MAGNETISM

10.09.2019 I DANIEL WORTMANN

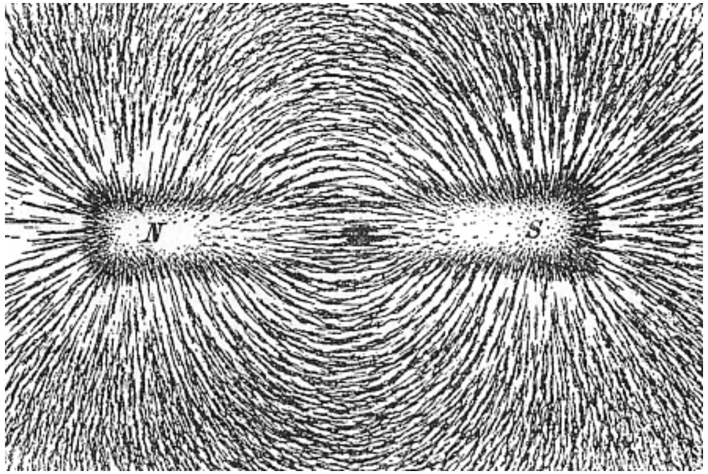
MAX DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

Mitglied der Helmholtz-Gemeinschaft

MAGNETISM

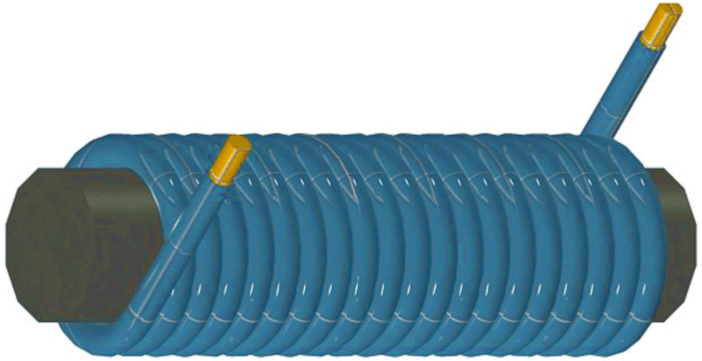
- Magnetic fields



N. H. Black, H. N. Davis (1913) *Practical Physics*, USA, p. 242, fig. 200

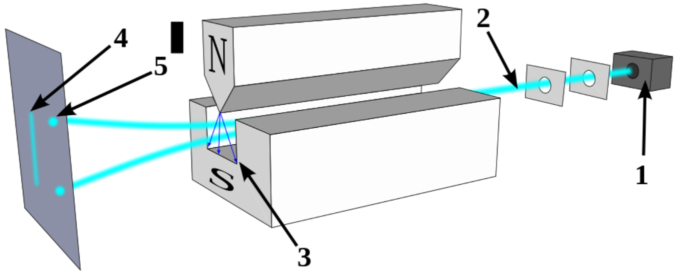
Frist source

- Electromagnetism
- Magnetic fields from electrical currents

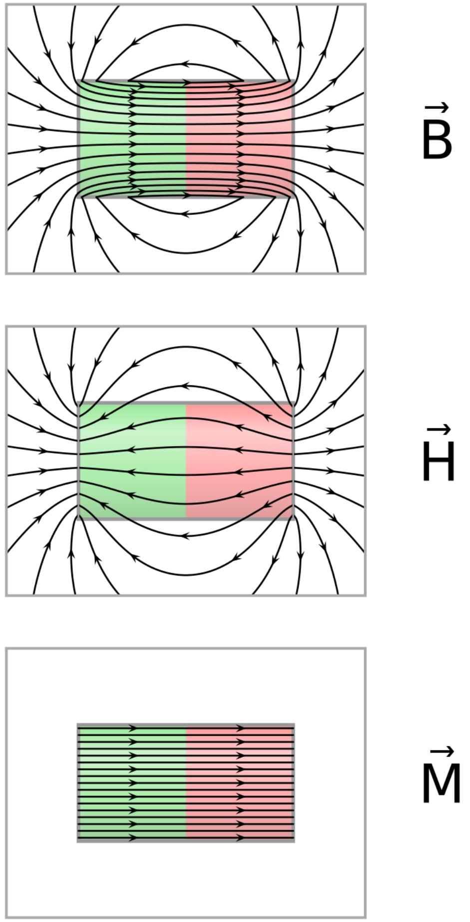


Second source:

- Intrinsic magnetic moments of elementary particles
- Spin of particles



B-FIELD AND MAGNETISATION



CC-Lizenz (Wikipedia)

- Materials react to magnetic fields:

$$\vec{B} = \mu_0(\vec{H} + \vec{M})$$

- Magnetisation positive/negative (Dia-,paramagnetism)
- Ferromagnetism: Magnetisation is present without external field

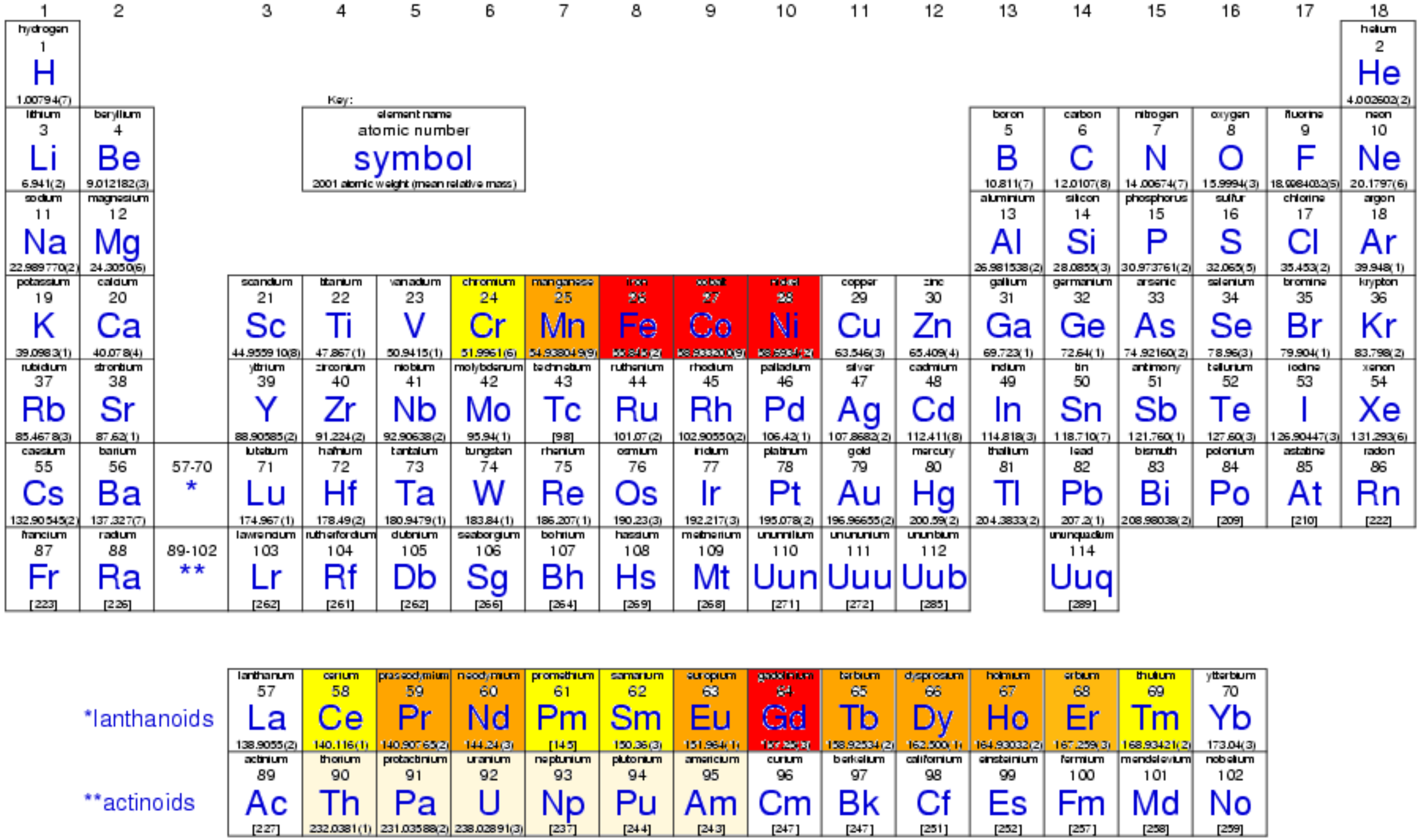
$$\vec{M} \approx -\mu_B \left\langle \Psi \left| \vec{\sigma} \right| \Psi \right\rangle$$

