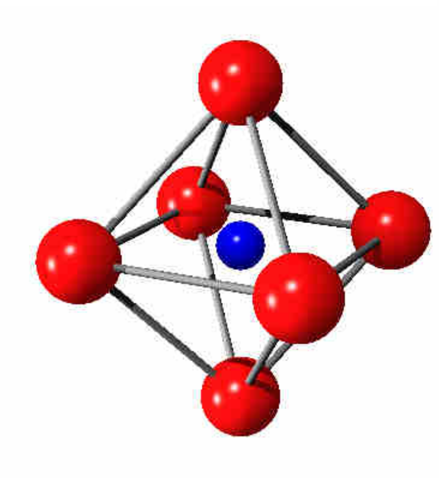
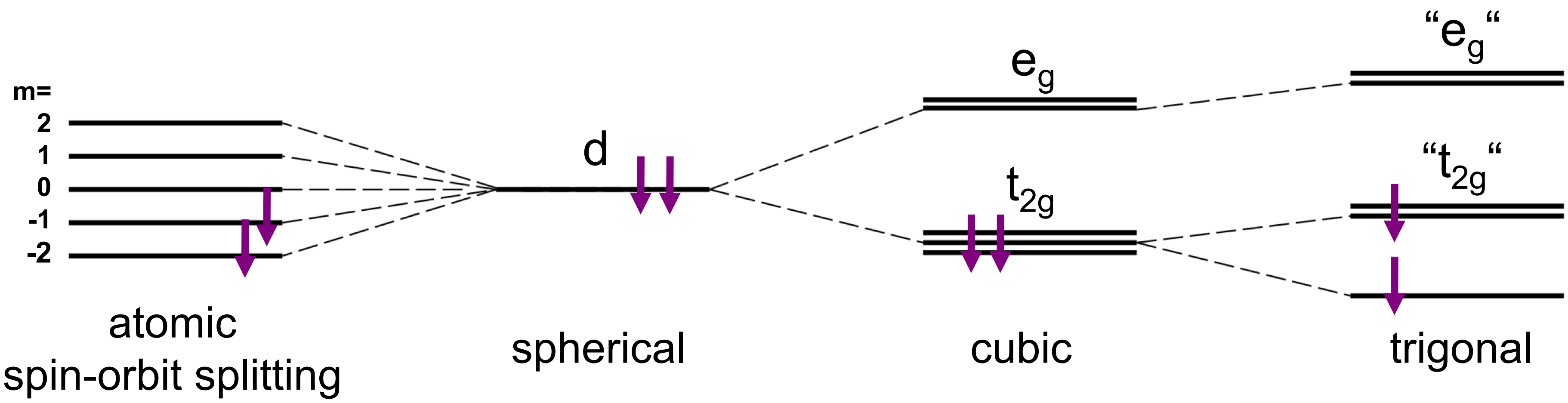
$Fe_3\ O_4$ $(Fe^{2+}O^{2-})(Fe_2^{3+}O_3^{2-})$ $K_1 = -2 \cdot 10^4$ $K_2 = -9 \cdot 10^3$ (J/m^{-3})

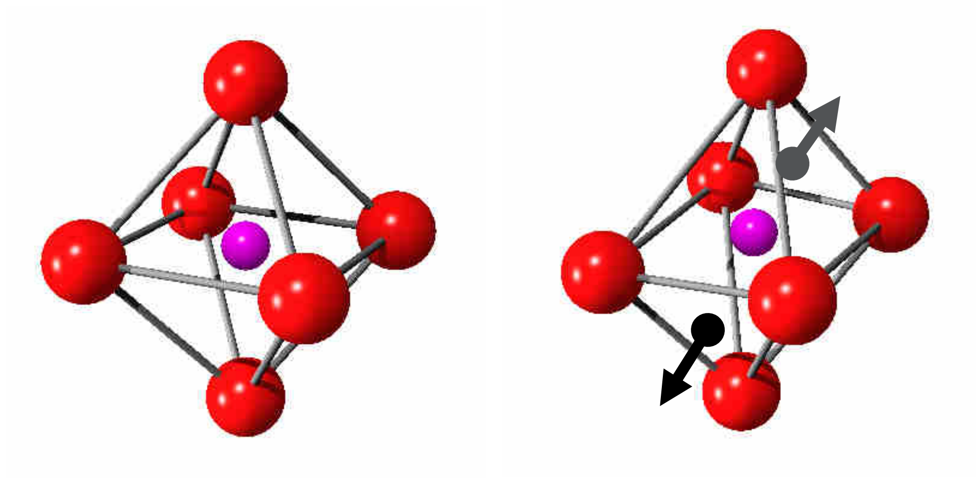




Example: Co mixed-spinel ferrite

$Fe_3\,O_4$	$(Fe^{2+}O^{2-})(Fe_2^{3+}O_3^{2-})$	$K_1 = -2 \cdot 10^4$	$K_2 = -9 \cdot 10^3$	(J/m^{-3})
$Co\,Fe_2\,O_4$	$(Co^{2+}O^{2-})(Fe_2^{3+}O_3^{2-})$	$K_1 \approx 10^6$	—	(J/m^{-3})





Unquenching the orbital moment by spin-orbit interaction

The spin-orbit interaction is in the wave function!

1st order perturbation theory: $$|o\rangle^{(1)} = |o\rangle + \sum_u \frac{\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$$

Orbital moment: $${}^{(1)}\langle o|\vec{L}|o\rangle^{(1)} \propto -\sum_{u(u\neq o)} \frac{\langle o|\vec{L}|u\rangle\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$$

MAE due to MCA: $$E_{\mathrm{MCA}} \propto \langle H_{\mathrm{SO}}\rangle \propto \xi\,\langle o|\vec{L}|o\rangle^{(1)}\langle\vec{S}\rangle$$

(2nd order perturbation) $$\propto -\sum_{u(u\neq o)} \frac{|\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle|^2}{(\epsilon_u - \epsilon_o)}$$

$|o\rangle :=$ occupied, ground states

$|u\rangle :=$ unoccupied, excited states

For d-states $|o\rangle, |u\rangle \in (|xy;\uparrow\rangle, |xz;\uparrow\rangle, |yz;\uparrow\rangle, |x^2-y^2;\uparrow\rangle, |3z^2-r^2;\uparrow\rangle$
$|xy;\downarrow\rangle, |xz;\downarrow\rangle, |yz;\downarrow\rangle, |x^2-y^2;\downarrow\rangle, |3z^2-r^2;\downarrow\rangle)$

Unquenching the orbital moment by spin-orbit interaction

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The spin-orbit interaction is in the wave function!

1st order perturbation theory:

$$|o\rangle^{(1)} = |o\rangle - \sum_{u(u\neq o)} \frac{\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)} |o\rangle$$

Symmetry-dependence
E.g. uniaxial symmetry

$$E(\theta) = K_0 + K_1 \sin^2\theta + K_2 \sin^4\theta$$

2nd 4th

$$G^V_{\mathrm{cryst}}(\hat{M}) = K_1(\alpha_1^2+\alpha_2^2) + K_2(\alpha_1^2+\alpha_2^2)^2$$

$$\alpha_1^4 \propto \widehat{M}\cdot\widehat{M}\cdot\widehat{M}\cdot\widehat{M} \propto \langle\vec{S}\rangle^4$$

MAE due to MCA:
(2nth order perturbation)

$$K_n \propto \langle H_{\mathrm{SO}}\rangle \propto -\sum_{u(u\neq o)} \frac{|\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle|^{2n}}{|(\epsilon_u-\epsilon_o)|^{(2n-1)}}$$

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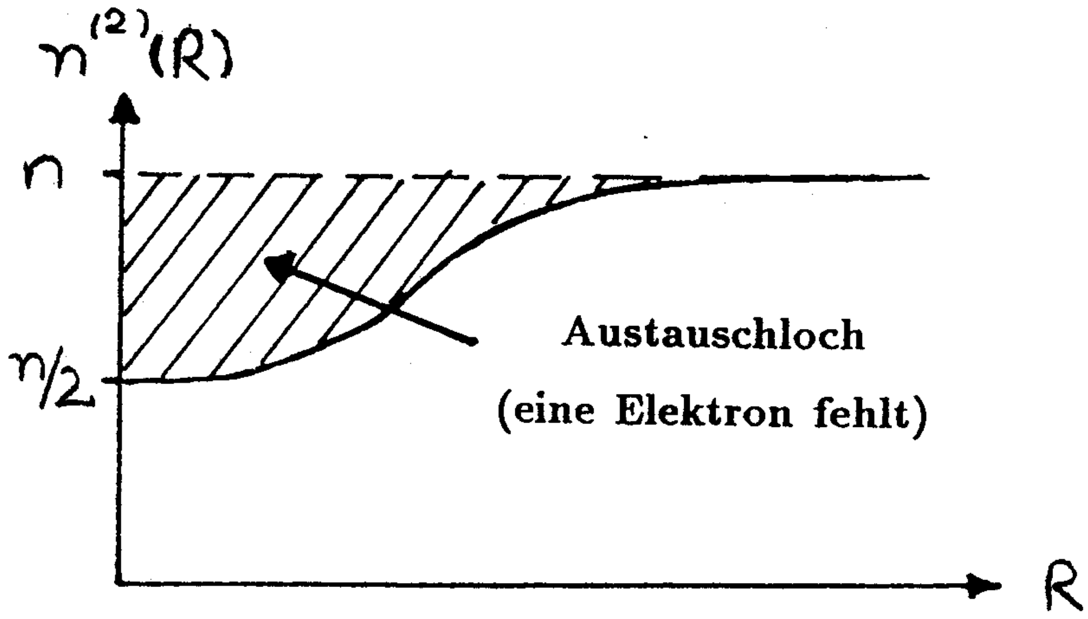
4. Homogeneous electron gas
(Hartree-Fock applied to plane wave functions)
Simple model for metal , but too simple

Discussed in lecture MM-1



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4. Stoner Model

Stoner Model for Ferromagnetism

- Xα approximation: only exchange (Hartree-Fock)

$$
\begin{aligned}
V_X^{\pm}(\mathbf{r}) &= -\alpha e^2 \left(\frac{6}{\pi}\right)^{1/3} \left(n^{\pm}(\mathbf{r})\right)^{1/3} \\
&= -\alpha e^2 \left(\frac{6}{\pi}\right)^{1/3} \left(n(\mathbf{r}) \pm m(\mathbf{r})\right)^{1/3} \\
&\approx V_X^0(\mathbf{r}) \mp m(\mathbf{r})\,\tilde{V}_X(\mathbf{r}) \qquad \text{(linearization)}
\end{aligned}
$$

- LSDA: $V_{xc}^{\pm}(\mathbf{r}) \approx V_{xc}^{0}(\mathbf{r}) \mp m(\mathbf{r})\,\tilde{V}_{xc}(\mathbf{r})$

- Model: $V_{xc}^{\pm}(\mathbf{r}) = V_{XC}^{o}(\mathbf{r}) \mp \frac{1}{2} IM$

$$M = \int_{V_{Atom}} m(\mathbf{r})\,d\mathbf{r}$$

$$I = 2 \int_{V_{Atom}} \tilde{V}_{xc}(\mathbf{r})\,d\mathbf{r}$$

Stoner Model for Ferromagnetism

- LSDA: $V_{xc}^{\pm}(\mathbf{r}) \approx V_{xc}^{0}(\mathbf{r}) \mp m(\mathbf{r})\tilde{V}_{xc}(\mathbf{r})$
- Model: $V_{xc}^{\pm}(\mathbf{r}) = V_{xc}^{o}(\mathbf{r}) \mp \frac{1}{2}IM$

$$M = \int_{V_{\text{Atom}}} m(\mathbf{r})d\mathbf{r}$$

$$I = 2\int_{V_{\text{Atom}}} \tilde{V}_{xc}(\mathbf{r})d\mathbf{r}$$

- Spin-dependent Hartree equations

$$\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 \mp V_{\text{eff}}([n_+, n_-]|\mathbf{r})\right]\varphi_{i\pm}(\mathbf{r}) = \epsilon_{i\pm}\varphi_{i\pm}(\mathbf{r})$$

$\Longrightarrow$ For Stoner model

$$\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V_{\text{eff}}^{o}(\mathbf{r}) \mp \frac{1}{2}IM\right]\varphi_{i\pm}(\mathbf{r}) = \epsilon_{i\pm}\varphi_{i\pm}(\mathbf{r})$$

Stoner Model for Ferromagnetism

- Model: $V_{xc}^{\pm}(\mathbf{r}) = V_{xc}^{o}(\mathbf{r}) \mp \frac{1}{2} IM \qquad M = \int_{V_{\text{Atom}}} m(\mathbf{r}) d\mathbf{r}$

- For Stoner model

$$\left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V_{\text{eff}}^{o}(\mathbf{r}) \mp \frac{1}{2} IM \right] \varphi_{i\pm}(\mathbf{r}) = \epsilon_{i\pm} \varphi_{i\pm}(\mathbf{r})$$

