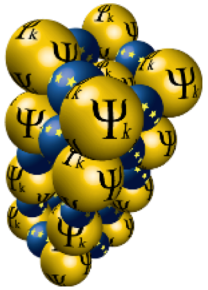
ADVANCED MAGNETISM

13.4.2021 I DANIEL WORTMANN

cecam
Centre Européen de Calcul Atomique et Moléculaire
Mitglied der Helmholtz-Gemeinschaft



MAX DRIVING THE EXASCALE TRANSITION

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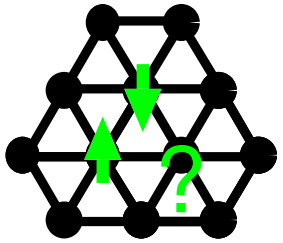
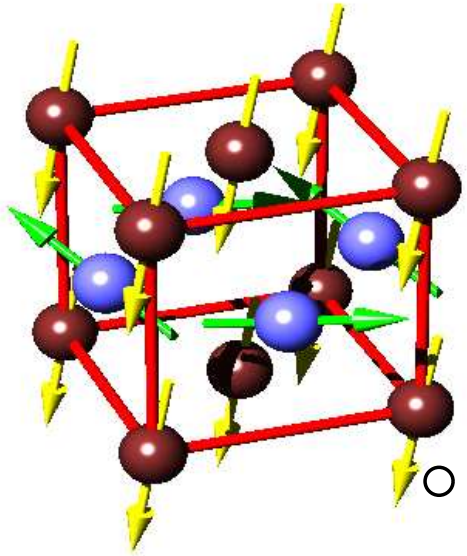
COLLINEAR VS NON-COLLINEAR

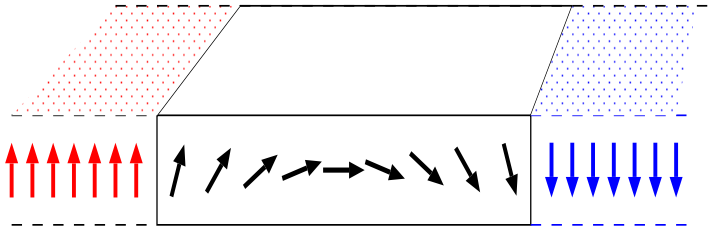


frustrated antiferromagnets
[e.g. Cr/Cu(111)]

ferro/antiferro
alloys
[e.g. FeMn]

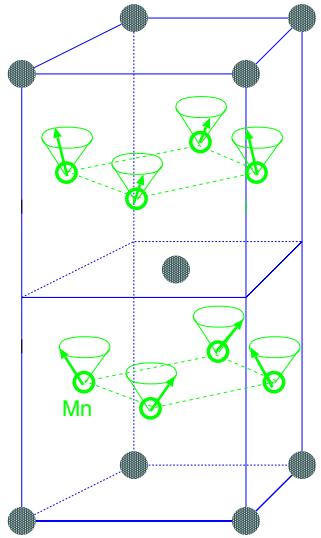


non-collinear
magnetic systems



domain walls in thin films
[e.g. Fe/W(110)]

incommensurate
spin spirals
[e.g. fcc Fe,
bcc Eu,
$LaMn_2Ge_2$]



MAGNETISM IN DFT

- Spin-dependent Kohn-Sham equation:

$$H\psi = \epsilon\psi$$

- Wave function consists of two component spinor

$$\psi = \begin{cases} \psi_\uparrow \\ \psi_\downarrow \end{cases}$$

- Hamiltonian becomes 2x2 matrix in spin

$$H = -\frac{1}{2}\nabla \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} V_{\uparrow\uparrow} & V_{\uparrow\downarrow} \\ V_{\downarrow\uparrow} & V_{\downarrow\downarrow} \end{pmatrix}$$

- Density:

$$n = \sum |\psi|^2$$

Magnetisation:

$$\vec{m} = \sum \psi^* \vec{\sigma} \psi$$

COLLINEAR MAGNETISM

- Magnetisation only in one direction:

$$\vec{m} = m_z \hat{e}_z$$

- Hamiltonian become spin-diagonal:

$$H = -\frac{1}{2}\nabla^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} V_{\uparrow\uparrow} & \cancel{V_{\uparrow\downarrow}} \\ \cancel{V_{\downarrow\uparrow}} & V_{\downarrow\downarrow} \end{pmatrix}$$