- Each electron carries a moment of approx. $-\mu_B$

- In addition: orbital moment $\vec{m}^{\mathrm{orb}}(\vec{r}) = -\mu_{\mathrm{B}} \sum_i \langle \phi_i | \vec{r} \times \vec{v} | \phi_i \rangle$

MAGNETISM IS RARE?

http://www.webelements.com/

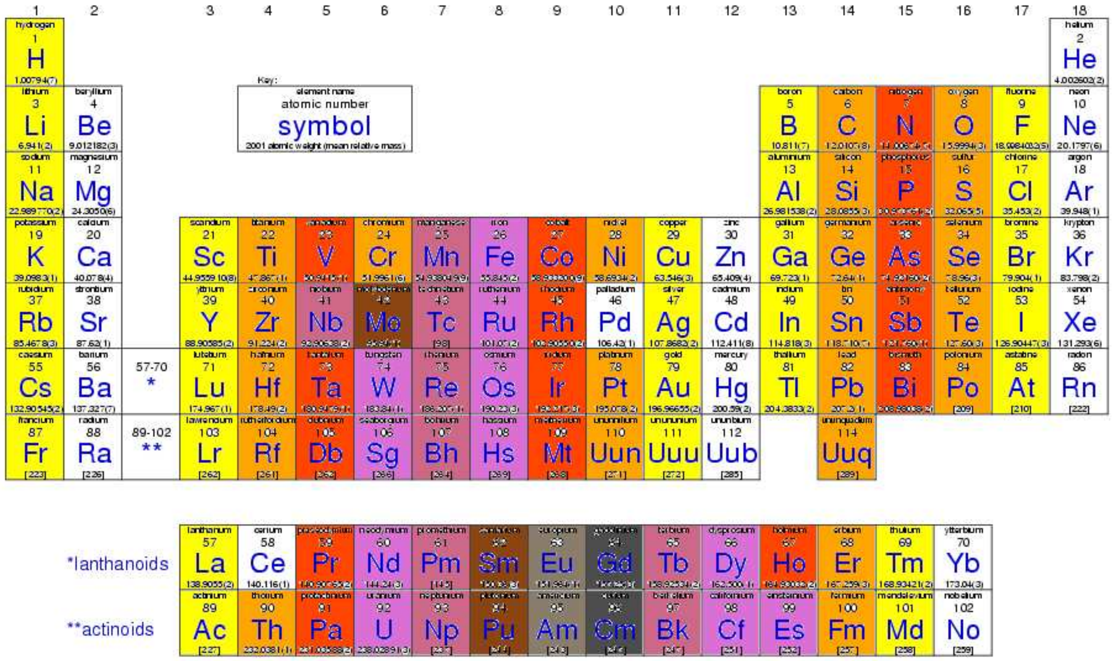


ATOMIC MAGNETISM

Isolated atoms:

- All atoms with incompletely filled shells are magnetic

http://www.webelements.com/



Simple counting:

- odd number of spins -> sum not zero

Hund's first rule:

- Spins are aligned to maximize total moment
- Example:

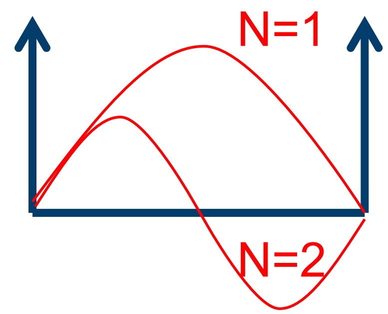
Vanadium: $4s^2\ 3d^3$

- Intra atomic exchange interaction!

WHAT DRIVES MAGNETISM?

- Some handwaving….

1D particles ”in a box”



- No interaction:
  - States quantized: $\epsilon = \frac{1}{2}k^2 \propto \frac{1}{\lambda^2} \propto N^2$
  - Kinetic energy
  - Each state hosts two electron with different spin
  - Two electrons: both N=1 with opposite spin

- Interaction:

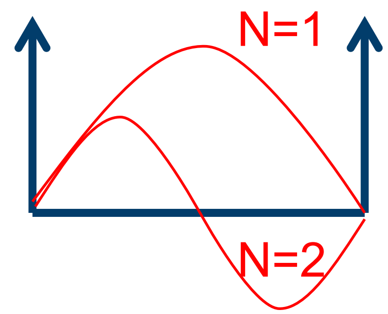
$$V_{ij} = \int \frac{\psi_i^2(r)\psi_j^2(r')}{|r - r'|}$$

- Prefers particles in different states
- Two electrons: one in N=1, one in N=2 ??

WHAT DRIVES MAGNETISM?

- Some handwaving….

1D particles ”in a box”



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    different spin
  - Two electrons:
    both N=1 with opposite s

- Interaction:

$$V_{ij} = \int \frac{\psi_i^2(r)\psi_j^2(r')}{|r - r'|}$$

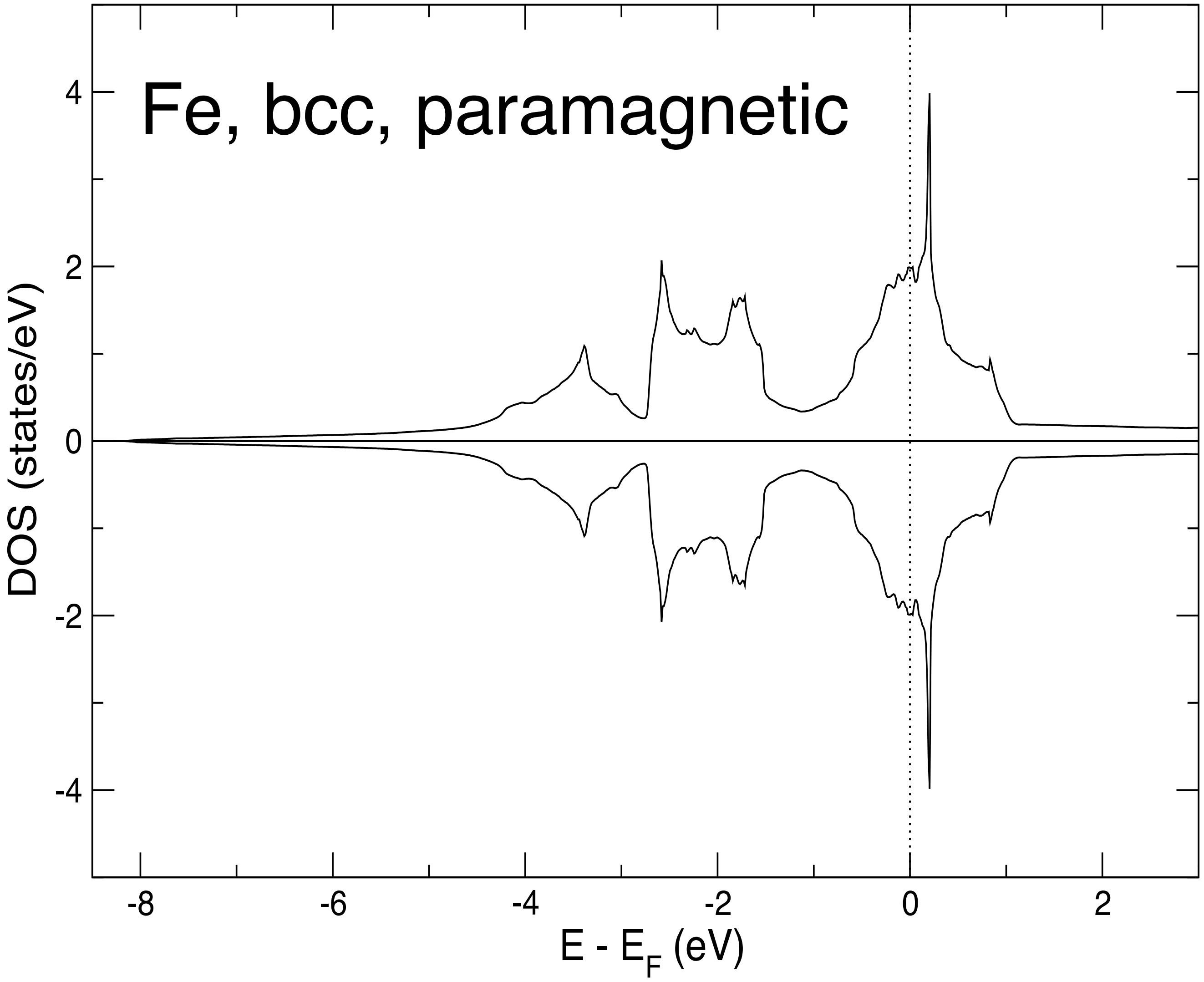
particles in different states

ctrons:

=1, one in N=2 ??

Magnetism is governed by competition between kinetic energy and (exchange) interaction

ITINERANT MAGNETS



- ~~Discrete atomic levels~~
- Continuous spectrum

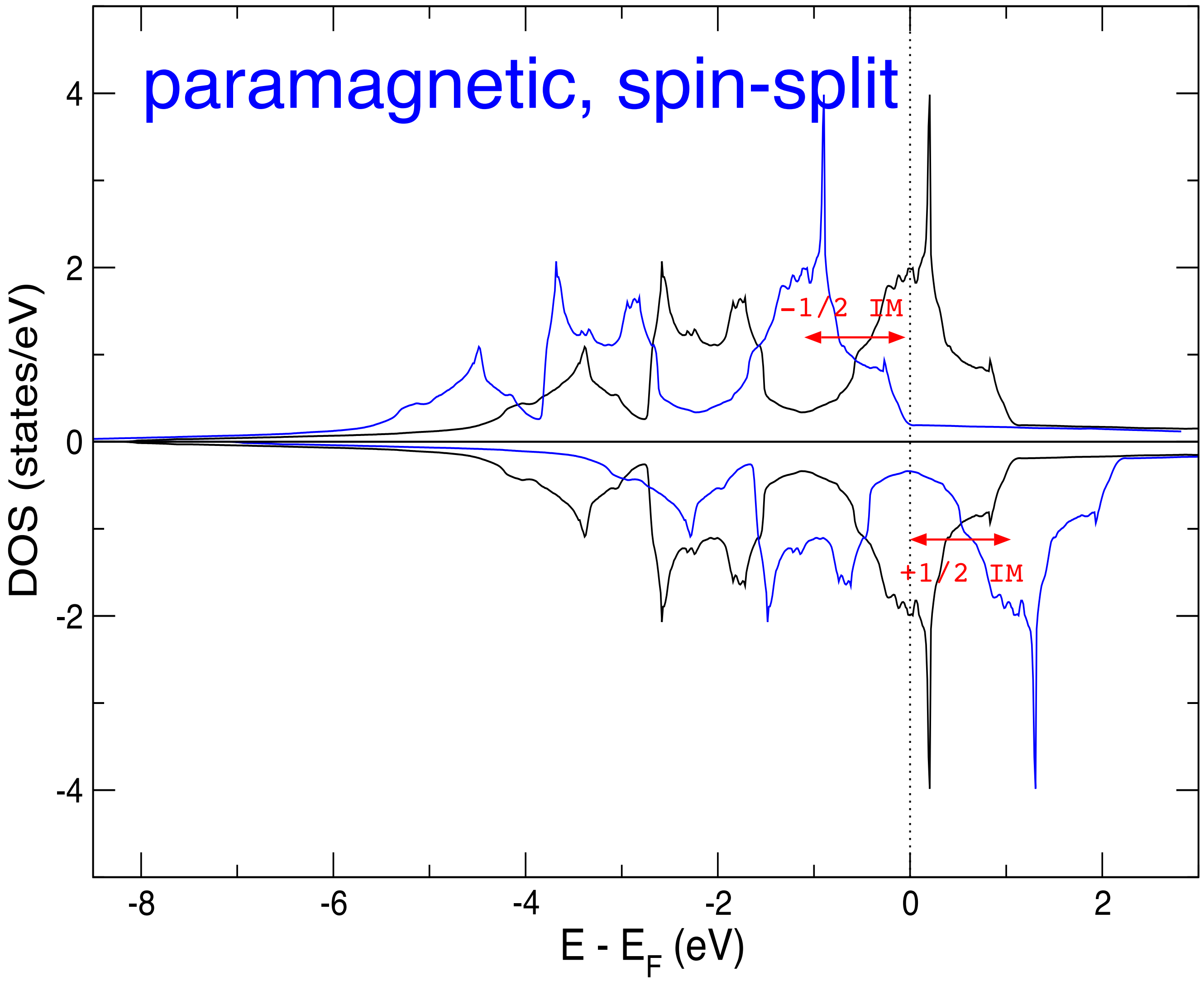
- Magnetisation will create B-Field

$$\vec{M} \rightarrow \vec{B}$$

$$B = I_0 * M + O(M^2)$$

$$\epsilon \approx \epsilon_0 \pm \mu_b B = \epsilon_0 \pm \frac{1}{2} IM$$

ITINERANT MAGNETS



- ~~Discrete atomic levels~~
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- Magnetisation will create B-Field
- B-Field will split energy levels