- *M* constant

$$\Longrightarrow \quad \varphi_{i\pm}(\mathbf{r}) = \varphi_{\mathbf{k}\nu\pm}(\mathbf{r}) = \varphi_{\mathbf{k}\nu}^{0}(\mathbf{r})$$

$$\epsilon_{i\pm} = \epsilon_{\mathbf{k}\nu\pm} = \epsilon_{\mathbf{k}\nu}^{0} \pm \frac{1}{2} IM$$

$$n_{\pm}(E) = \sum_{\nu} \int_{\text{BZ}} \delta(E - \epsilon_{\mathbf{k}\nu\pm})\, d\mathbf{k} = n^0 \left(E \pm \frac{1}{2} IM \right)$$

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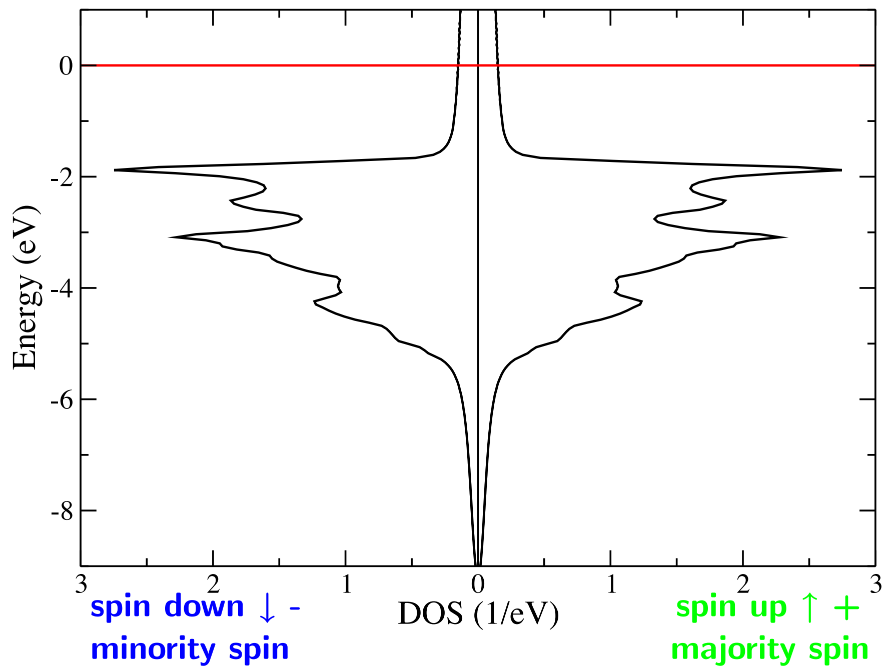
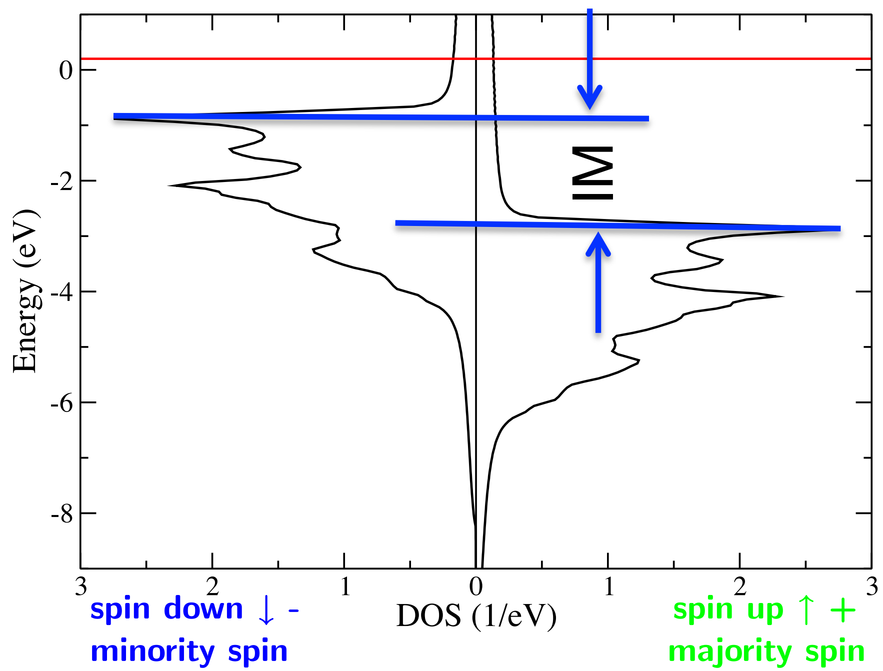
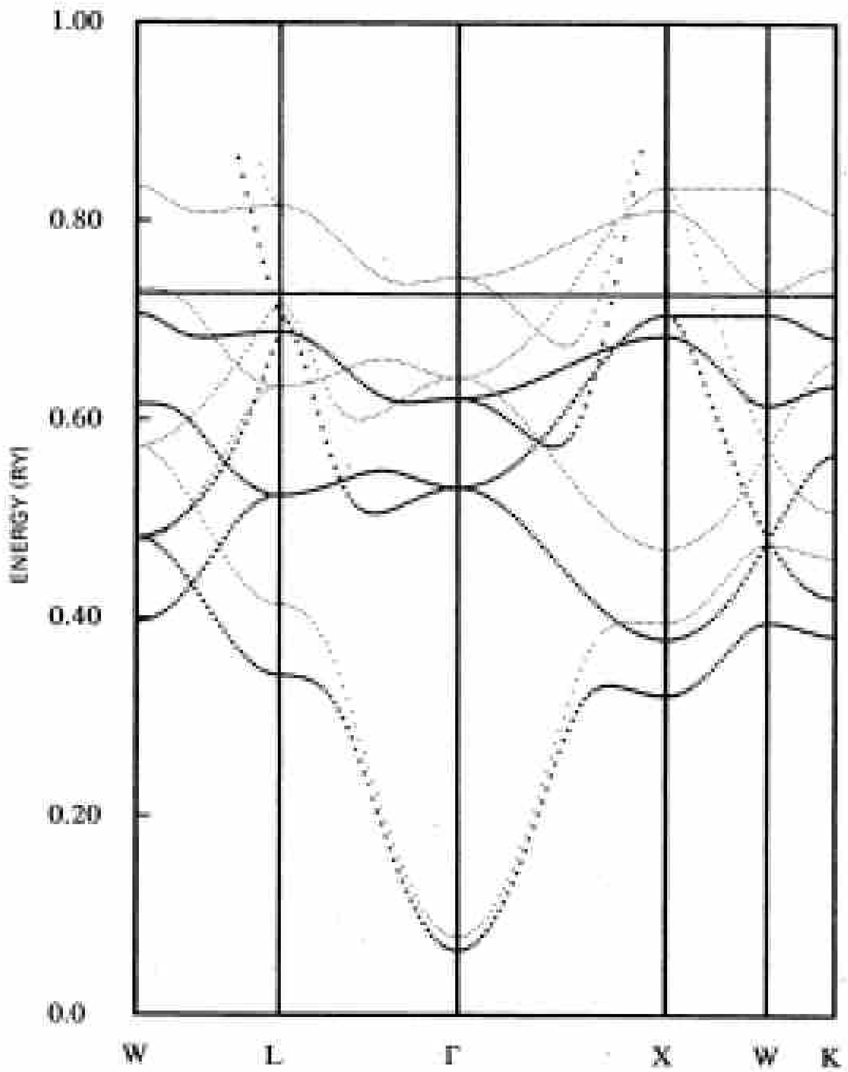
Exchange split density of states





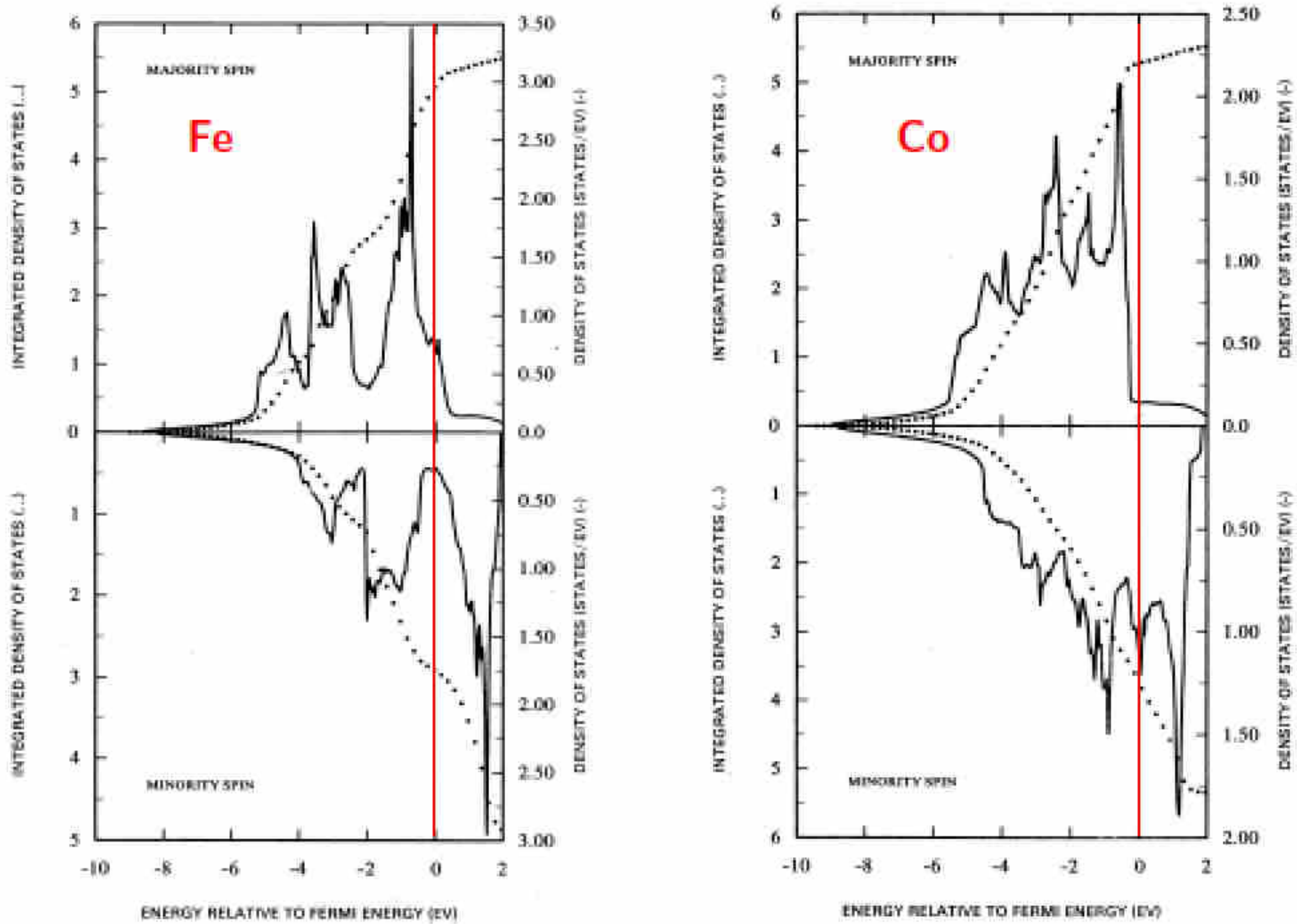
Band structure of ferromagnetic fcc-Co

bandstructure
for fcc Co



Moruzzi, Janak, Williams (1978)

Density of States of Fe and Co



Moruzzi, Janak, Williams (1978)

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Derivation of Stoner criterion

- Self-consistency condition

$$N = \int^{E_F} \left[n^0(E + \frac{1}{2}IM) + n^0(E - \frac{1}{2}IM) \right] dE$$

$$M = \int^{E_F} \left[n^0(E + \frac{1}{2}IM) - n^0(E - \frac{1}{2}IM) \right] dE$$

- Two equations: $\Longrightarrow$ $E_F = E_F(M)$ and $M = F(M)$

1. $E_F(M)$ is even function in M: $E_F = E_F(M) \approx E_F(0) + \frac{1}{2} E_F''(0) M^2$

Side remark

One calculates $\frac{dE_F}{dM}$ from $dN = 0$

$$dN = 0 = \frac{\partial N}{\partial E_F} dE_F + \frac{\partial N}{\partial M} dM = \left(n_+^0 + n_-^0\right) dE_F + \frac{I}{2}\left(n_+^0 - n_-^0\right) dM$$

2.