- Two independent KS equations:

$$H_\uparrow \psi_\uparrow = \left(-\frac{1}{2}\nabla^2 + V_{\uparrow\uparrow} \right) \psi_\uparrow = \epsilon \psi_\uparrow$$

COMPUTATIONAL EFFORT

	non-magnetic	collinear	non-collinear
EV Problem :	$(H_0 + v)\,\phi_i = \epsilon_i \phi_i$	$\begin{matrix}(H_0+v+B^{\uparrow})\phi_i^{\uparrow}=\epsilon_i^{\uparrow}\phi_i^{\uparrow} \\ (H_0+v+B^{\downarrow})\phi_i^{\downarrow}=\epsilon_i^{\downarrow}\phi_i^{\downarrow}\end{matrix}$	$\left(H_0 + \begin{array}{c\|c} V_{\uparrow\uparrow} & V_{\uparrow\downarrow} \\ \hline V_{\downarrow\uparrow} & V_{\downarrow\downarrow} \end{array}\right) \begin{pmatrix}\phi_i^{\uparrow} \\ \phi_i^{\downarrow}\end{pmatrix} = \epsilon_i \begin{pmatrix}\phi_i^{\uparrow} \\ \phi_i^{\downarrow}\end{pmatrix}$
Inversion sy. :	real-symmetric	real-symmetric	complex-hermitian
Unit cell :	small	large	large
irreducible BZ :	small	small	large

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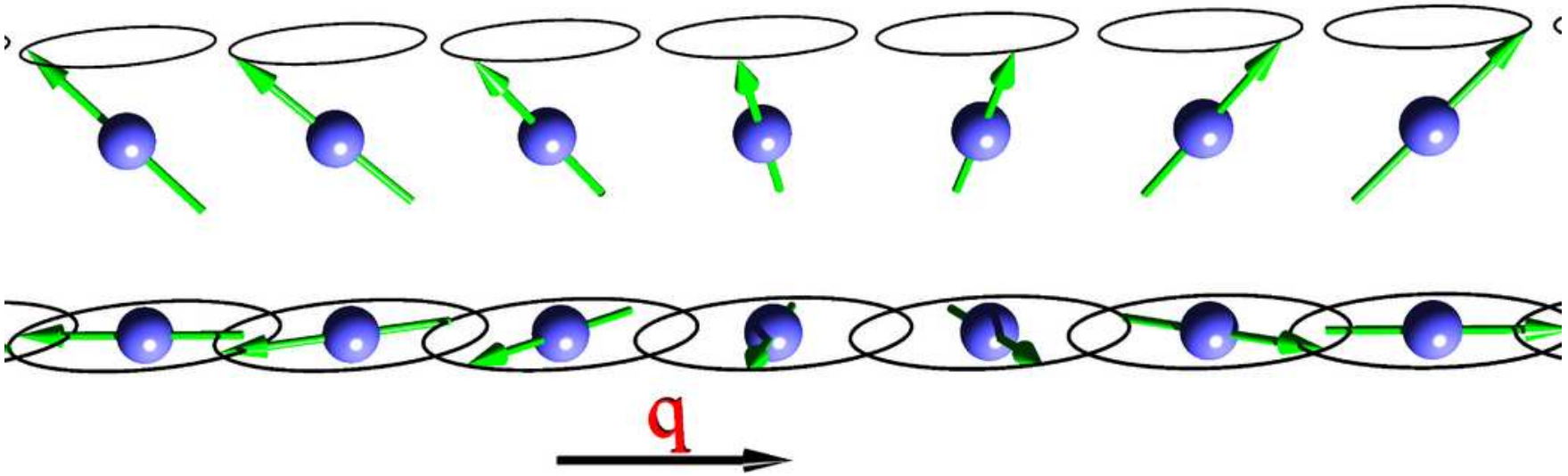
SPIN SPIRALS