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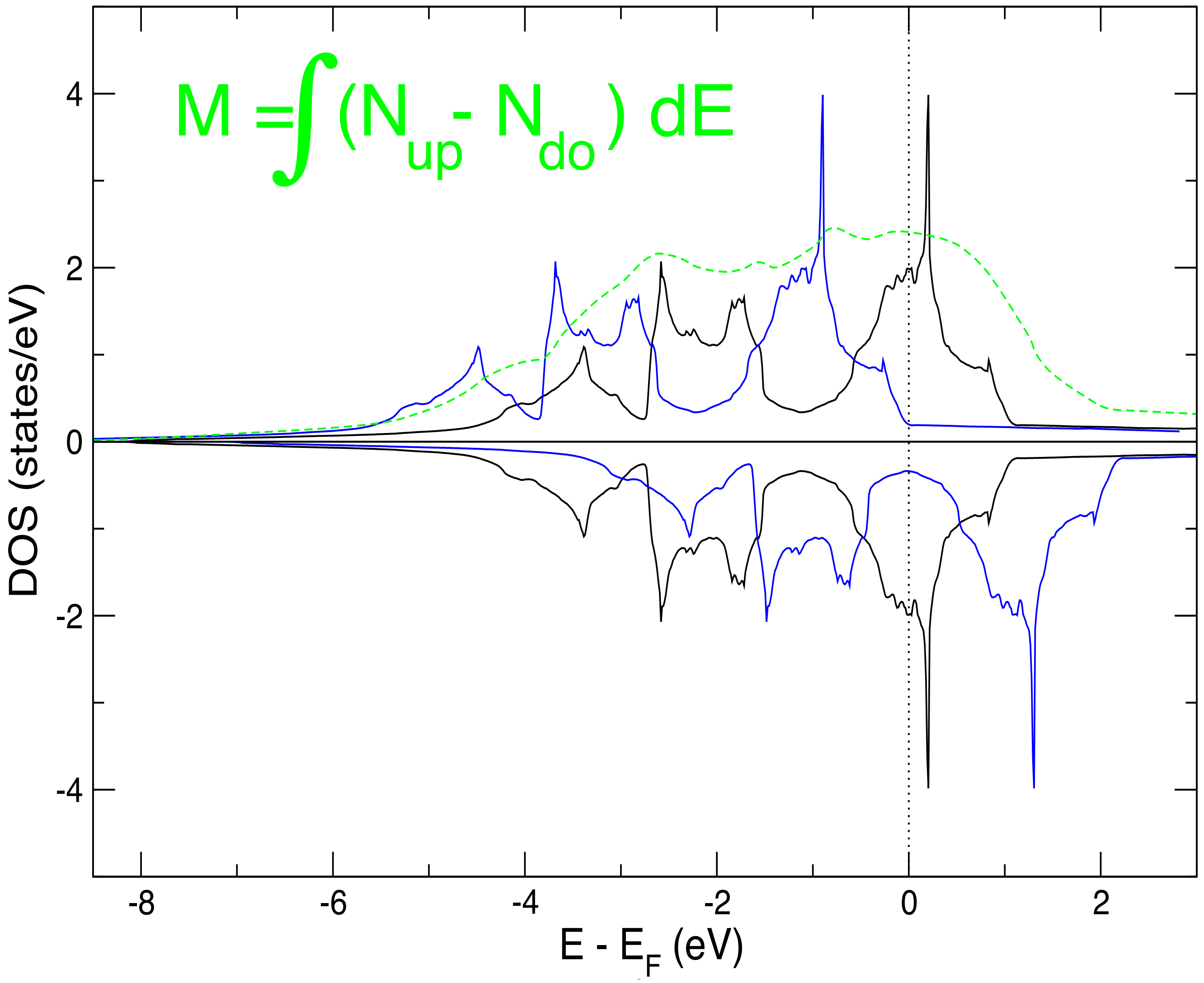


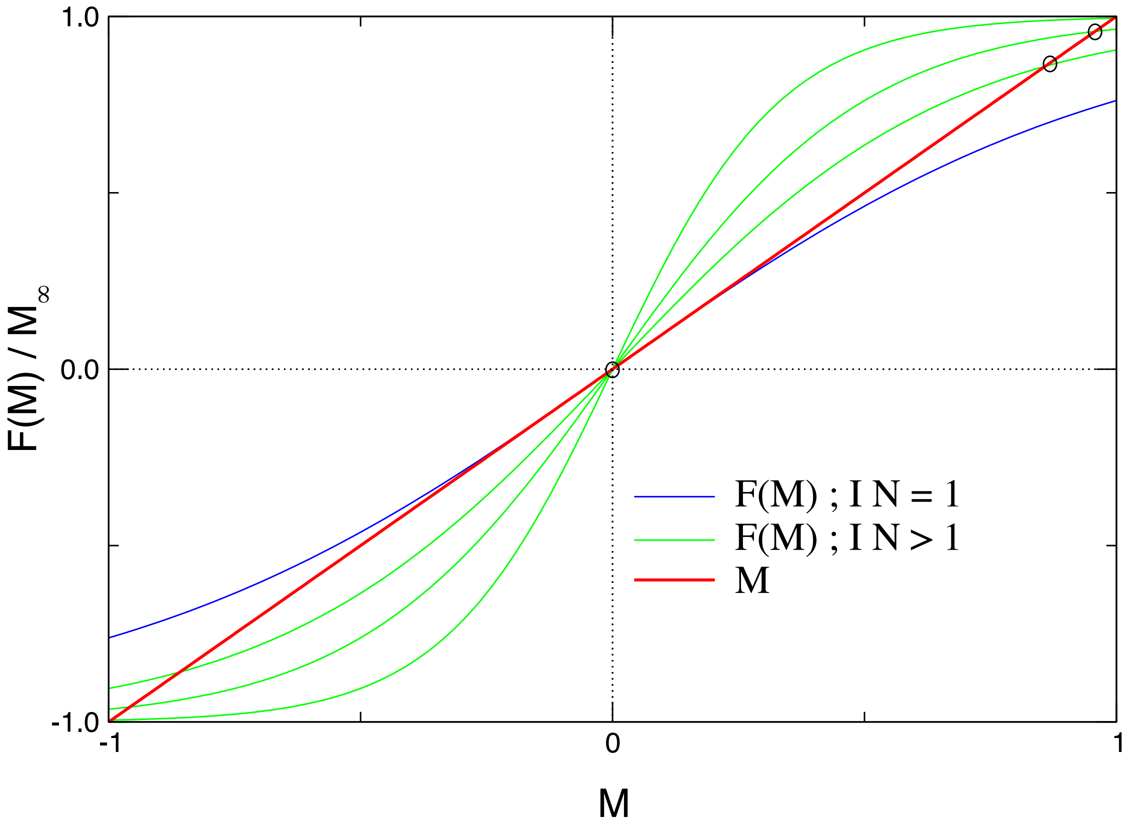
- ~~Discrete atomic levels~~
- Continuous spectrum

- Magnetisation will create B-Field
- B-Field will split energy levels
- Split will lead to magnetisation

$$F(M) = \int^{e_F} N^{\uparrow}(\epsilon) - N^{\downarrow}(\epsilon) d\epsilon$$