$$\Longrightarrow F'(M) = \frac{I}{2}\left(n_+^0 + n_-^0\right)\left\{1 - \left(\frac{n_+^0 - n_-^0}{n_+^0 + n_-^0}\right)^2\right\} \geq 0$$

where $$n_\pm^0 = n^0\left(E_F \pm \frac{IM}{2}\right) \geq 0$$

Derivation of Stoner criterion

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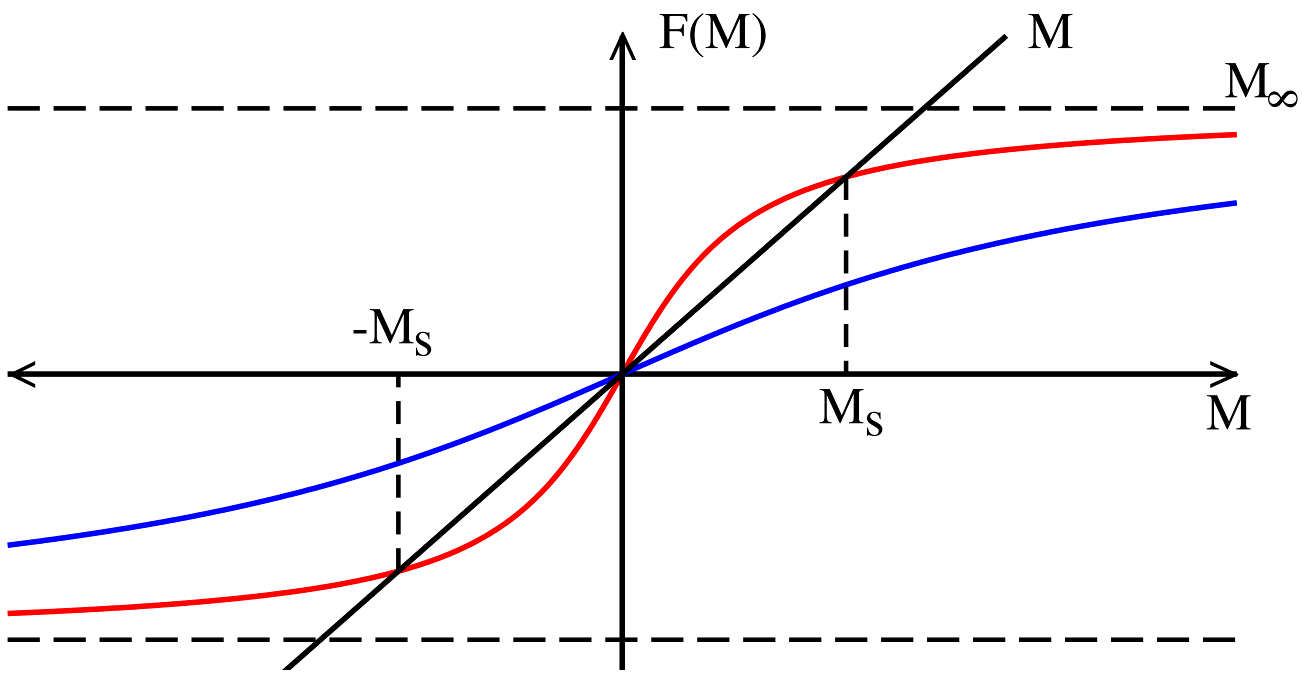
- Self-consistency condition

$$N = \int^{E_F} \left[n^0(E + \frac{1}{2}IM) + n^0(E - \frac{1}{2}IM) \right] dE$$

$$M = \int^{E_F} \left[n^0(E + \frac{1}{2}IM) - n^0(E - \frac{1}{2}IM) \right] dE$$



Derivation of Stoner criterion

1. One solution M=0 if $F'(M)$<1
2. Three solutions M=0 and $M=\pm M_s$ if $F'(M)$>1

➢ The derivative $F'(M)$ is

$$F'(M) = \frac{I}{2}\left[n^0(E_F + \frac{1}{2}IM) + n^0(E_F - \frac{1}{2}IM)\right] + \left[n^0(E_F + \frac{1}{2}IM) - n^0(E_F - \frac{1}{2}IM)\right]\frac{dE_F}{dM}$$

=0 for M=0

which for M=0 leads to $F'(0) = In^0(E_F)$ and
the sufficient condition for magnetic solutions is $F'(0)>1$, which implies the Stoner criterion

⟹Stoner criterion: $$In^0(E_F) = 1$$

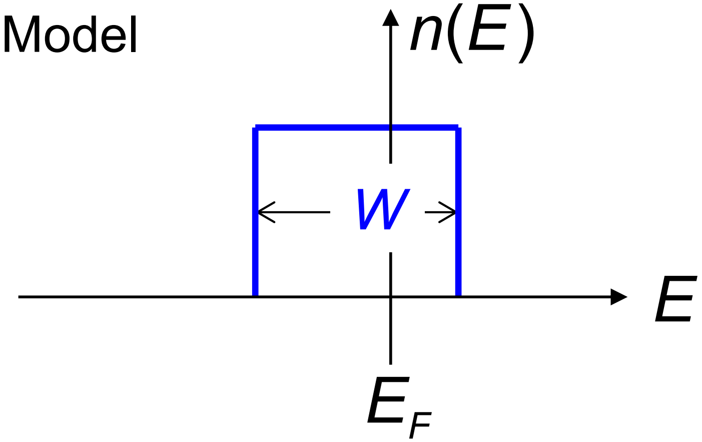
2. Evaluation of Stoner Model for bulk materials

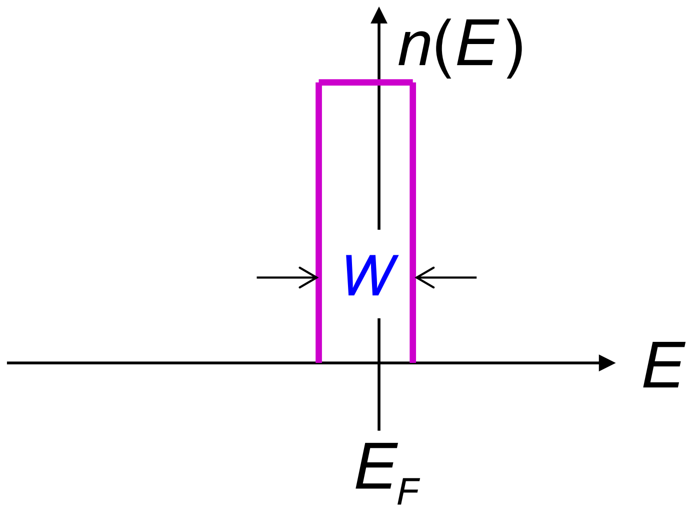
Stoner Model for Ferromagnetism

- Stoner criterion: $I \bullet n(E_F) > 1$
  (for d-electrons)

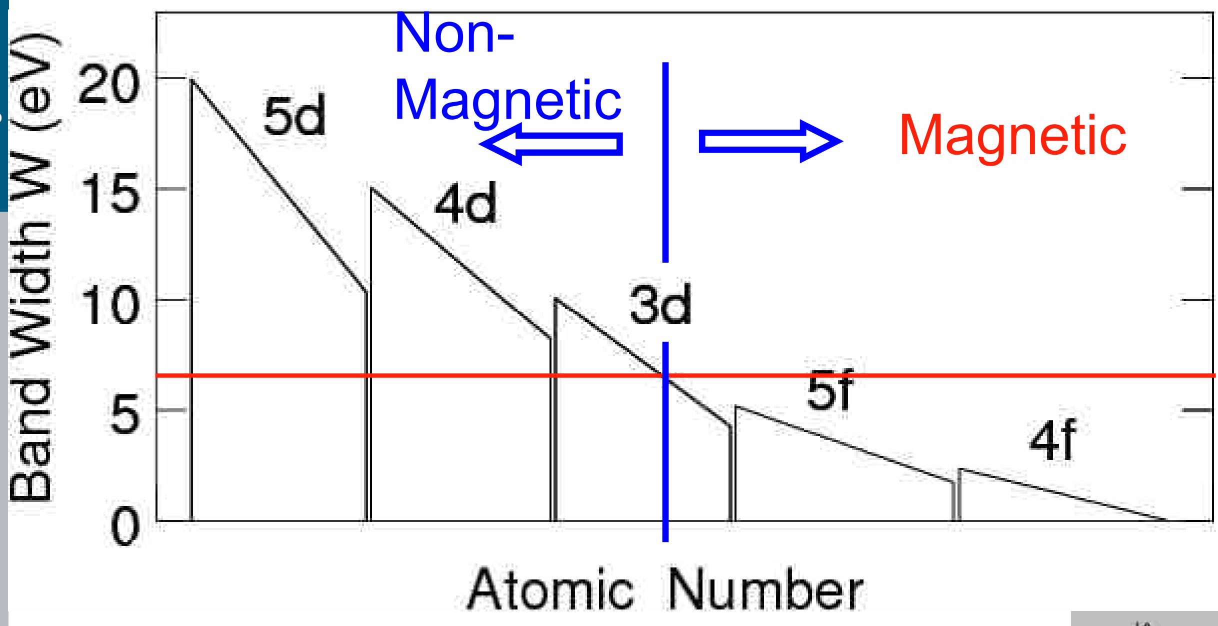
- Density of states: $n(E_F) \sim \frac{1}{W}$ $\quad [\ n \bullet W = 5\ ]$

