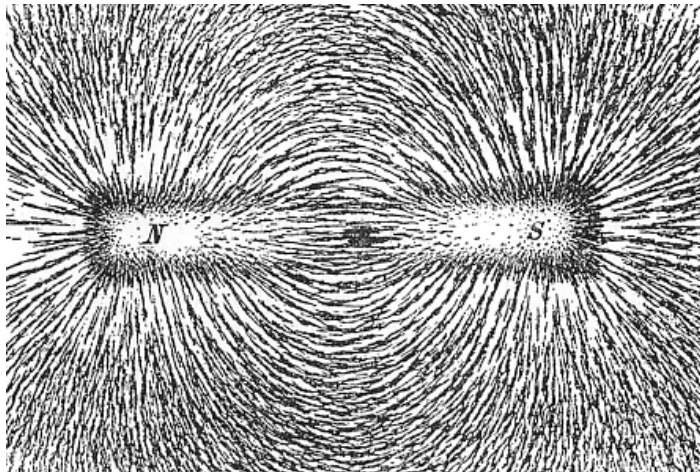


MAGNETISM

10.09.2019 | DANIEL WORTMANN

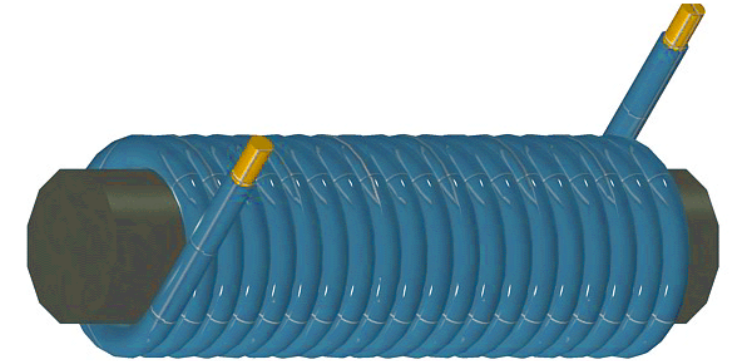
- Magnetic fields



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

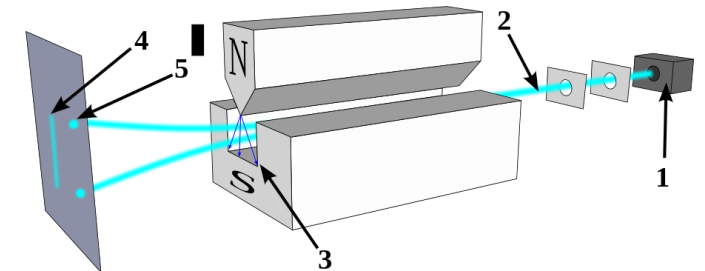
First source

- Electromagnetism
- Magnetic fields from electrical currents

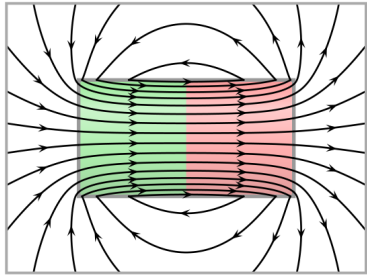


Second source:

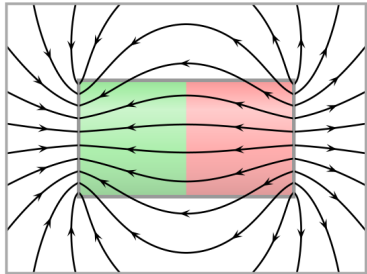
- Intrinsic magnetic moments of elementary particles
- Spin of particles



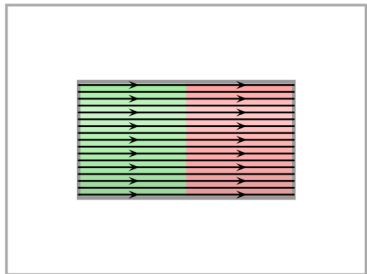
CC-Lizenz (Wikipedia)



\vec{B}



\vec{H}



\vec{M}

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

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

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

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

MAGNETISM IS RARE?