STONER CRITERION

$$M = F(M) = \int^{E_F} [N(E + \frac{1}{2}IM) - N(E - \frac{1}{2}IM)]dE$$



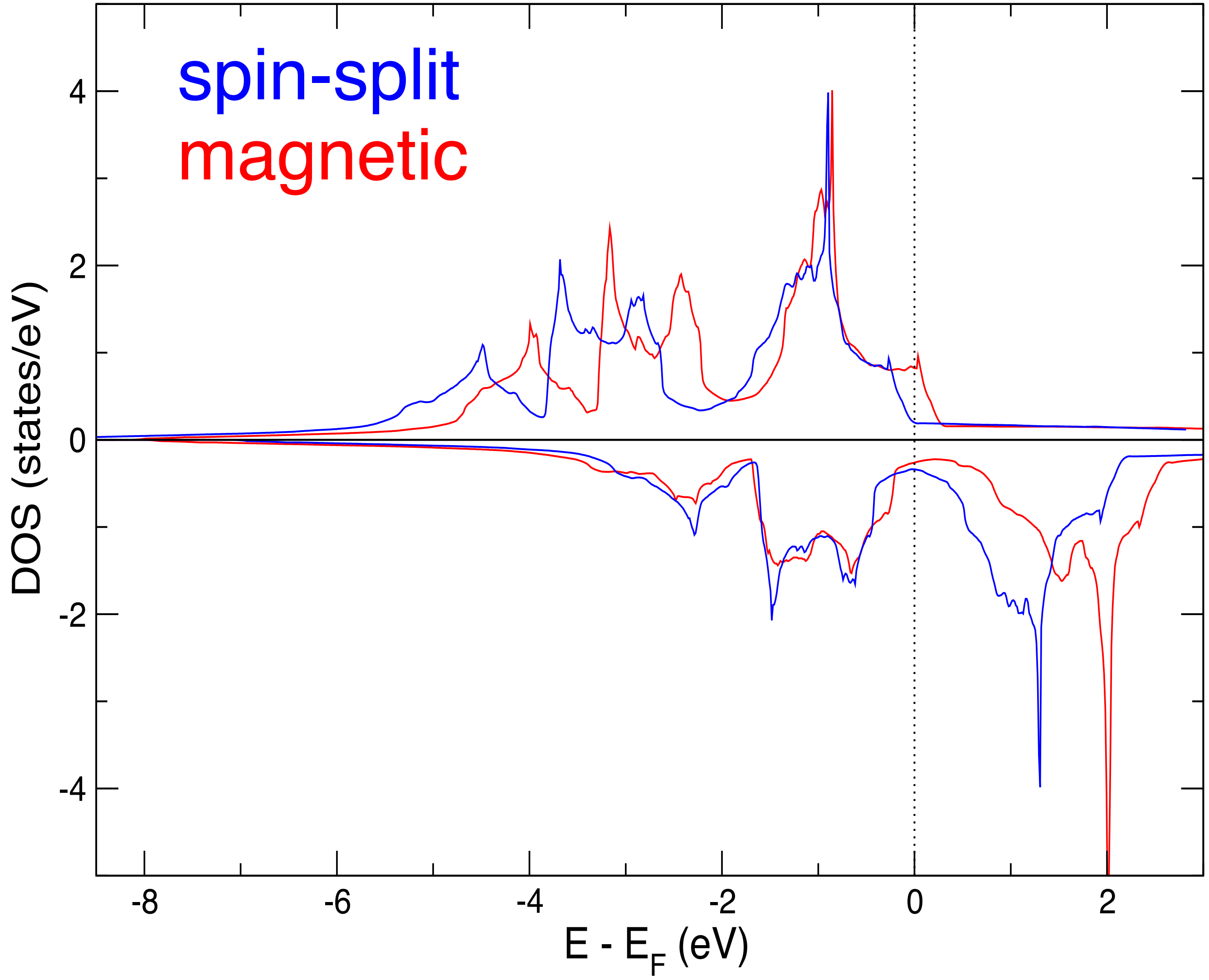
- ~~Different possible solutions~~

$$\frac{dF(M)}{dM}|_0 > 1 \quad \rightarrow IN(E_F) > 1$$

- Magnetic solution is lower in energy
- Typical values for Stoner parameter

$$I = 0.4 - 0.5eV$$

ITINERANT MAGNETS



Comparison:

- Stoner model
- Magnetic DFT calculation

Interpretation:

- Kinetic energy favours non-magnetic state
- Exchange interaction favours magnetic state
- High DOS at e_F leads to instability

MAGNETISM IN DFT

- Reminder the ”D” in DFT:

$$E = E\{n\}$$

- Potential is a functional of the density as well:

$$V_{\mathrm{eff}} = V_{\mathrm{ext}} + V_{\mathrm{Hartree}}\{n\} + V_{\mathrm{ex}}\{n\}$$

- In the magnetic case we add a dependency on the magnetisation of the system

$$V_{\mathrm{xc}}\{n\} \rightarrow V_{\mathrm{xc}}\{n, \vec{m}\}$$

MAGNETISM IN DFT

DRIVING THE EXASCALE TRANSITION

- Does it work?

$$V_{\mathrm{xc}}\{n\} \rightarrow V_{\mathrm{xc}}\{n, \vec{m}\}$$

- (Spin-)Magnetisation obtained in DFT

$$M_{\mathrm{spin}} = \int \vec{m}(\vec{r})d\vec{r} = \int [n^{\uparrow}(\vec{r}) - n^{\downarrow}(\vec{r})]d\vec{r}.$$

Property	source	Fe (bcc)	Co (fcc)	Ni (fcc)	Gd (hcp)
M_{spin}	LSDA	2.15	1.56	0.59	7.63
M_{spin}	GGA	2.22	1.62	0.62	7.65
M_{spin}	experiment	2.12	1.57	0.55	
$M_{\mathrm{tot.}}$	experiment	2.22	1.71	0.61	7.63

ORBITAL MOMENTS

Expectation value of orbital momentum operator $\mathbf{L} = \vec{r} \times \vec{v}$:

$$\vec{m}^{\mathrm{orb}}(\vec{r}) = -\mu_{\mathrm{B}} \sum_i \langle \phi_i | \vec{r} \times \vec{v} | \phi_i \rangle.$$

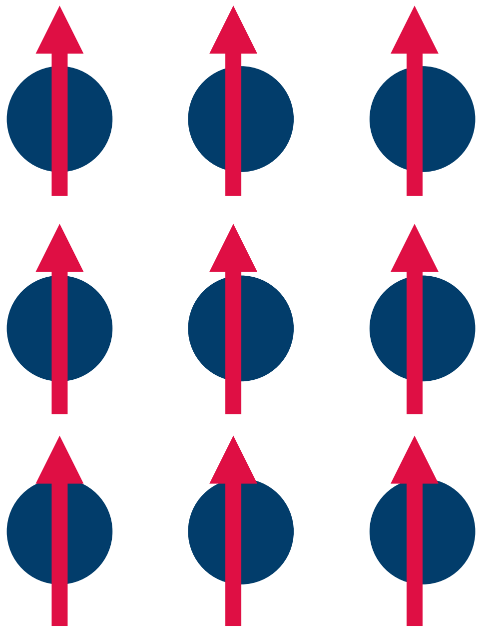
At a certain atom ν, the orbital moment M_ν^{orb} is:

$$M_\nu^{\mathrm{orb}} = -\mu_{\mathrm{B}} \sum_i \langle \phi_i | \mathbf{L} | \phi_i \rangle_\nu.$$

Property	source	Fe (bcc)	Co (fcc)	Ni (fcc)
M_{orb}	LSDA	0.05	0.08	0.05
M_{orb}	experiment	0.09	0.16	0.05