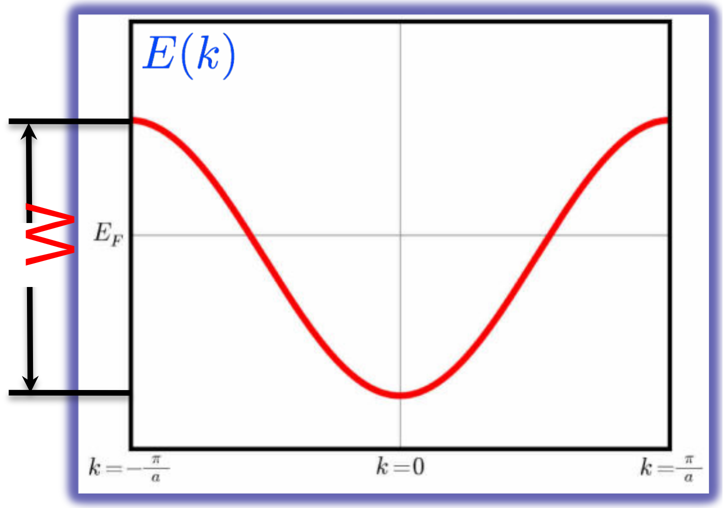
Model

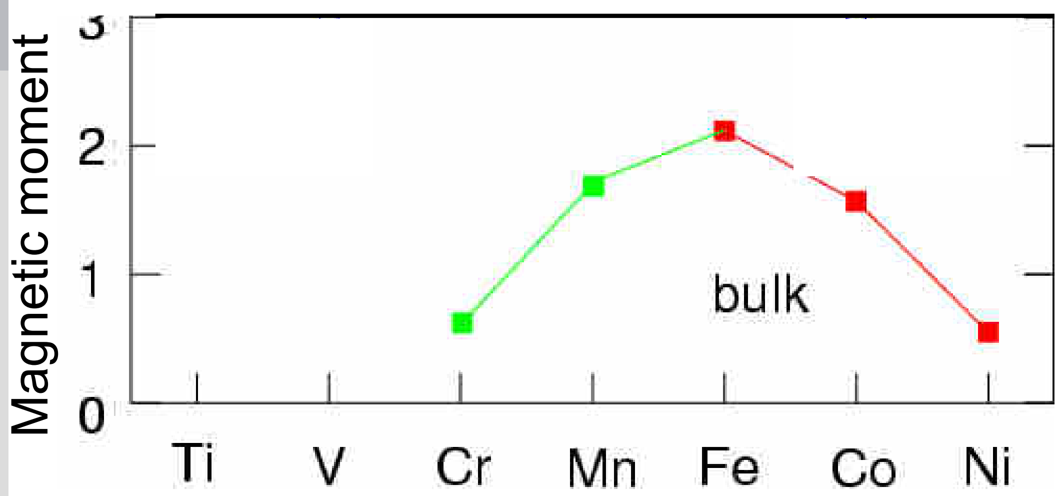


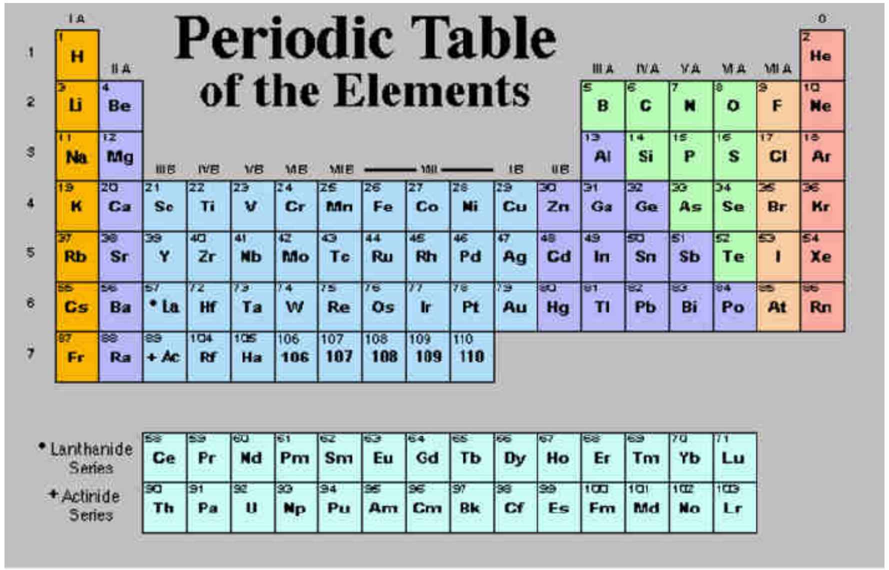


Bandwidths of metals

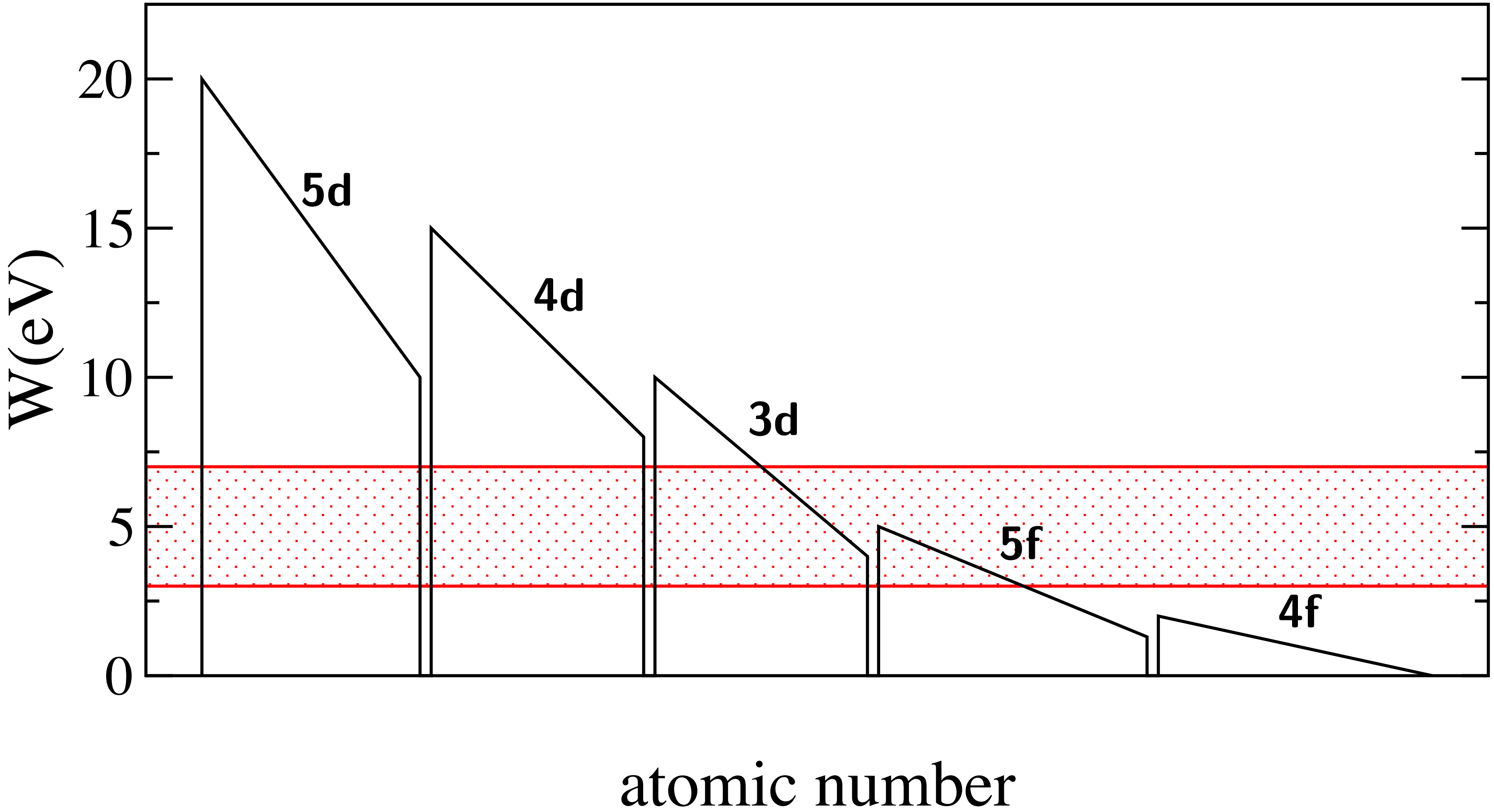








Band width *W* as measure for localization



Stoner Parameter

metal	$n^o(E_F)[eV^{-1}]$	$I[eV]$	$In^o(E_F)$	$S = \chi/\chi_0$
Na	0.23	1.82	0.41	1.71
Al	0.21	1.22	0.25	1.34
Cr	0.35	0.76	0.27	1.36
Mn	0.77	0.82	0.63	2.70
Fe	1.54	0.93	1.43	-2.34
Co	1.72	0.99	1.70	-1.43
Ni	2.02	1.01	2.04	-0.97
Cu	0.14	0.73	0.11	1.12
Pd	1.14	0.68	0.78	4.44
Pt	0.79	0.63	0.50	2.00

Gunnarson (1976), Janak (1977)

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4. Heisenberg Model

The Heisenberg Model

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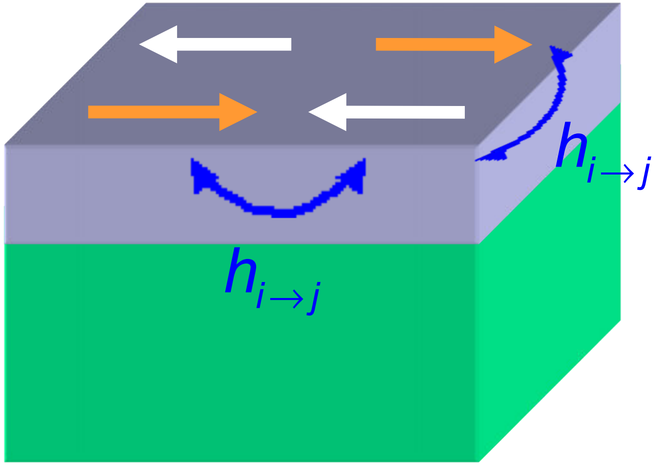
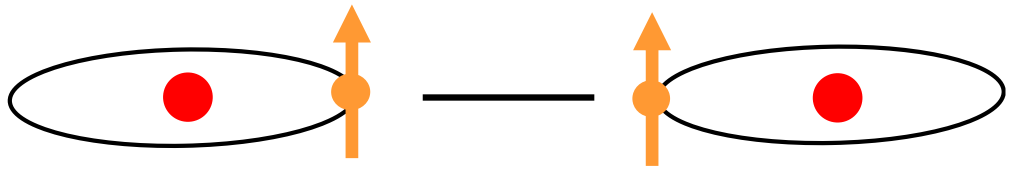
(Derivation of an effective spin model) **H_2-molecule**





$$s_1 = \frac{1}{2} \qquad s_2 = \frac{1}{2}$$

$$|s_1 - s_2| \leq S \leq s_1 + s_2$$

Singlet state: $\vec{S}^2 \chi_0 = 0$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_S(\vec{r}_1; \vec{r}_2)\chi_0$$

Triplet state: $\vec{S}^2 \chi_1 = 2\chi_1$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_T(\vec{r}_1; \vec{r}_2)\chi_1$$

The Heisenberg Model

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Singlet: S=0

$$\chi_0 = \sqrt{1/2}\,(\,|+,-\rangle - |-,+\rangle\,)$$

Triplet: S=1

$$\begin{cases} \chi_{1,1} = |+,+\rangle \\ \chi_{1,0} = \sqrt{1/2}\,(\,|+,-\rangle + |-,+\rangle\,) \\ \chi_{1,-1} = |-,-\rangle \end{cases}$$

- singlet is anti-symmetric in the spin variables
- triplet is symmetric.
- Pauli principle allows only totally antisymmetric wavefunctions,

➔ (Orbital-) real space wavefunction

singlet: $\phi_S(\mathbf{r}_1,\mathbf{r}_2)$, symmetric,

triplet: $\phi_T(\mathbf{r}_1,\mathbf{r}_2)$, anti-symmetric

Singlet state: $\vec{S}^2\chi_0 = 0$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_S(\vec{r}_1; \vec{r}_2)\chi_0$$

- Energies E_S for ϕ_s and E_T for ϕ_T are different

➔ Exchange energy:

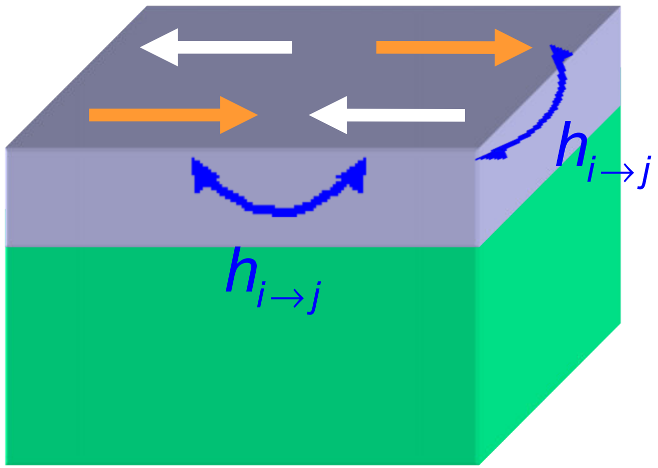
$$J = E_{\text{triplet}} - E_{\text{singlet}}$$

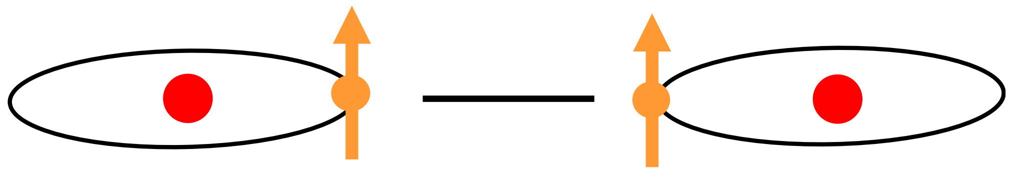
Triplet state: $\vec{S}^2\chi_1 = 2\chi_1$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_T(\vec{r}_1; \vec{r}_2)\chi_1$$

The Heisenberg Model

(Derivation of an effective spin model) **H_2-molecule**





$$s_1 = \frac{1}{2} \qquad s_2 = \frac{1}{2}$$

$$|s_1 - s_2| \leq S \leq s_1 + s_2$$

Singlet state: $\vec{S}^2\chi_0 = 0$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_S(\vec{r}_1; \vec{r}_2)\chi_0$$

Triplet state: $\vec{S}^2\chi_1 = 2\chi_1$

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \Phi_T(\vec{r}_1; \vec{r}_2)\chi_1$$

Energy of eigenstate: E_S or E_T

$$\mathcal{H}_S = \begin{cases} E_S & \text{if} \quad \vec{S}^2\chi_0 = 0 \\ E_T & \text{if} \quad \vec{S}^2\chi_1 = 2\chi_1 \end{cases}$$

The Heisenberg Model

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Energy of eigenstate: E_S or E_T

$$\mathcal{H}_S = \begin{cases} E_S & \text{if} \quad \vec{S}^2\chi_0 = 0 \\ E_T & \text{if} \quad \vec{S}^2\chi_1 = 2\chi_1 \end{cases}$$

$$J := E_S - E_T$$

$$\vec{s}_1\vec{s}_2 = 1/2\left(\vec{S}^2 - \vec{s}_1^{\,2} - \vec{s}_2^{\,2}\right)$$

$$\vec{S}^2 \;\hat{=}\; (\vec{s}_1 + \vec{s}_2)^2$$

$$\mathcal{H}_s = -J_{12}\vec{s}_1 \cdot \vec{s}_2 + 3/4E_T + 1/4E_s$$

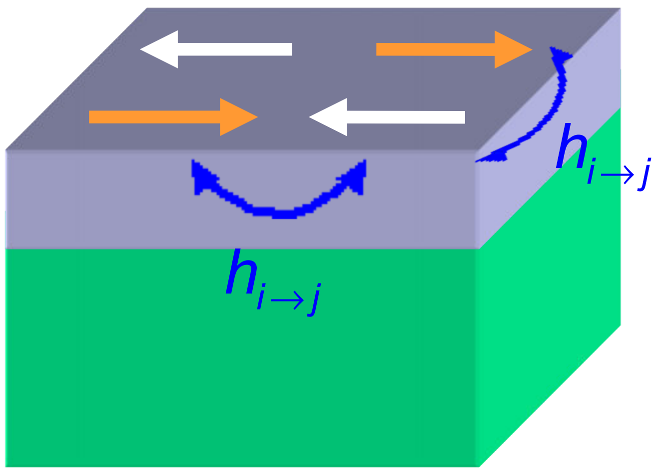
$$\vec{s}_1 \cdot \vec{s}_2\chi_0 = \frac{1}{2}\left(0 - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right)\right)\chi_0 = -\frac{3}{4}\chi_0$$

$$\mathcal{H}_S\chi_0 = -(E_S - E_T)(-3/4)\chi_0 + (3/4E_T + 1/4E_S)\chi_0 = E_S\chi_0$$