- Special non-collinear state

- Magnetisation rotates homogenously $\phi = \vec{q}\vec{R}$



SPIN SPIRALS

In absence of spin-orbit coupling: generalised Bloch theorem holds:

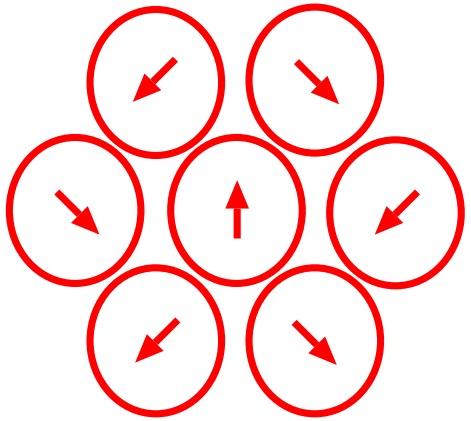
Bloch theorem	generalised Bloch theorem
translation $\vec{R}_n$	translation + spin rotation U_φ $U_\varphi = \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0 \\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix}; \varphi = \vec{q}\cdot\vec{R}_n$
$\mathsf{T}_n \Psi_{\vec{k}}(\vec{r}) = \Psi_{\vec{k}}(\vec{r}+\vec{R}_n) = e^{i\vec{k}\cdot\vec{R}_n}\Psi_{\vec{k}}$	$\mathcal{T}_n \Phi_{\vec{k}}(\vec{r}) = U_\varphi \Phi_{\vec{k}}(\vec{r}+\vec{R}_n) = e^{i\vec{k}\cdot\vec{R}_n}\ \Phi_{\vec{k}}(\vec{r})$
$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$	$\Phi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} e^{-\frac{i\vec{q}\cdot\vec{r}}{2}} u_\uparrow(\vec{r}) \\ e^{\frac{i\vec{q}\cdot\vec{r}}{2}} u_\downarrow(\vec{r}) \end{pmatrix}$

allows to use small unit cells for spin-spiral calculations!

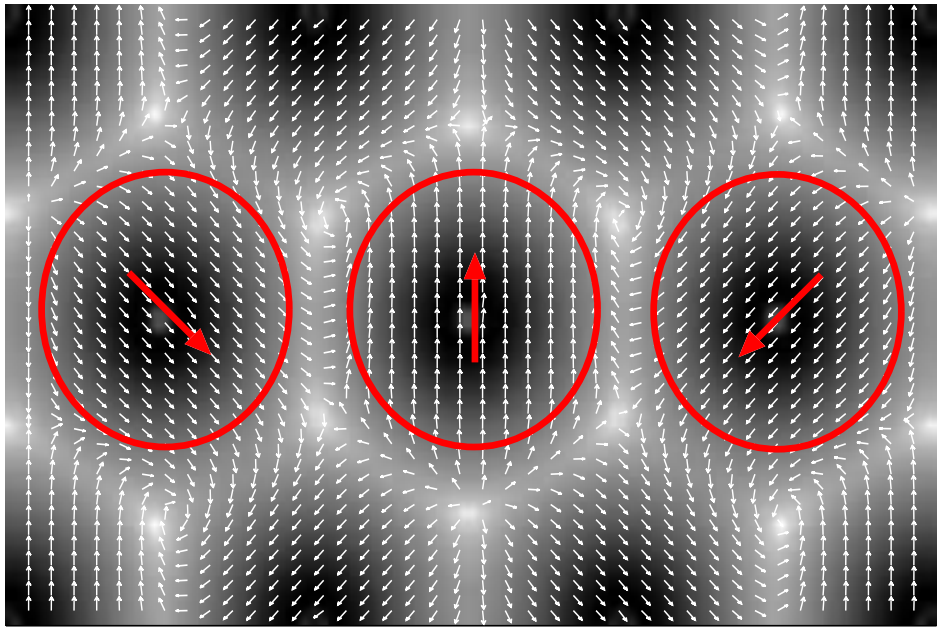
LOCAL MOMENTS

Cr monolayer on Cu(111): Néel structure
Inside the red spheres:

$$\vec{m}(\vec{r}) = M_\nu \hat{\mathbf{e}}_\nu$$



Nèel structure



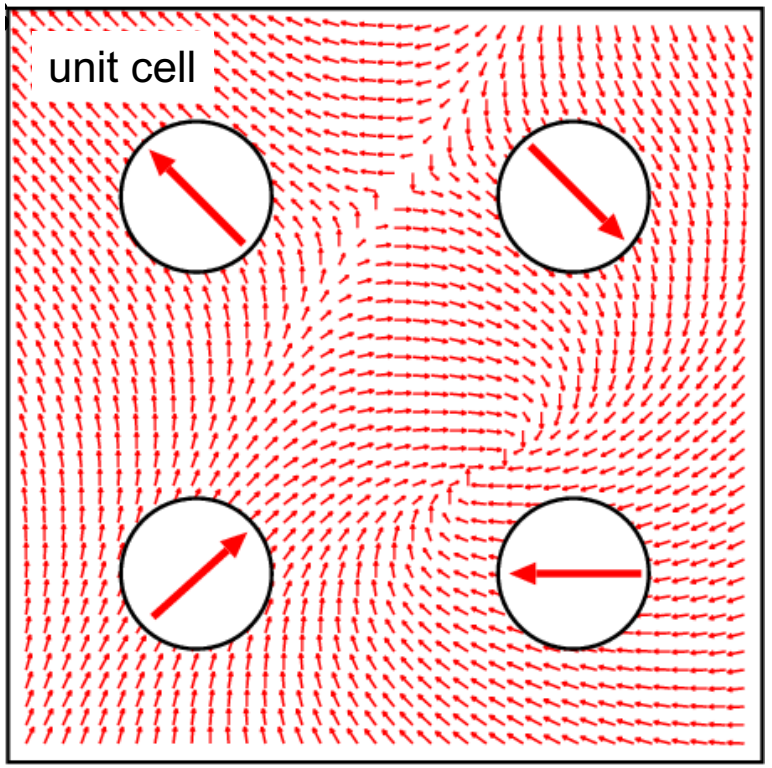
CONSTRAINED LOCAL MOMENTS

Approximation:

- Within the MT-sphere we assume the charge to be collinear
- Different atoms => different spin-quantization axis

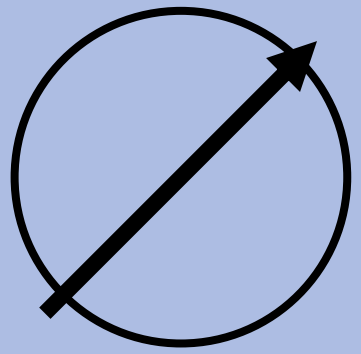
Default approximation in FLEUR

- Significant reduction of degrees of freedom
- Clearer physical interpretation
- More efficient calculations



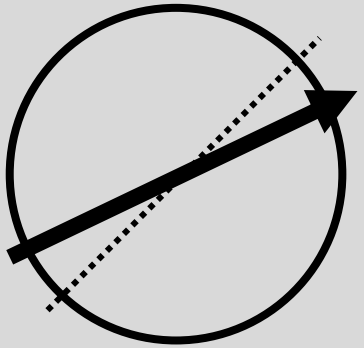
MAGNETIC MOMENTS DIRECTION

Input magnetisation:



(Remember we might constrain the density to be collinear in the sphere)

Output magnetisation:



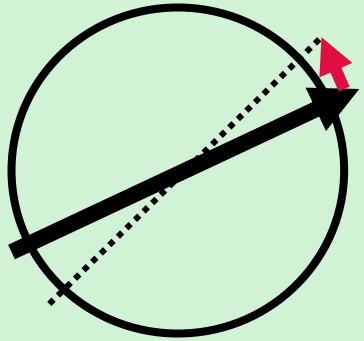
Might have a different direction, i.e. there is an angle between input and output magnetisation

Three choices:

a) Neglect rotation

b) Rotate magnetisation

c) Constrain direction



Add B-Field to ensure

$$\vec{M}_{\text{in}} \parallel \vec{M}_{\text{out}}$$

RELAXATION OF LOCAL DIRECTIONS

In a „unconstraint local moment calculation“ the moment direction will relax „automatically“