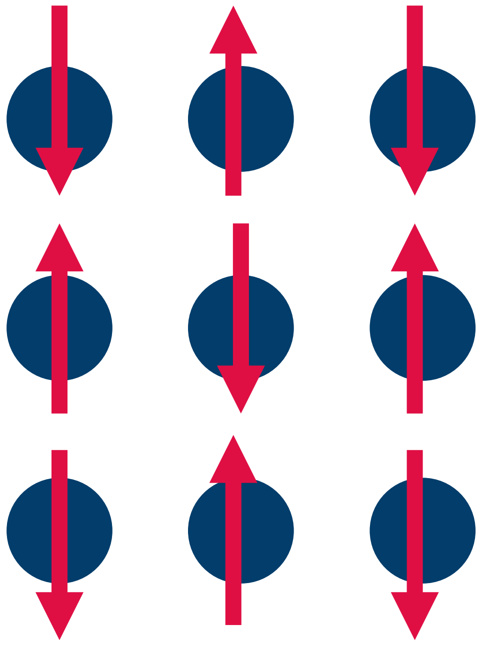
MAGNETIC ORDER

Ferromagnets



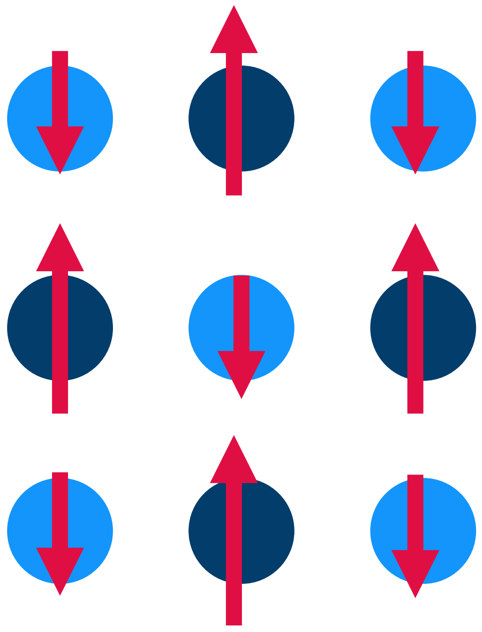
M>0

Anti-Ferromagnets



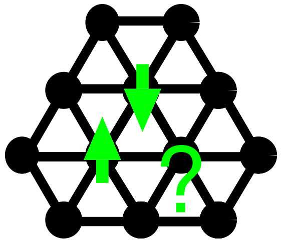
M=0

Ferrimagnets



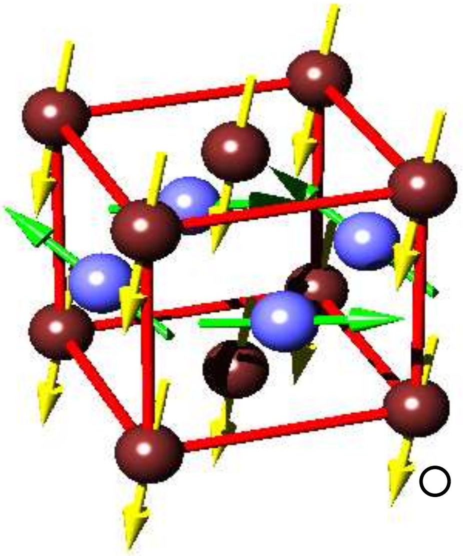
M>0

COLLINEAR VS NON-COLLINEAR

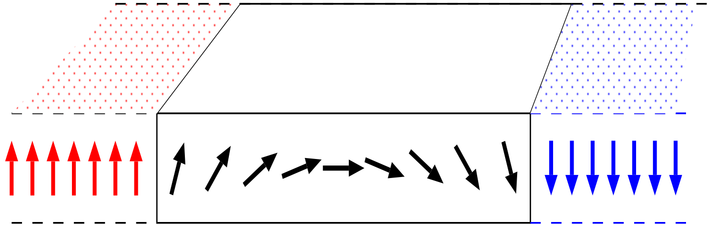


frustrated antiferromagnets
[e.g. Cr/Cu(111)]

ferro/antiferro
alloys
[e.g. FeMn]

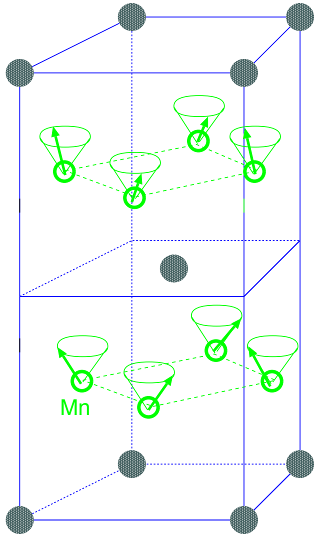


non-collinear
magnetic systems



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

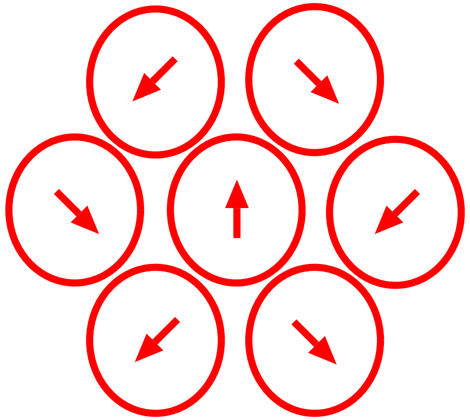
incommensurate
spin spirals
[e.g. fcc Fe,
bcc Eu,
$LaMn_2Ge_2$]



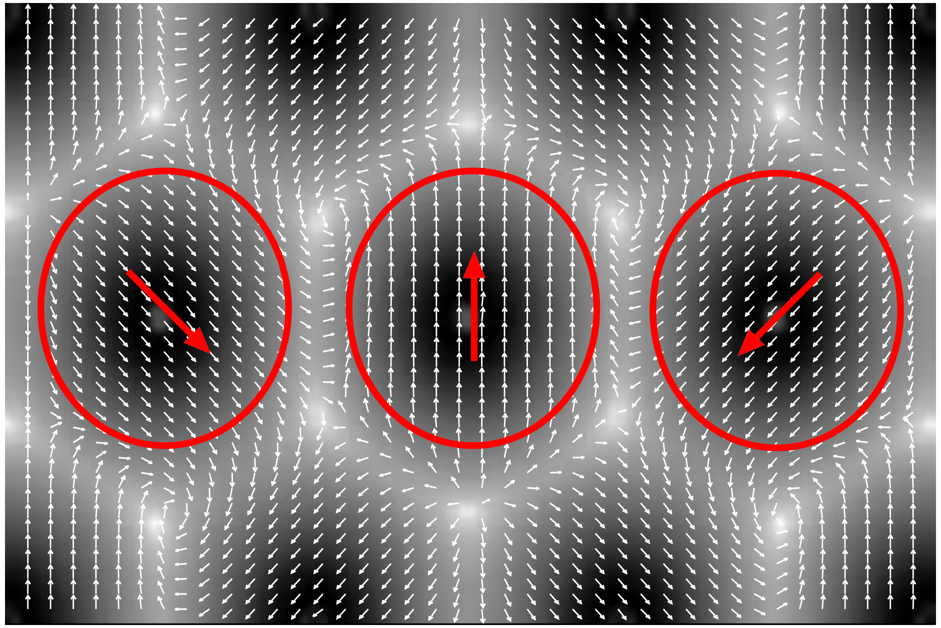
LOCAL MOMENTS

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

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

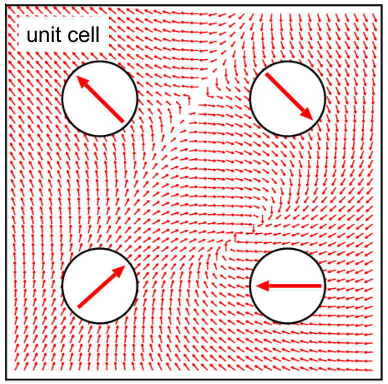


Nèel structure



Approximation:

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



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

MAX DRIVING THE EXASCALE TRANSITION

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

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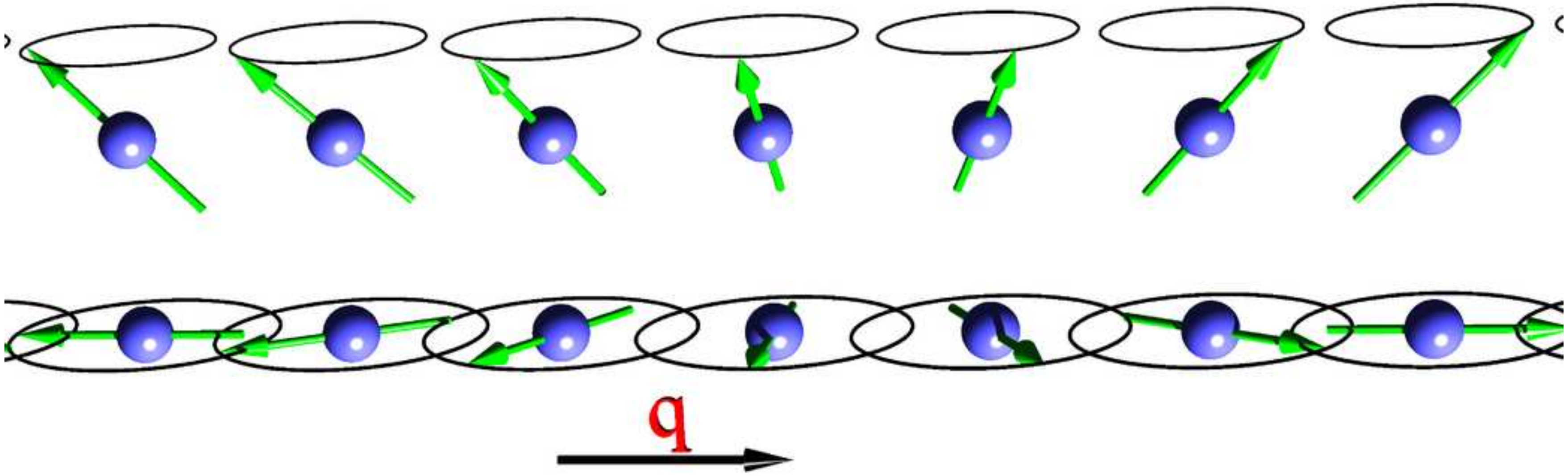
SPIN SPIRALS