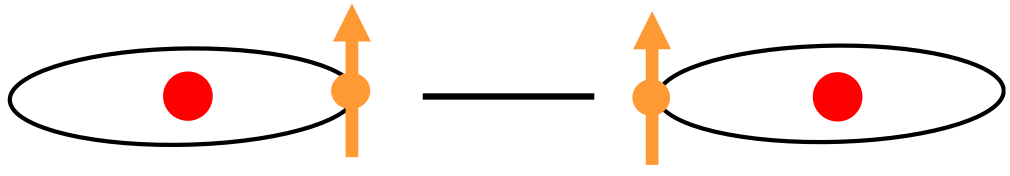
$$\mathcal{H}_S\chi_1 = -(E_S - E_T)(+1/4)\chi_1 + (3/4E_T + 1/4E_S)\chi_1 = E_T\chi_1$$

The Heisenberg Model

(Derivation of an effective spin model)



H_2-molecule



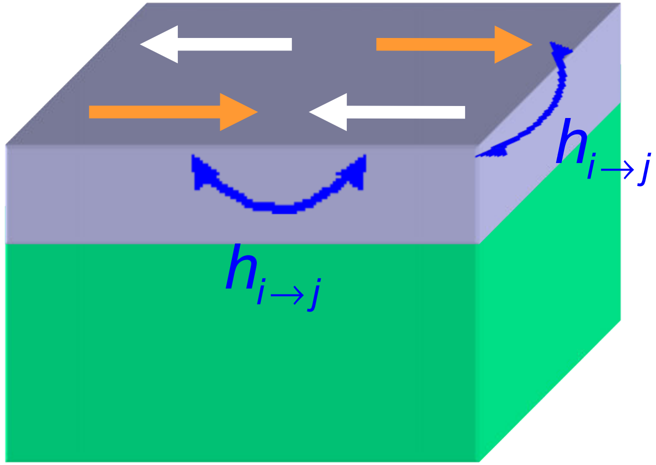
Energy of eigenstate: E_S or E_T

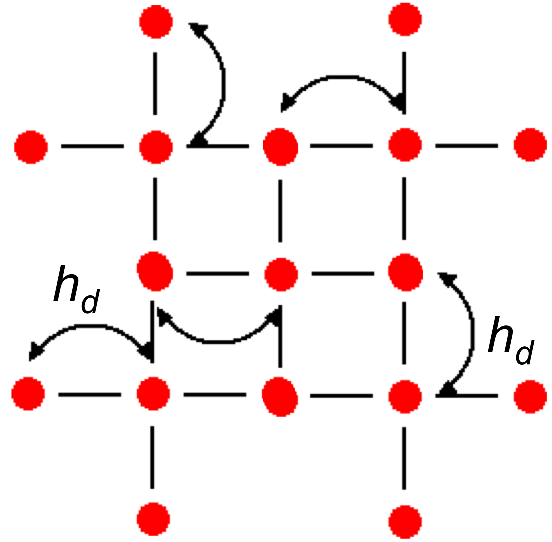
$$\mathcal{H}_S = \begin{cases} E_S & \text{if} \quad \vec{S}^2\chi_0 = 0 \\ E_T & \text{if} \quad \vec{S}^2\chi_1 = 2\chi_1 \end{cases}$$

$$\mathcal{H}_s = -J_{12}\vec{s}_1 \cdot \vec{s}_2 + 3/4 E_T + 1/4 E_s$$

The Heisenberg Model

(Derivation of an effective spin model)





→ generalization

Heisenberg Model:

$$\mathcal{H}_s = -\frac{1}{2}\sum_{i,j} J_{ij}\vec{s}_i \cdot \vec{s}_j$$

Energy of eigenstate: E_S or E_T

$$\mathcal{H}_S = \begin{cases} E_S & \text{if} \quad \vec{S}^2\chi_0 = 0 \\ E_T & \text{if} \quad \vec{S}^2\chi_1 = 2\chi_1 \end{cases}$$

$$\mathcal{H}_s = -J_{12}\vec{s}_1 \cdot \vec{s}_2 + 3/4E_T + 1/4E_s$$

Heisenberg Model

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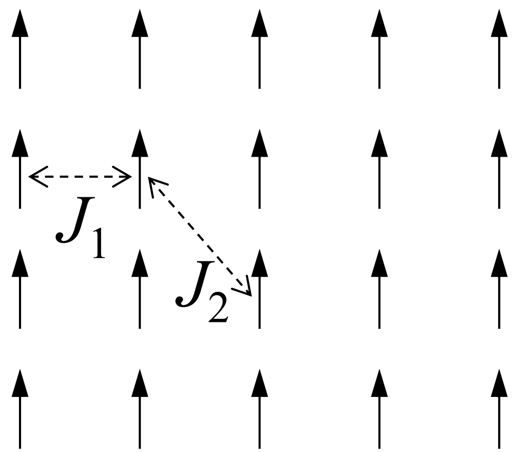
Heisenberg model

$$\mathcal{H}_s = -\frac{1}{2}\sum_{i,j} J_{ij}\,\vec{\mathcal{S}}_i \cdot \vec{\mathcal{S}}_j$$

$J > 0$: Ferromagnetism
$J < 0$: Antiferromagnetism

Applications:

- o Search of magnetic ground states
- o Thermodynamical properties
- o Magnetic excitations
- o Magnetization dynamics



$$J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)$$

Heisenberg Model

Quantum Heisenberg model $\mathcal{S} = \frac{1}{2}, 1, \frac{3}{2}, \cdots$

$$\mathcal{H}_S = -\frac{1}{2}\sum_{i,j} J_{ij}\,\vec{\mathcal{S}}_i \cdot \vec{\mathcal{S}}_j \qquad M_S = -S, -S+1, \ldots, S-1, S$$

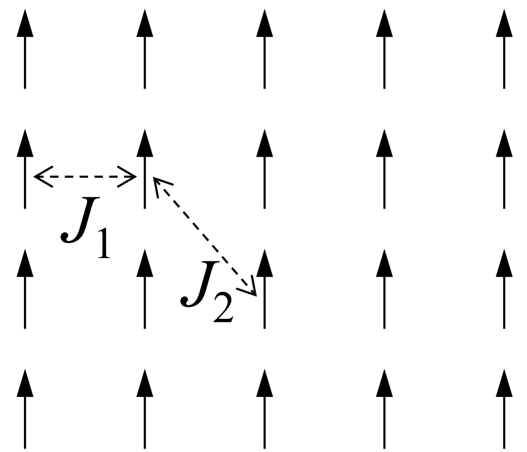
Applications:

o Search of magnetic ground states

o Thermodynamical properties

o Magnetic excitations

o Magnetization dynamics



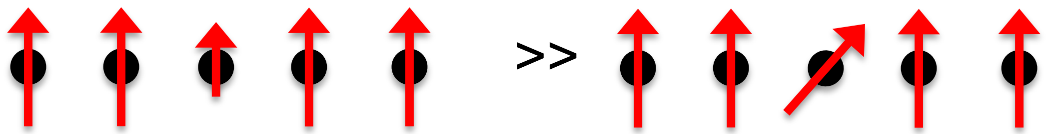
$$J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)$$

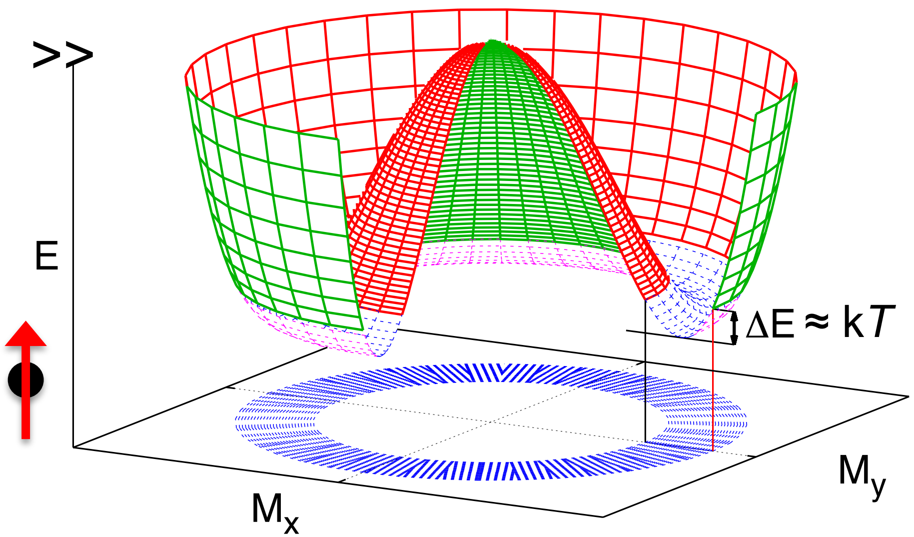
Conditions for classical Heisenberg model

Magnetic moments are localized within muffin-tin sphere

Energy for moments magnitude (1- 2 eV) >>
energy for moments rotation (0.1-0.2 eV)

Magnitude change   Rotation





Adiabatic principle:
Time-scale of moment rotations (ps) >> time-scale of electron hopping (fs)

See e.g. You and Heine 1982; Staunton et al. 1985; Antropov et al. 1996; Halilov et al. 1998

Classical Heisenberg Model

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Classical Heisenberg model: $\vec{\mathcal{S}} \rightarrow \vec{S} = \langle \vec{\mathcal{S}} \rangle$

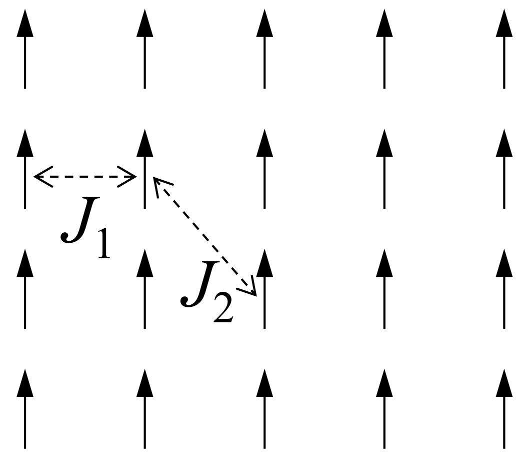
$$H_S = -\frac{1}{2} \sum_{i,j} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$

$J > 0$: Ferromagnetism

$J < 0$: Antiferromagnetism

Applications:

- o Search of magnetic ground states
- o Thermodynamical properties
- o Magnetic excitations
- o Magnetization dynamics



$$J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)$$

Classical Heisenberg Model

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Classical Heisenberg model: $\vec{\mathcal{S}} \rightarrow \vec{S} = \langle \vec{\mathcal{S}} \rangle = \mathbf{S}$

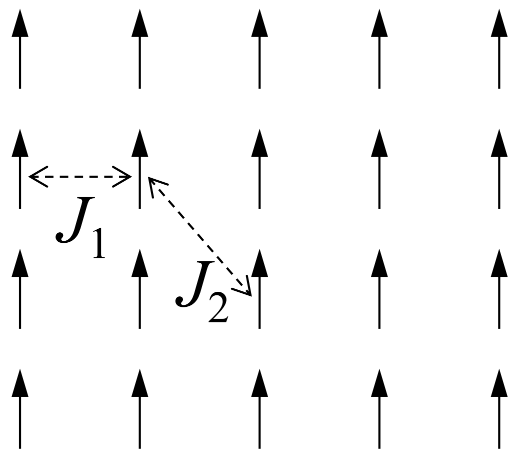
$$H_S = -\frac{1}{2}\sum_{i,j} J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j$$

$J > 0$: Ferromagnetism

$J < 0$: Antiferromagnetism

Applications:

- o Search of magnetic ground states
- o Thermodynamical properties
- o Magnetic excitations
- o Magnetization dynamics



$$J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)$$

Frustrated Magnetism

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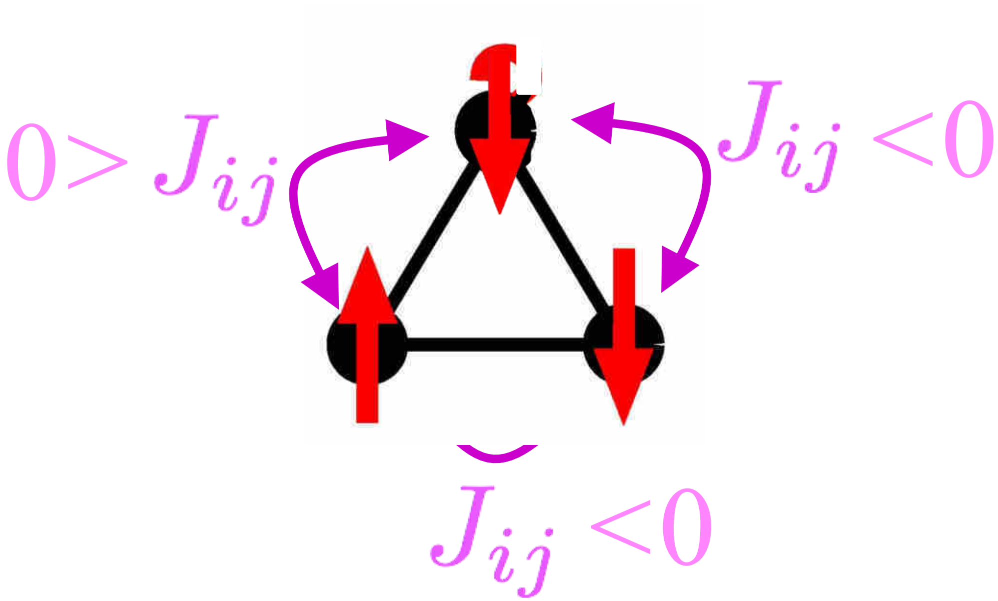
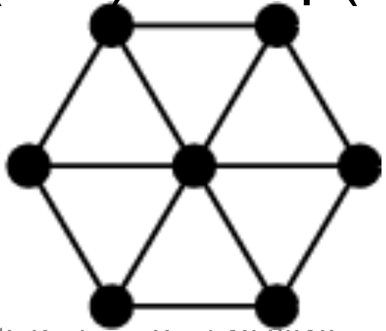
Geometrical Frustration