But:

Global Spin

Spin rotation

Local Spin

LAPW basis functions:

$$\phi_{\vec{G},\sigma} = \chi_{\sigma,s} \sum_{L} (a_{\vec{G},L} u_{s,L} + b_{\vec{G},L} \dot{u}_{s,L}) Y_L$$

Basis set will depend on ch

New and experimental features in MaX releases of FLEUR

Solution: Adjust local direc ction of average magnetic moment

MODEL HAMILTONIAN

Calculating magnetic structures with DFT works great but:

- The phase-space of possible structures is gigantic
- Time-dependence can be hard to include

Heisenberg Model Hamiltonian:

$$H = -\sum_{nn'} J_{nn'} \vec{S}_n \cdot \vec{S}_{n'}$$

- (classical) Model in which S_n are local spins
- $J_{nn'}$ are interaction constants

SOLUTIONS OF THE HEISENBERG MODEL

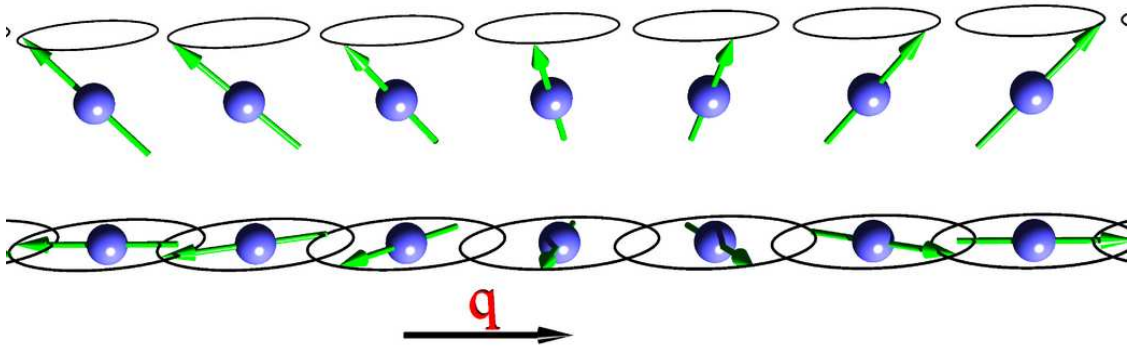
Simplify $H = -\sum_{nn'} J_{nn'} \vec{S}_n \cdot \vec{S}_{n'}$ by Fourier-transformation:

$$\vec{S}(\vec{q}) = \frac{1}{N} \sum_n \vec{S}_n e^{-i\vec{q}R_n} \quad \text{and} \quad J(\vec{q}) = \sum_n J_{0n} e^{-i\vec{q}R_n}.$$