- Special non-collinear state

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



SPIN SPIRALS

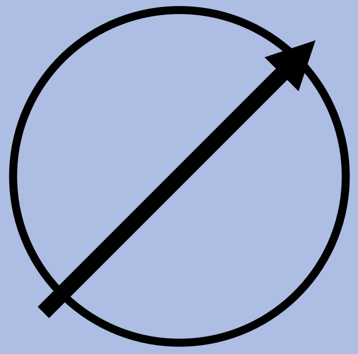
In absence of spin-orbit coupling: generalised Bloch theorem holds:

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

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

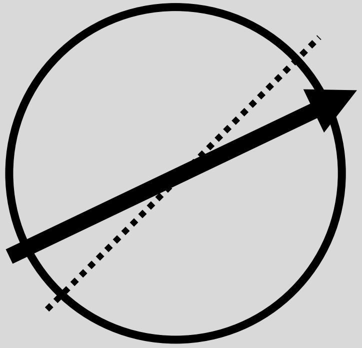
MAGNETIC MOMENTS DIRECTION

Input magnetisation:



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

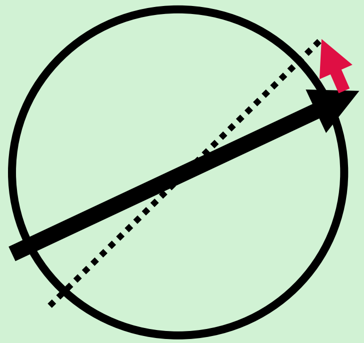
Output magnetisation:



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

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

FLEUR INPUT

Within the <calculationSetup> -tag there is a <magnetism> tag:

<magnetism jspins="2" l_noco="F" />

- jspins: determine number of spins to consider
- l_noco: is this a non-collinear setup

For a "noco" calculation:

in the <calculationSetup> tag:

<nocoParams l_ss="T" l_mperp="F" …>

<qss> 0.0 0.0 0.2 </qss>

</nocoParams>

in the <atomGroup> tag:

<nocoParams alpha="0.0" beta="1.2" …/>

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<magnetism jspins="2" l_noco="F" />

- jspins: determine number of spins to consider
- l_noco: is this a non-collinear setup

Hint: Use inpgen –noco to obtain these switches in inp.xml

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in the <calculationSetup> tag:

```
<nocoParams l_ss="T" l_mperp="F" …>
    <qss> 0.0 0.0 0.2 </qss>
  </nocoParams>
```

in the <atomGroup> tag:

```
<nocoParams alpha="0.0" beta="1.2" …/>
```

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

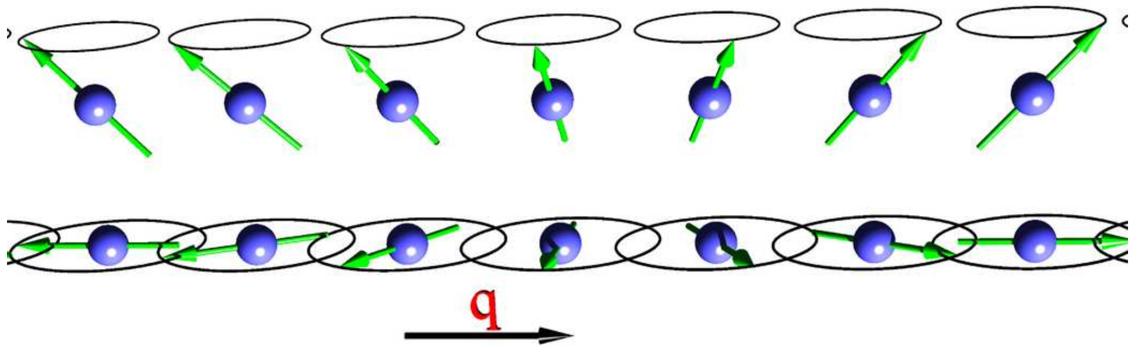
Simplify $H = -\sum_{nn'} J_{nn'} \vec{S}_n \cdot \vec{S}_{n'}$ by Fourier-transformation:

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

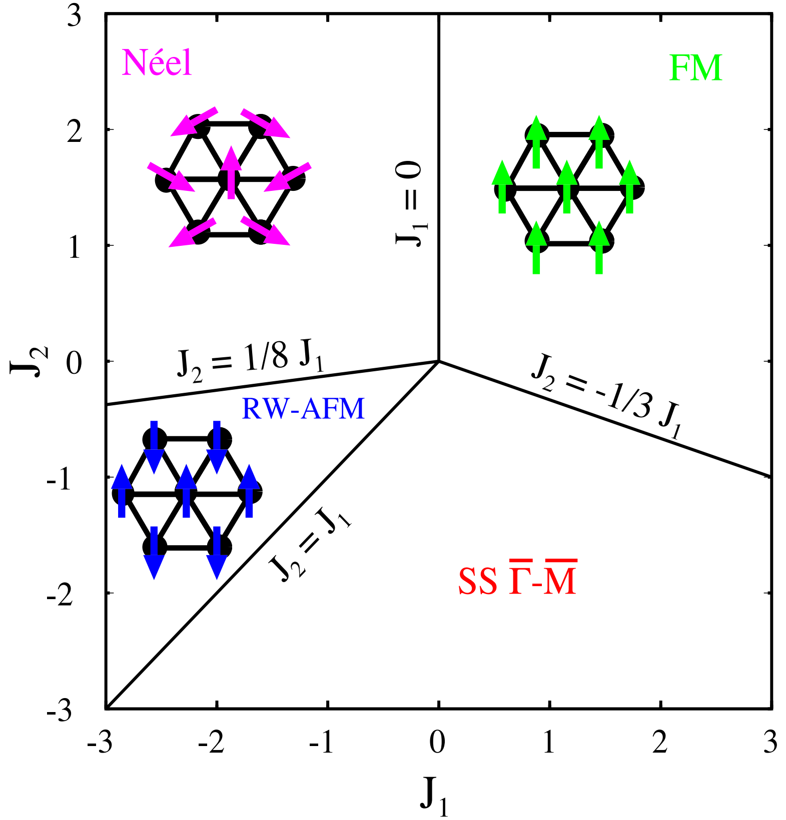
leads to

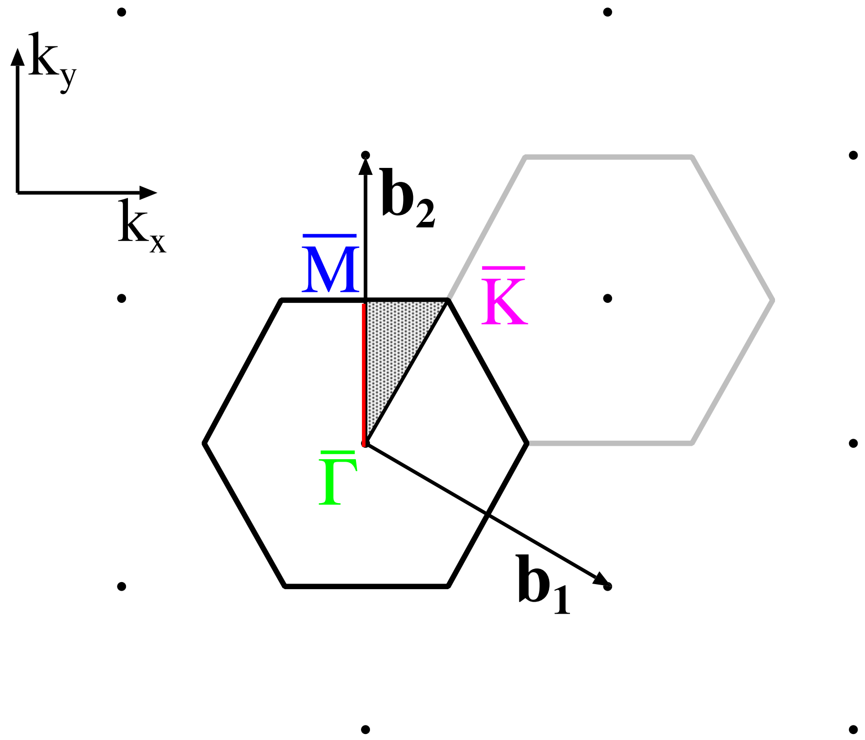
$$H = -N \sum_{\vec{q}} J(\vec{q}) \vec{S}(\vec{q}) \cdot \vec{S}(-\vec{q})$$