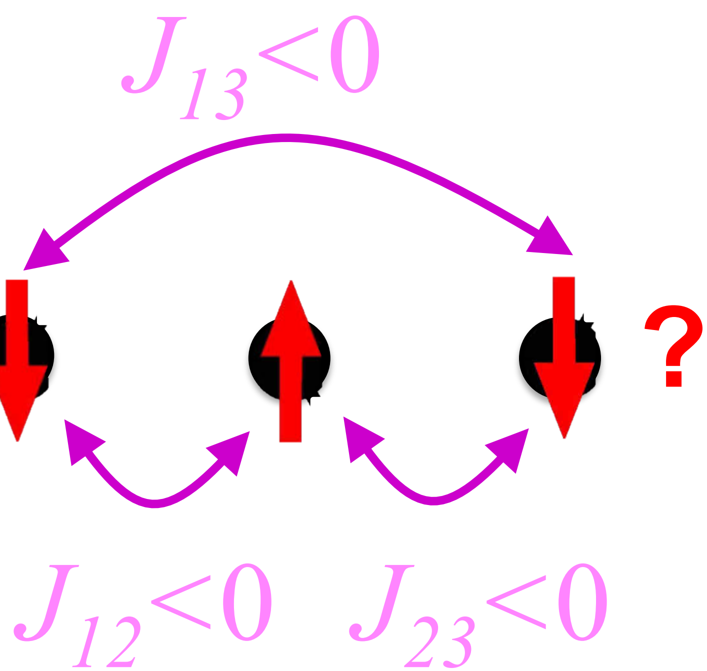
Cr/Mn on fcc(111) or hcp(0001)



Frustration of Exchange interactions

Heisenberg Model

$$H = -\sum_{i,j} J_{ij} \mathbf{S}_i \mathbf{S}_j$$



Fermi surface of transition metals

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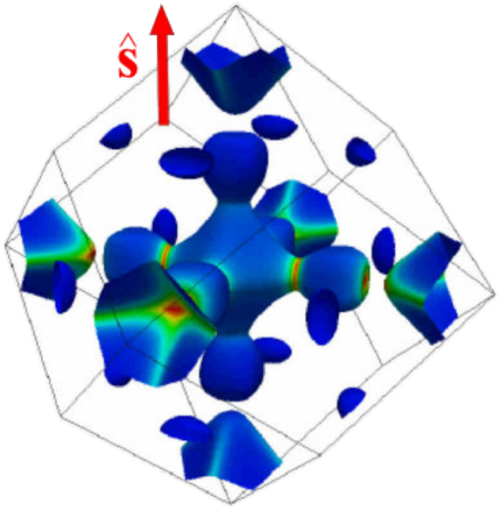
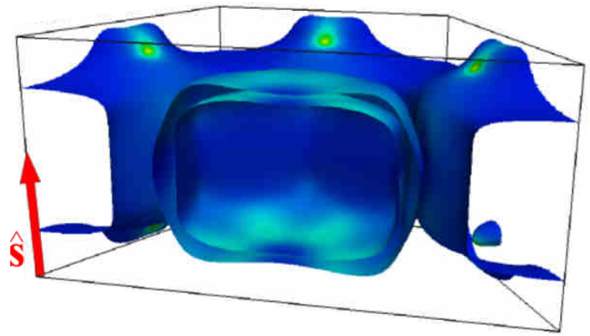
bcc W (Z=74)



hcp Os (Z=76)



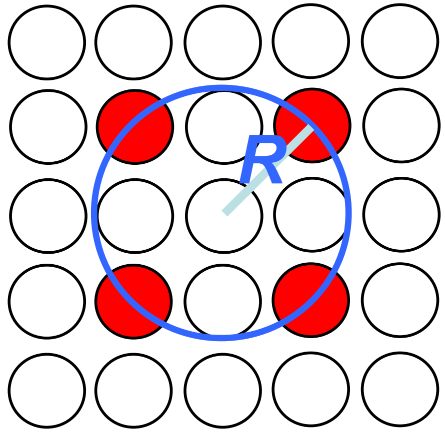
details matter !

$$J_{ij} \propto \frac{\cos(2k_F|\mathbf{R}_i - \mathbf{R}_j|)}{|\mathbf{R}_i - \mathbf{R}_j|^3}$$

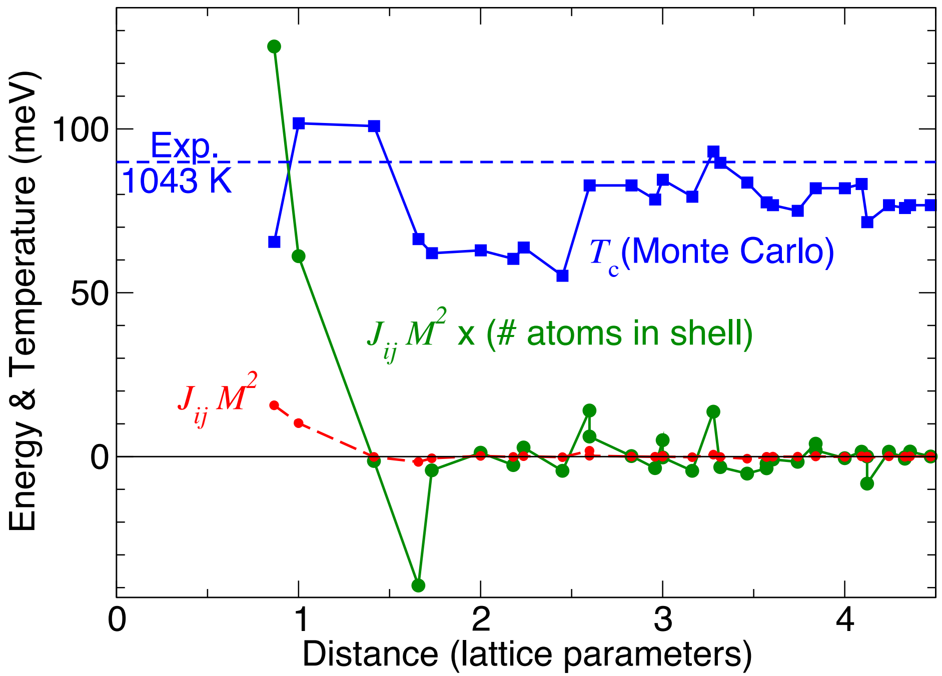
Oscillatory exchange interaction

$$J_{ij} \propto \frac{\cos(2k_F|\mathbf{R}_i - \mathbf{R}_j|)}{|\mathbf{R}_i - \mathbf{R}_j|^3} e^{-2\sqrt{E_g}|\mathbf{R}_i - \mathbf{R}_j|}$$

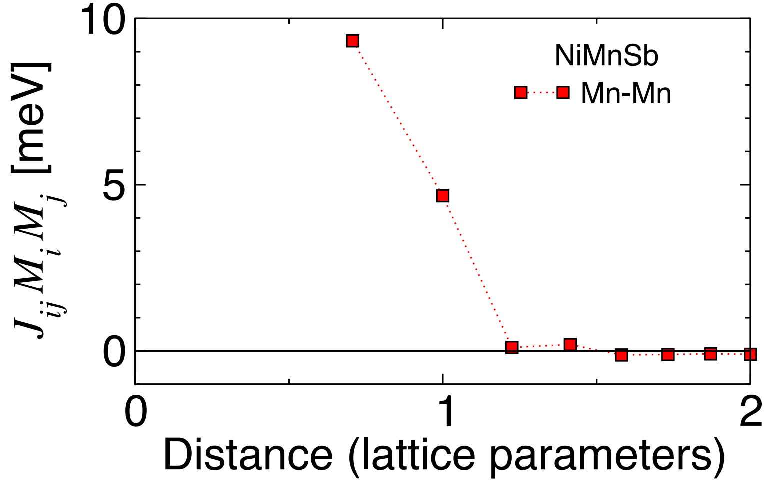
Shell of equivalent atoms at a distance



Exchange interactions and Curie temperature in bcc Fe



Exchange interactions in NiMnSb



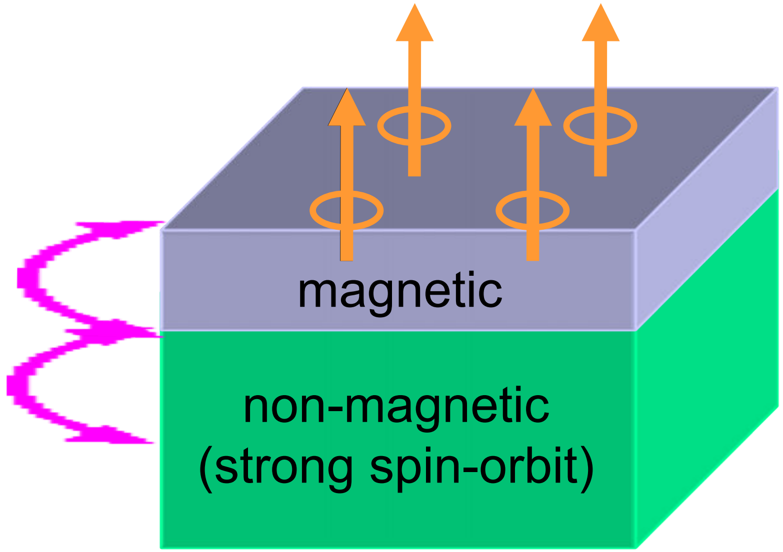
An other exotic magnetic interaction: Dzyaloshinsky Moriya Interaction

- Magnetism is a field with many different types of interactions at different length and energy scales.

Dzyaloshinskii-Moriya Interaction

Break of inversion symmetry

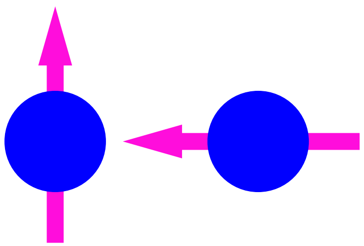
$P(z) \neq P(-z)$

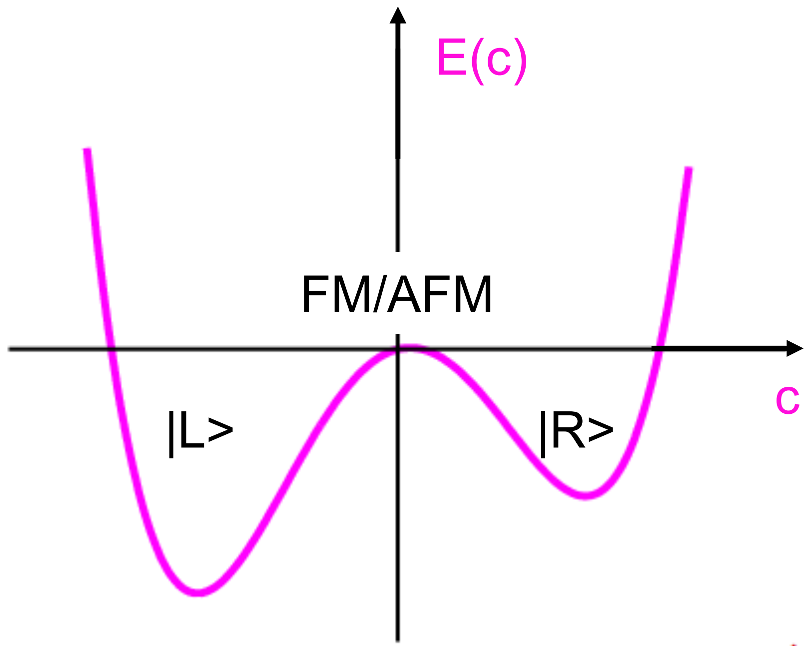


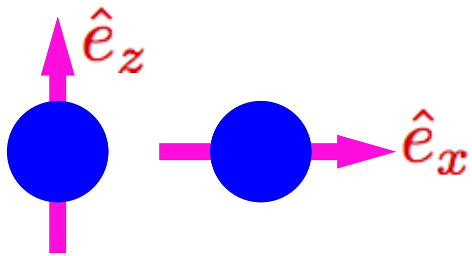
$$H_{\mathrm{DM}} = \sum_{ij} \mathbf{D}_{ij} \underbrace{\mathbf{m}_i \times \mathbf{m}_j}_{\mathbf{c}_{ij}}$$