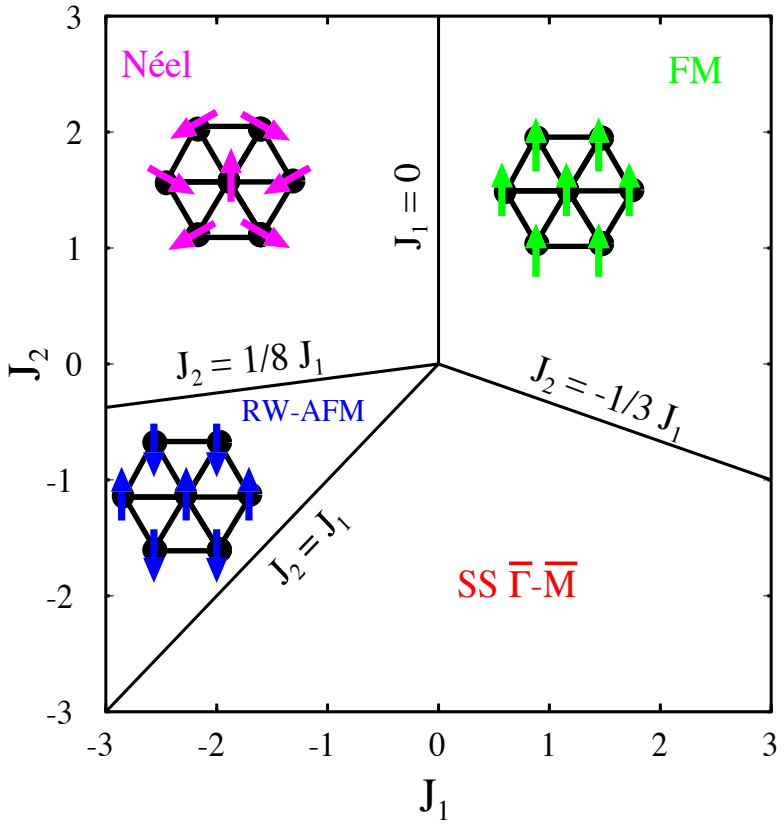
leads to

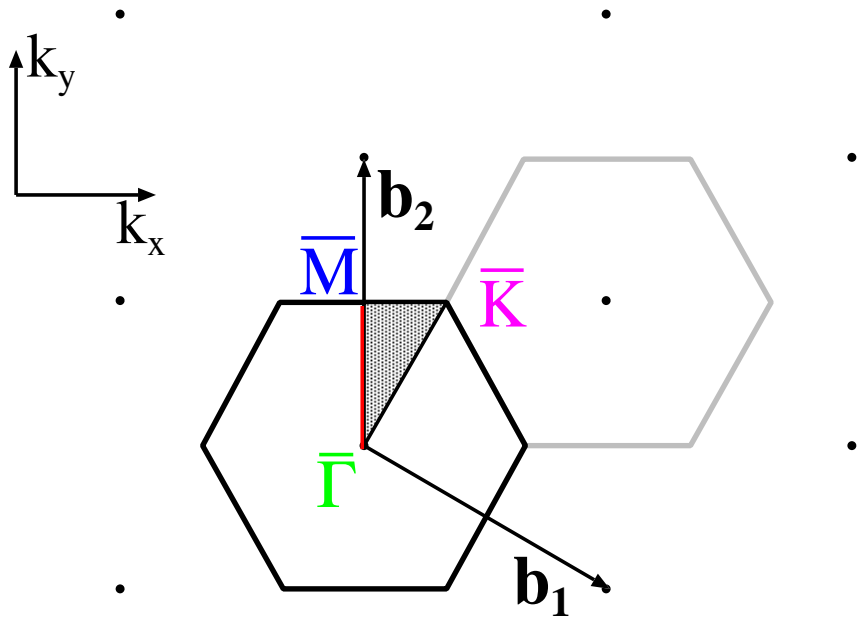
$$H = -N \sum_{\vec{q}} J(\vec{q}) \vec{S}(\vec{q}) \cdot \vec{S}(-\vec{q})$$

If $\vec{S}_n^2 = S^2$, solutions are: $\vec{S}_n = \sqrt{2}S \left(\hat{\vec{e}}_x \cos(\vec{q} \cdot \vec{R}_n) + \hat{\vec{e}}_y \sin(\vec{q} \cdot \vec{R}_n) \right)$:



SPIN SPIRALS





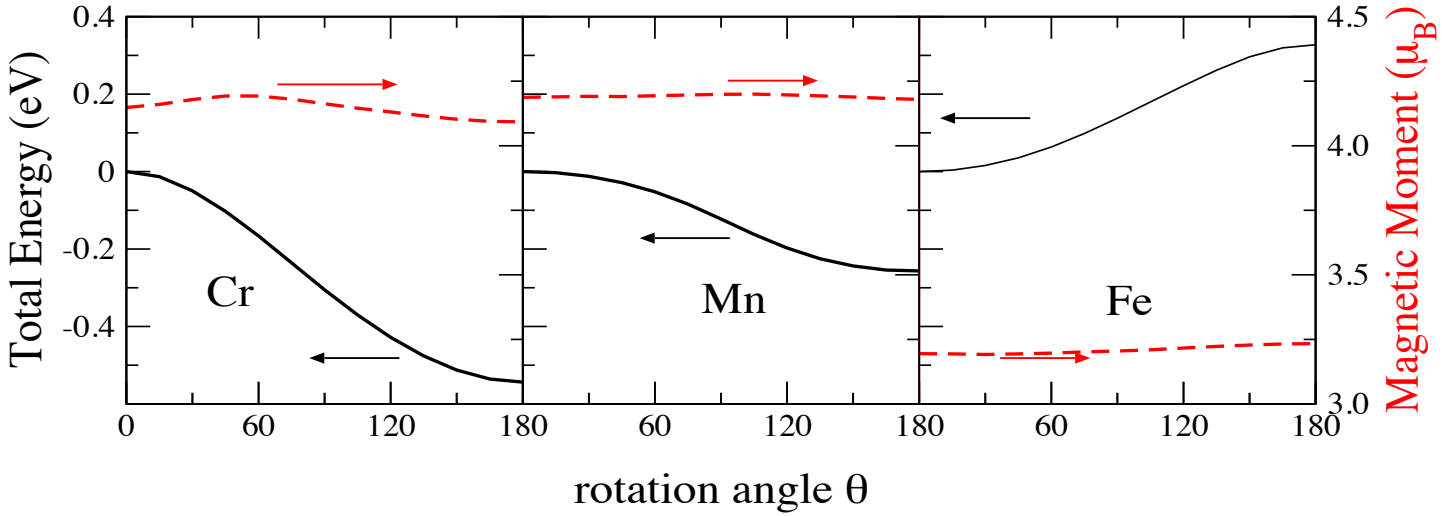
Ferromagnetic state: $\vec{q} = (0, 0)$

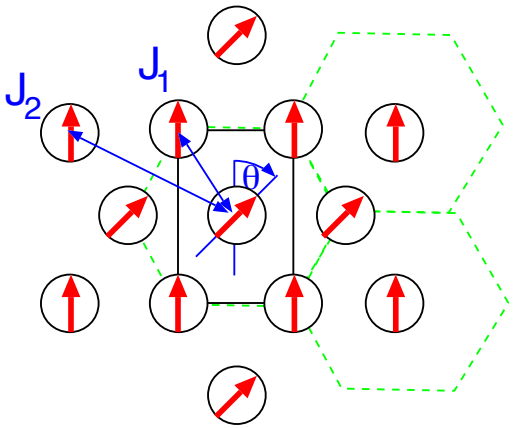
Row-wise antiferro. state: $\vec{q} = 1/2, 1/2$

Néel state: $\vec{q} = (1/3, 2/3)$

Spin-spiral $\vec{q} = (\alpha, \alpha)$

DETERMINING MODEL PARAMETERS





neighbor	#	J	prefactor
nearest	4	J_1	$\cos\theta$
	2	J_1	1
next-nearest	2	J_2	1
	4	J_2	$\cos\theta$

$$E = -S^2(J_1 + J_2)(2 + 4\cos\theta)$$

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FORCE THEOREM CALCULATIONS

A change in the total energy

$$E = \sum_i \varepsilon_i - \frac{1}{2} \int \int \frac{n(\vec{r}) n(\vec{r}')}{\vec{r} - \vec{r}'} d\vec{r}' d\vec{r} + \int [e_{\mathrm{xc}}(\vec{r}) - V_{\mathrm{eff}}(\vec{r})] n(\vec{r}) d\vec{r}$$

due to a change in the density is to first order perturbation theory:

$$\delta E = \sum_i \delta \varepsilon_i$$

- $(+)$ no self-consistency required
- $(-)$ perturbation has to be small

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FORCE THEOREM MODES IN FLEUR

MAE mode:

- Calculation with different magnetisation directions and SOC
- Enables the evaluation of the Magnetocrystaline Anisotropy Energy

SS-Dispersion mode:

- Calculations with spin-spirals of different q-vectors
- Evaluation of spin-spiral dispersion

DMI mode:

- Calculations of SOC for spin-spirals (1st order perturbation theory)

SUMMARY

Using FLEUR, over time you will be experts on:

Magnetic Order

Spin-moment

Collinear Magnetism

Spin-Spirals

Orbital-moment

Exchange interaction

Non-collinear magnetism

Heisenberg model