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





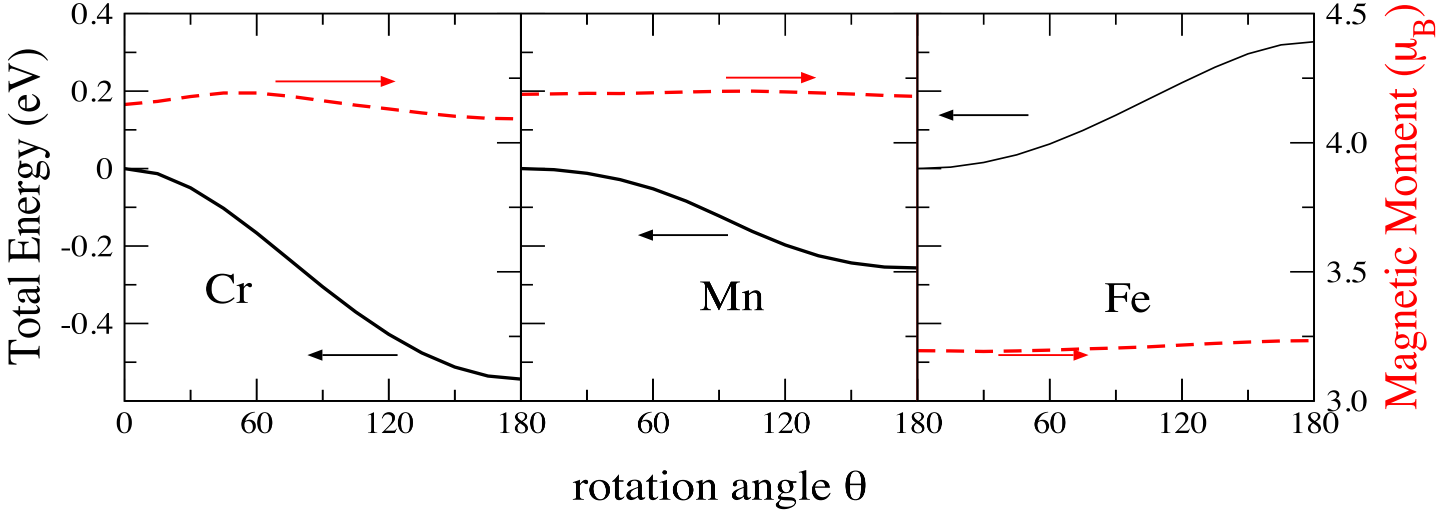
Ferromagnetic state: $\vec{q} = (0, 0)$

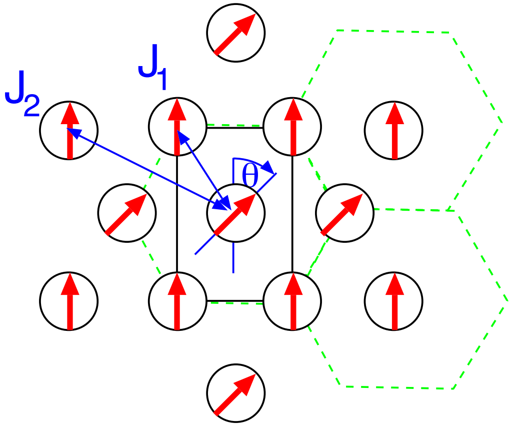
Row-wise antiferro. state: $\vec{q} = 1/2, 1/2$

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	$\cos\theta$

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

FORCE THEOREM CALCULATIONS

A change in the total energy

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

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

USING MODEL TO DETERMINE TC

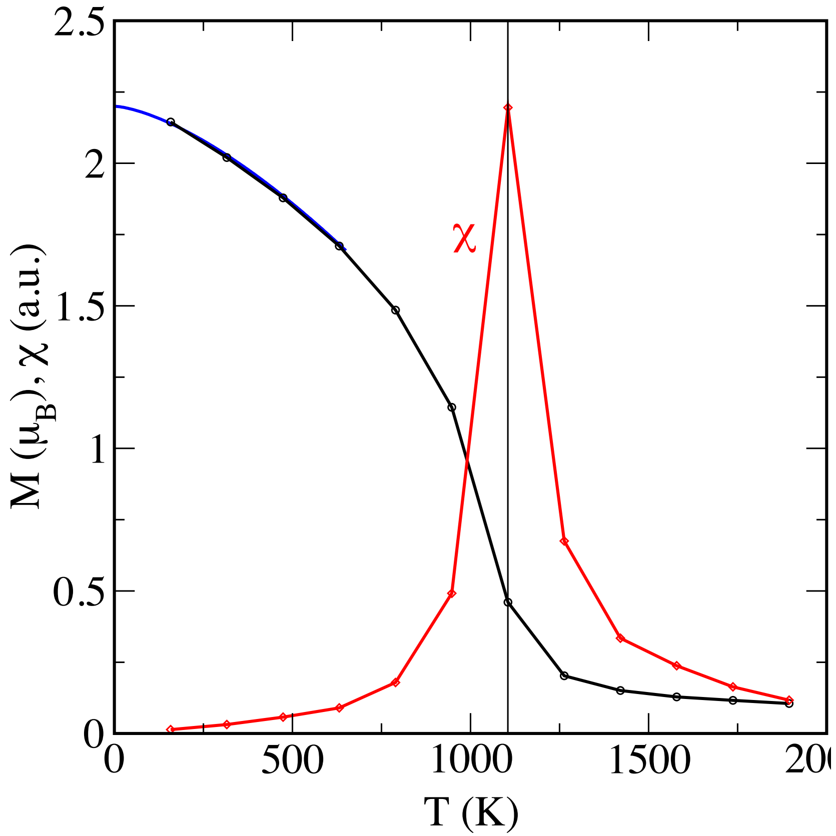
DRIVING THE EXASCALE TRANSITION

From $J_{nn'}$ one can:

- calculate J_0 and do MFA
- calculate $J(\vec{q})$ and do RPA
- make Monte Carlo simulations $\rightarrow$

to estimate T_C.

In all cases:
Check convergence w.r.t.
number of neighbor shells ($J_{nn'}$'s).



$$k_\mathrm{B}T_\mathrm{C}^\mathrm{MFA} = \frac{2}{3}J_0 \qquad k_\mathrm{B}T_\mathrm{C}^\mathrm{RPA} = \frac{2}{3}\left(\sum_{\vec{q}} \frac{1}{J(\vec{q})}\right)^{-1}$$

OUTLOOK

Heisenberg model:

- magnetic exchange
- Iteraction between two spins (magnetic sites)

Extended models, more physics:

- Further spin-interactions
- Interaction parameters including Spin-orbit interaction:
  - Magnetic anisotropy energy
  - Asymmetric exchange

Complex ground states, time dependence, …:

  - Spin dynamics

SUMMARY

You are experts on:

Magnetic Order

Spin-moment

Collinear Magnetism

Spin-Spirals

Orbital-moment

Exchange interaction

Non-collinear magnetism

Heisenberg model