Dzyaloshinskii-Moriya
Antisymmetric Exchange
Chiral magnetic interaction

Dzyaloshinskii-Moriya Interaction







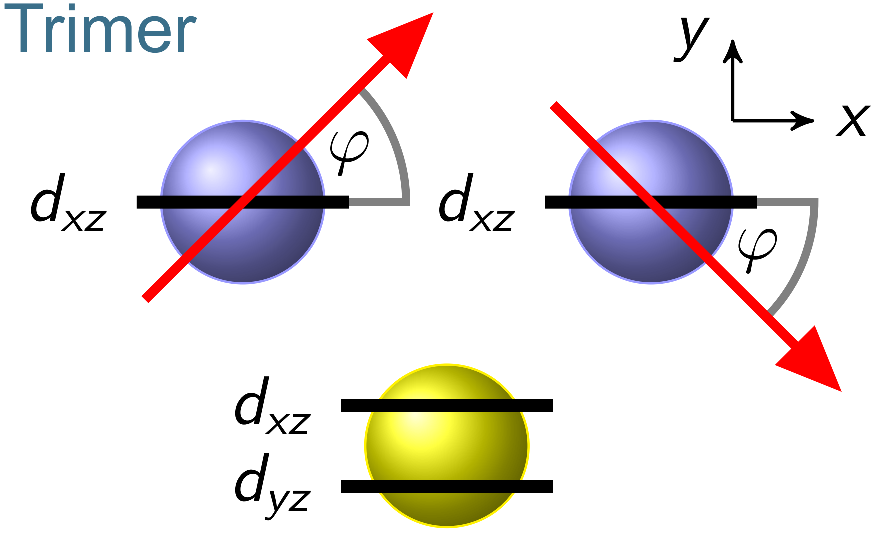
$$\vec{c} = -\hat{e}_y$$

$$\vec{c} = \vec{m}_i \times \vec{m}_j = \hat{e}_y$$

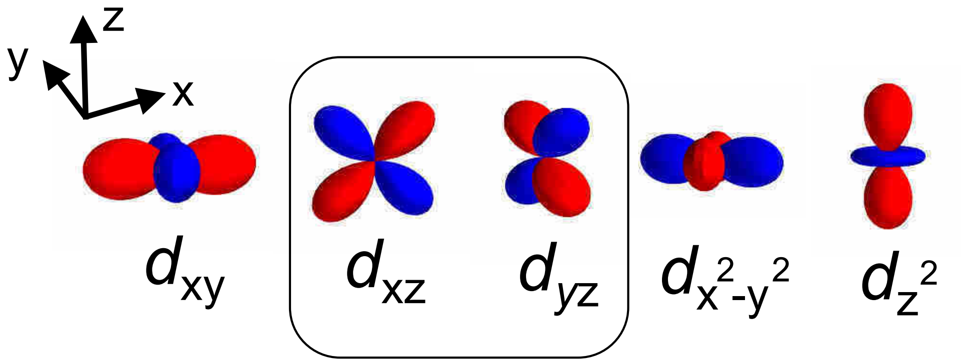
$$H_{\mathrm{DM}} = \sum_{i,j} \vec{D}_{i,j} \underbrace{\vec{S}_i \times \vec{S}_j}_{\vec{c}}$$

DMI: Tight-binding model

❖ Isosceles Trimer



❖ Basis

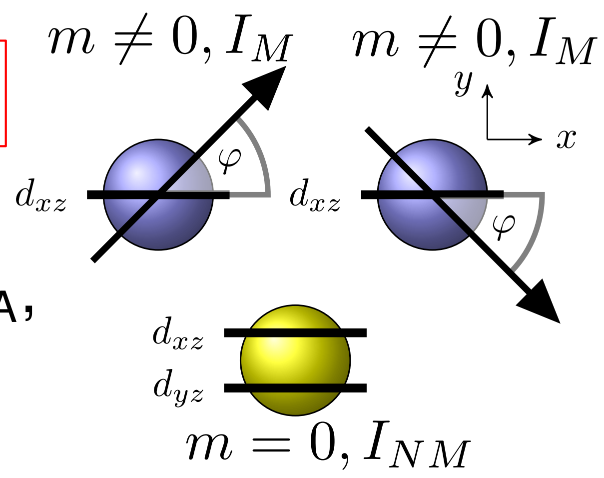


- two magnetic atoms and one non-magnetic atom
- one orbital (d_{xz}) on magnetic and two orbitals (d_{xz},d_{yz}) on non-magnetic atom
- non-collinear magnetic configuration: rotation within *x*-*y* plane
- no SOI on magnetic and large SOI on non-magnetic atoms

Minimal system and model covering non-vanishing DMI inspired by model
A. Fert and P. M. Levy, PRL **44** 1538 (1980)

Perturbative solution for NC case

TB Hamiltonian: $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm mag}(\varphi \neq 0)$



Perturbation $\Delta V = -\Theta_{\rm A}^{\dagger} \boldsymbol{\sigma} \mathbf{B}\, \Theta_{\rm A} = -\gamma \sigma_y \delta_{\rm AA}$,

Eigenstate in first order perturbation :

$$|\tilde{n}\rangle = |n^{\sigma}\rangle + \sum_{\substack{n' \,(\neq n)\\ (\sigma' \neq \sigma)}} \frac{\langle n'^{\sigma'} | \Delta V | n^{\sigma}\rangle}{\varepsilon_n^{\sigma} - \varepsilon_{n'}^{\sigma'}} |n'^{\sigma'}\rangle$$

$$= |n^{\sigma}\rangle - \mathrm{i}\gamma \sum_{\substack{n' \,(\neq n)\\ (\sigma' \neq \sigma)}} \frac{\delta S_{n'^{\sigma'} n^{\sigma}}}{\varepsilon_n^{\sigma} - \varepsilon_{n'}^{\sigma'}} |n'^{\sigma'}\rangle$$

Perturbative solution for SOC

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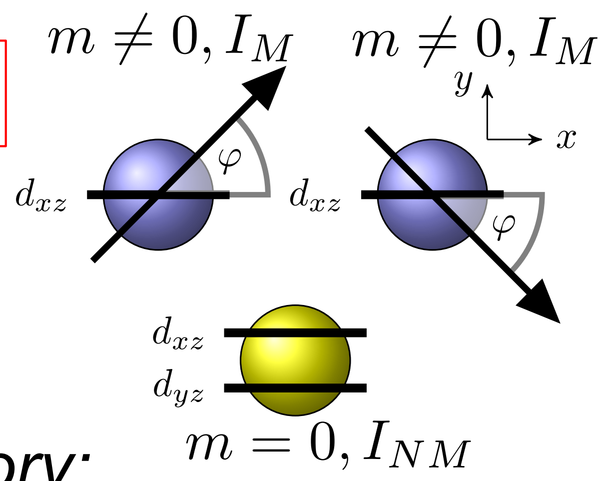
TB Hamiltonian: $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{mag}}(\varphi \neq 0)$



Perturbation $\mathcal{H}_{\text{SOI}} \sim \xi \mathbf{L} \cdot \boldsymbol{\sigma} = \xi L_z \sigma_z$

Energy shift in first order perturbation theory:

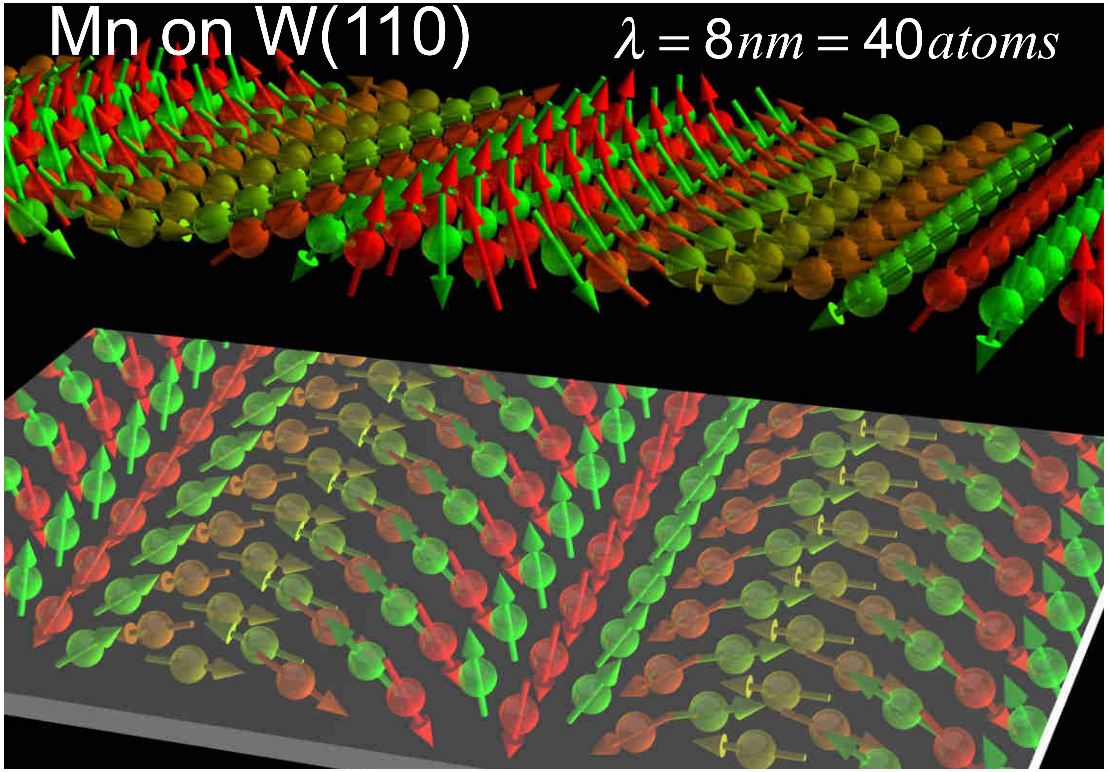
$$\delta\varepsilon_n = \langle \tilde{n} | \mathcal{H}_{\text{SO}} | \tilde{n} \rangle \qquad E_{\text{DMI}} = \sum \delta\varepsilon_n \cdot f(\varepsilon_n)$$

$$\delta\varepsilon_n = -\gamma\xi \sum_{\substack{n' \, (\neq n) \\ (\sigma' \neq \sigma)}} \frac{\mathrm{i}\langle n'^{\sigma'} | \sigma_y | n^{\sigma} \rangle_{\mathrm{A}} \langle n^{\sigma} | L_{\mp}\sigma_{\pm} | n'^{\sigma'} \rangle_{\mathrm{C}}}{\varepsilon_n^{\sigma} - \varepsilon_{n'}^{\sigma'}}$$

$$= -\gamma\xi t_1 t_2 (-1)^i \sigma \sum_{\substack{n' \, (\neq n) \\ (i' \neq i)}} \frac{\tau \, \delta_{\sigma,-\sigma'} \tau'}{W_n^{\sigma} (\varepsilon_n^{\sigma} - \varepsilon_{n'}^{\sigma'}) W_{n'}^{\sigma'}}$$

Example 7:
Homo-chiral magnetic structure

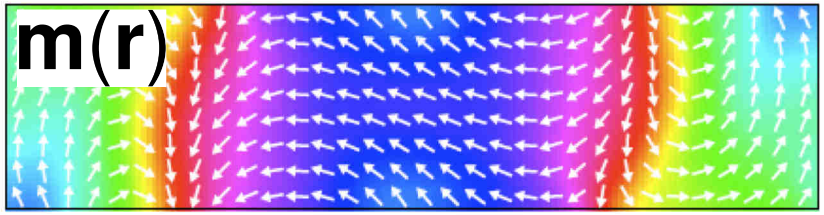
Formation of homochiral (cycloidal) magnetism ground state



Mn/W(110): M. Bode *et al*., Nature **447**, 190 (2007).
Mn/W(100): P. Ferriani *et al*., PRL **101**, 027201 (2008).
Cr/W(110): B. Zimmermann *et al.* PRB **90**, 115427 (2014).
Fe/Ir(100): M. Menzel *et al*., PRL **108**, 197204 (2012).

Theoretical scale bridging models

Mitglied der Helmholtz Gemeinschaft

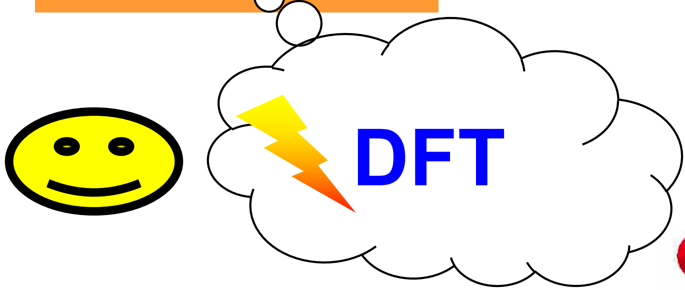


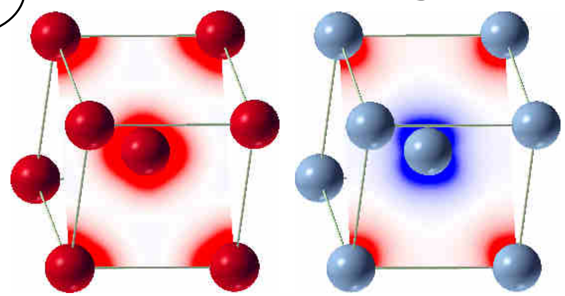
❖ Micromagnetic-model (≈μm):

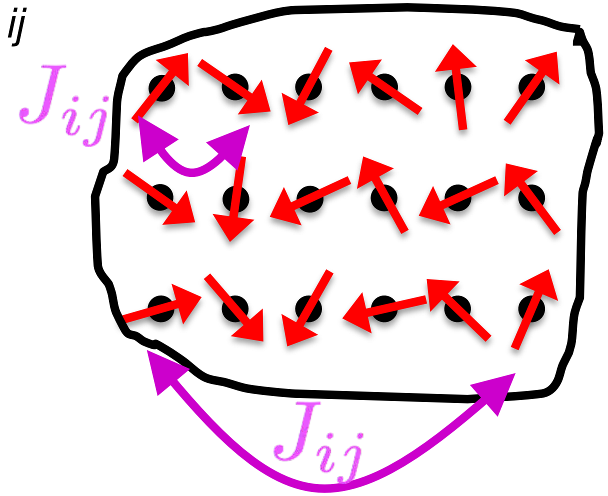
$$E(\mathbf{m}) = \int \left[A\,|\nabla \mathbf{m}|^2 + \mathbf{D}\cdot(\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m}\cdot \underline{\mathbf{K}} \cdot \mathbf{m} \right] dr$$

❖ Spin-Lattice Model: (≅c 10nm)

$$H = \frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{m}_i\mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij}\,\overbrace{\mathbf{m}_i \times \mathbf{m}_j} + \sum_i \mathbf{m}_i\,\underline{\mathbf{K}}\,\mathbf{m}_i + \sum_{ij} \frac{1}{r_{ij}^3}\left[\mathbf{m}_i\mathbf{m}_j - (\mathbf{m}_i\hat{\mathbf{e}}_i)(\mathbf{m}_j\hat{\mathbf{e}}_i)\right]$$







❖ DFT-model: $E[n, \mathbf{m}]$

Beyond micromagnetic modeling

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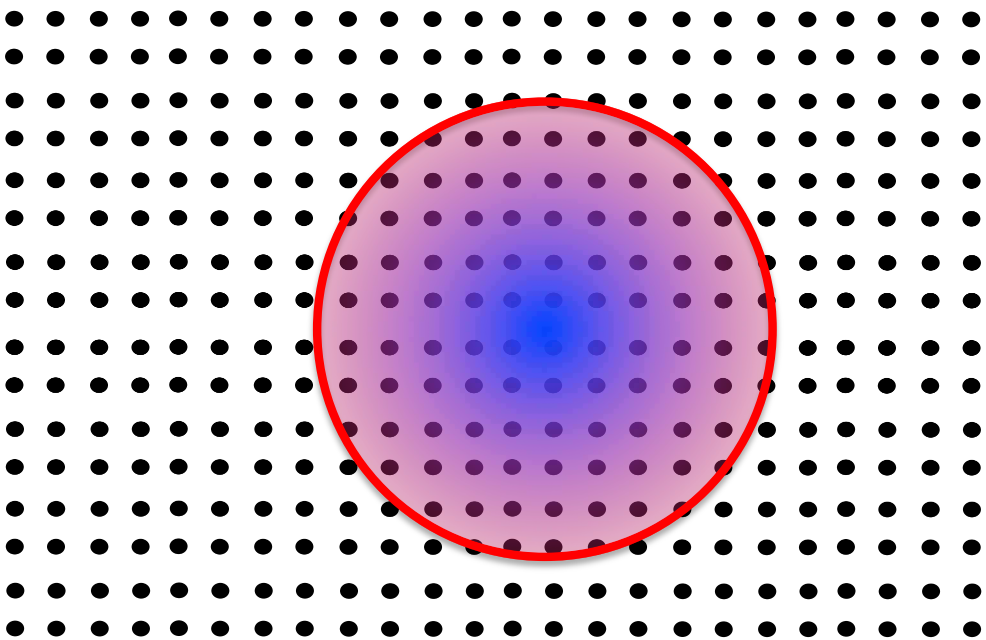
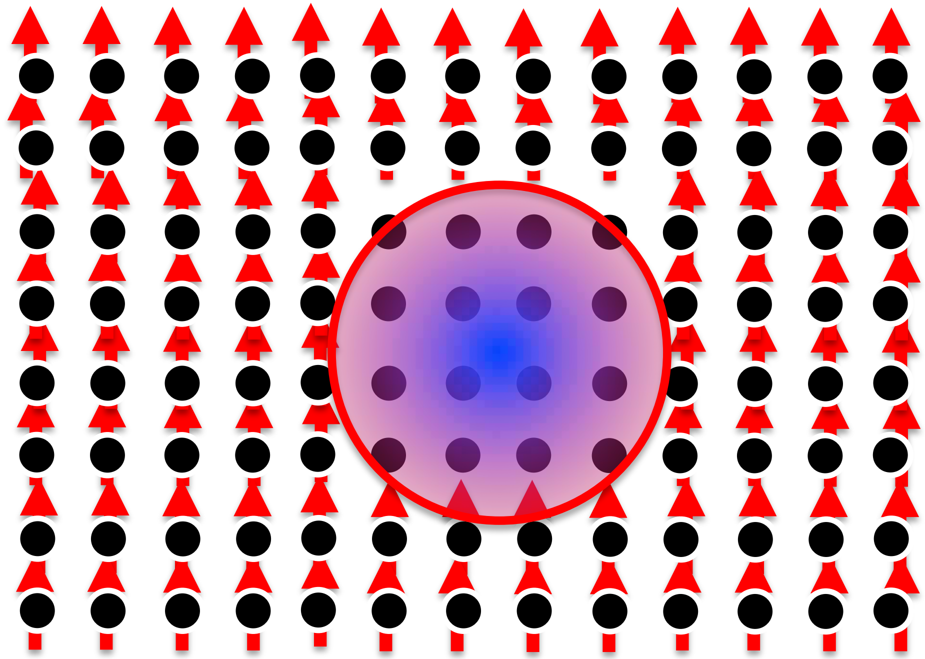
❖ Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] \, dr$$

- Approximate in materials specificity
- Limited accuracy for small skyrmions or skyrmion stability



❖ Atomistic Model



Continuum approximation

$$\mathbf{m}(\mathbf{r} = \mathbf{R}_j) \approx \mathbf{m}(\mathbf{R}_i) + (\mathbf{R}_j - \mathbf{R}_i)\nabla \mathbf{m}(\mathbf{r}) \quad \Longleftarrow \quad \mathbf{m}_i = \mathbf{m}(\mathbf{R}_i)$$

Mitglied der Helmholtz Gemeinschaft

Multiscale approach

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❖ Micromagnetic-model:

Continuum Approximation $\mathbf{m}_i = \mathbf{m}(\mathbf{R}_i) \Longrightarrow \mathbf{m}(\mathbf{r}) = \mathbf{m}_i$ for $\mathbf{r} = \mathbf{R}_i$

$$E(\mathbf{m}) = \int \left[A \, |\nabla \mathbf{m}|^2 + \mathbf{D} \cdot (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} \right] \, d\mathbf{r}$$

- Spin Stiffness

$$A = \frac{1}{A_\Omega} \sum_{j>0} J_{0j} R_{0j}^2$$

- Spiralization (micromagnetic D)

$$\mathbf{D} = \frac{1}{A_\Omega} \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

❖ Spin-Lattice Model:

$$H = \frac{1}{2} \sum_{ij} J_{ij} \, \mathbf{m}_i \mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij} \overbrace{\mathbf{m}_i \times \mathbf{m}_j}^{c} + \sum_i \mathbf{m}_i \, \underline{\mathbf{K}} \, \mathbf{m}_i + \sum_{ij} \frac{1}{r_{ij}^3} \left[\mathbf{m}_i \mathbf{m}_j - (\mathbf{m}_i \hat{\mathbf{e}}_i)(\mathbf{m}_j \hat{\mathbf{e}}_i) \right]$$

❖ DFT-model: $\mathbf{m}$, J_{ij}, , $\mathbf{D}_{ij}$, $\underline{\mathbf{K}}$

Multiscale modeling

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- Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] dr$$

- Atomistic / Spin-Lattice Model:

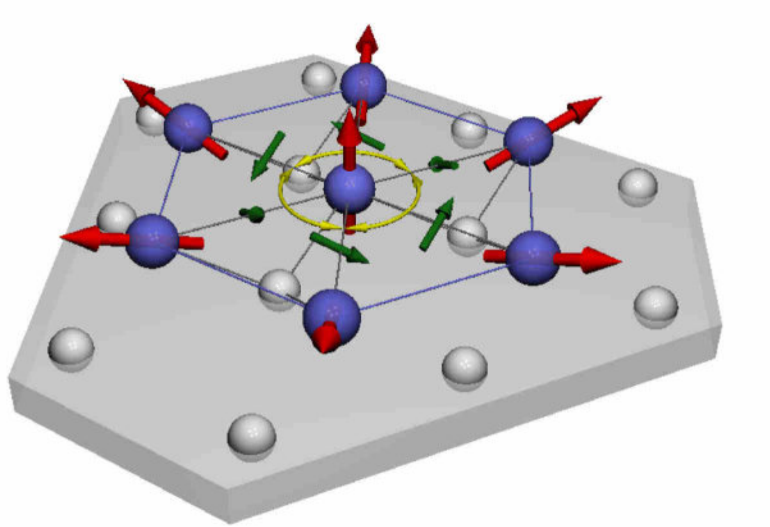
$$H = \frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{m}_i\mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij}\,\overbrace{\mathbf{m}_i \times \mathbf{m}_j}^{c} + \sum_i \mathbf{m}_i\,\underline{\mathbf{K}}\,\mathbf{m}_i + \sum_{ij} \frac{1}{r_{ij}^3}\left[\mathbf{m}_i\mathbf{m}_j - (\mathbf{m}_i\hat{\mathbf{e}}_i)(\mathbf{m}_j\hat{\mathbf{e}}_i)\right]$$

- Dzyaloshinskii-Moriya vector $\mathbf{D}_{ij} = (D^x, D^y, D^z)_{ij}$

C_{3v}: (111) – Surface

mirror planes ➔

D inplane $\mathbf{D}_{ij} = (D^x, 0, D^z)_{ij}$



Multiscale modeling

JÜLICH FORSCHUNGSZENTRUM

- Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] dr$$

- Atomistic / Spin-Lattice Model:

https://spirit-code.github.io/

$$H = \frac{1}{2} \sum_{ij} J_{ij}\, \mathbf{m}_i \mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij} \overbrace{\mathbf{m}_i \times \mathbf{m}_j}^{\mathbf{c}} + \sum_i \mathbf{m}_i\, \underline{\mathbf{K}}\, \mathbf{m}_i + \sum_{ij} \frac{1}{r_{ij}^3} \left[\mathbf{m}_i \mathbf{m}_j - (\mathbf{m}_i \hat{\mathbf{e}}_i)(\mathbf{m}_j \hat{\mathbf{e}}_i) \right]$$

- Spin Stiffness:

$$A \propto \sum_{j>0} J_{0j} R_{0j}^2$$

- Spiralization (micromagnetic D)

$$\underline{\mathbf{D}} \propto \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

- DFT-model: From *ab initio* total energy:

$$E_{\text{tot}}^{\text{DFT}}(\mathbf{q}, \hat{\mathrm{e}}_{\text{rot}}) = E_{\text{noSOC}}^{\text{DFT}}(\mathbf{q}) + \Delta E_{\text{SOC}}^{\text{DFT}}(\mathbf{q}, \hat{\mathrm{e}}_{\text{rot}})$$

- A, $\underline{\mathbf{D}}$, $\underline{\mathbf{K}}$
- J_{ij}, $\mathbf{D}_{ij}$

www.flapw.de Fleur

M. Heide, G. Bihlmayer, and S. Blügel, Physica B **404**, 2678 (2009)
B. Zimmermann, M. Heide, G. Bihlmayer, and S. Blügel, PRB **90**, 115427 (2014)
B. Schweflinghaus, B. Zimmermann, G. Bihlmayer and S. Blügel, PRB **94**, 024403 (2016)

Determine the spin-textures yourselves

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https://www.juDFT.de

https://spirit-code.github.io/

Thanks !