<http://www.webelements.com/>

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
hydrogen 1 H 1.00794(7)																	helium 2 He 4.002603(2)	
lithium 3 Li 6.941(2)	beryllium 4 Be 9.012182(3)											boron 5 B 10.811(7)	carbon 6 C 12.0107(8)	nitrogen 7 N 14.00674(7)	oxygen 8 O 15.9994(3)	fluorine 9 F 18.9984032(5)	neon 10 Ne 20.1797(6)	
sodium 11 Na 22.989770(2)	magnesium 12 Mg 24.3050(6)											aluminum 13 Al 26.981538(2)	silicon 14 Si 28.0855(3)	phosphorus 15 P 30.973761(2)	sulfur 16 S 32.065(3)	chlorine 17 Cl 35.453(2)	argon 18 Ar 39.948(1)	
potassium 19 K 39.0983(1)	calcium 20 Ca 40.078(4)	scandium 21 Sc 44.955910(8)	titanium 22 Ti 47.867(1)	vanadium 23 V 50.9415(1)	chromium 24 Cr 51.9961(6)	manganese 25 Mn 54.938043(9)	iron 26 Fe 55.845(2)	cobalt 27 Co 58.933195(7)	nickel 28 Ni 58.933195(7)	copper 29 Cu 63.546(3)	zinc 30 Zn 65.409(4)	gallium 31 Ga 69.723(1)	germanium 32 Ge 72.64(1)	arsenic 33 As 74.92160(2)	selenium 34 Se 78.96(3)	bromine 35 Br 79.904(1)	krypton 36 Kr 83.798(2)	
rubidium 37 Rb 85.4678(3)	strontium 38 Sr 87.62(1)	yttrium 39 Y 88.90585(2)	zirconium 40 Zr 91.224(2)	niobium 41 Nb 92.90638(2)	molybdenum 42 Mo 95.94(1)	technetium 43 Tc [98]	ruthenium 44 Ru 101.07(2)	rhodium 45 Rh 102.90550(2)	palladium 46 Pd 106.42(1)	silver 47 Ag 107.8682(2)	cadmium 48 Cd 112.411(8)	indium 49 In 114.818(3)	tin 50 Sn 118.710(7)	antimony 51 Sb 121.760(1)	tellurium 52 Te 127.60(3)	iodine 53 I 126.90447(3)	xenon 54 Xe 131.293(6)	
caesium 55 Cs 132.90545(2)	barium 56 Ba 137.327(7)	57-70 *	lutetium 71 Lu 174.967(1)	hafnium 72 Hf 178.49(2)	tantalum 73 Ta 180.9479(1)	tungsten 74 W 183.84(1)	rhenium 75 Re 186.207(1)	osmium 76 Os 190.23(3)	iridium 77 Ir 192.217(3)	platinum 78 Pt 195.078(2)	gold 79 Au 196.96655(2)	mercury 80 Hg 200.59(2)	thallium 81 Tl 204.3833(2)	lead 82 Pb 207.2(1)	bismuth 83 Bi 208.98038(2)	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnium 110 Uun [271]	ununium 111 Uuu [272]	unubium 112 Uub [285]		ununquadium 114 Uuq [289]				

Key:
 element name
 atomic number
 symbol
 2001 atomic weight (mean relative mass)

*lanthanoids

**actinoids

lanthanum 57 La 138.9055(2)	cerium 58 Ce 140.116(1)	praseodymium 59 Pr 140.90763(2)	neodymium 60 Nd 144.24(3)	promethium 61 Pm [145]	samarium 62 Sm 150.36(3)	europium 63 Eu 151.964(1)	gadolinium 64 Gd 157.25(3)	terbium 65 Tb 158.92534(2)	dysprosium 66 Dy 162.500(1)	holmium 67 Ho 164.93032(2)	erbium 68 Er 167.259(3)	thulium 69 Tm 168.93421(2)	ytterbium 70 Yb 173.04(3)
actinium 89 Ac [227]	thorium 90 Th 232.0381(1)	protactinium 91 Pa 231.03688(2)	uranium 92 U 238.02891(3)	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendeleevium 101 Md [258]	nobelium 102 No [259]

ATOMIC MAGNETISM

Isolated atoms:

- All atoms with incompletely filled shells are magnetic

<http://www.webelements.com/>

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Hydrogen 1 H 1.00794(7)																	Helium 2 He 4.0026032(3)
Lithium 3 Li 6.941(2)	Beryllium 4 Be 9.0121832(3)											Boron 5 B 10.811(7)	Carbon 6 C 12.010(8)	Nitrogen 7 N 14.00643(4)	Oxygen 8 O 15.9994(4)	Fluorine 9 F 18.9984032(3)	Neon 10 Ne 20.1797(6)
Sodium 11 Na 22.98976928(2)	Magnesium 12 Mg 24.30409(4)											Aluminum 13 Al 26.9815385(3)	Silicon 14 Si 28.0855(3)	Phosphorus 15 P 30.973761998(5)	Sulfur 16 S 32.065(5)	Chlorine 17 Cl 35.453(2)	Argon 18 Ar 39.948(1)
Potassium 19 K 39.0983(1)	Calcium 20 Ca 40.078(4)	Scandium 21 Sc 44.9559108(6)	Titanium 22 Ti 47.88(7)	Vanadium 23 V 50.9415(2)	Chromium 24 Cr 51.9961(6)	Manganese 25 Mn 54.938044(1)	Iron 26 Fe 55.845(2)	Cobalt 27 Co 58.933195(5)	Nickel 28 Ni 58.6934(4)	Copper 29 Cu 63.546(3)	Zinc 30 Zn 65.408(4)	Gallium 31 Ga 69.723(1)	Germanium 32 Ge 72.64(1)	Arsenic 33 As 74.921595(6)	Selenium 34 Se 78.96(3)	Bromine 35 Br 79.904(1)	Krypton 36 Kr 83.798(2)
Rubidium 37 Rb 85.4678(3)	Sr 87.62(1)	Yttrium 39 Y 88.90585(2)	Zirconium 40 Zr 91.224(2)	Niobium 41 Nb 92.90638(2)	Molybdenum 42 Mo 95.94(1)	Technetium 43 Tc [98]	Ruthenium 44 Ru 101.07(2)	Rhodium 45 Rh 102.90550(2)	Palladium 46 Pd 106.42(1)	Silver 47 Ag 107.8682(2)	Cadmium 48 Cd 112.411(8)	Indium 49 In 114.818(3)	Tin 50 Sn 118.710(7)	Antimony 51 Sb 121.757(3)	Tellurium 52 Te 127.60(3)	Iodine 53 I 126.90447(3)	Xenon 54 Xe 131.29(3)
Cesium 55 Cs 132.9054519(3)	Ba 137.327(7)	Lanthanum 57 La 138.90549(3)	Hafnium 72 Hf 178.49(2)	Tantalum 73 Ta 180.94788(2)	Tungsten 74 W 183.84(1)	Rhenium 75 Re 186.207(1)	Osmium 76 Os 190.23(4)	Iridium 77 Ir 192.222(1)	Platinum 78 Pt 195.078(2)	Gold 79 Au 196.966569(4)	Mercury 80 Hg 200.59(2)	Thallium 81 Tl 204.3833(2)	Lead 82 Pb 207.2(1)	Bismuth 83 Bi 208.980386(2)	Polonium 84 Po [209]	Astatine 85 At [210]	Rn [222]
Francium 87 Fr [223]	Radium 88 Ra [226]	Lr [262]	Rf [261]	Db [262]	Sg [263]	Bh [264]	Hs [265]	Mt [266]	Uun [271]	Uuu [272]	Uub [285]	Uuq [289]					

Key:
element name
atomic number
symbol
2001 atomic weight (mean relative mass)

*lanthanoids

57	58	59	60	61	62	63	64	65	66	67	68	69	70
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
138.90549(3)	140.116(1)	140.90768(2)	144.242(3)	[147]	150.358(2)	151.964(1)	157.254(1)	158.92534(2)	162.500(1)	164.930329(2)	167.259(2)	168.93421(2)	173.054(3)
89	90	91	92	93	94	95	96	97	98	99	100	101	102
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No
[227]	232.0381(1)	231.036888(2)	238.02891(3)	[237]	[244]	[247]	[250]	[252]	[257]	[258]	[261]	[269]	[289]

**actinoids

Simple counting:

- odd number of spins -> sum not zero

Hund's first rule:

- Spins are aligned to maximize total moment
- Example:

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

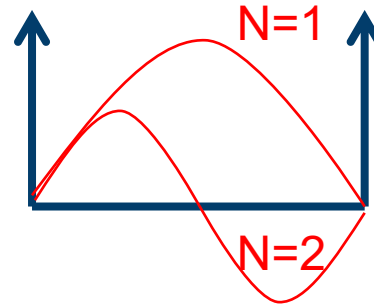


- Intra atomic exchange interaction!

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:

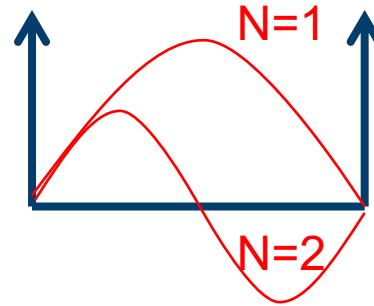
$$V_{ij} = \int \frac{\psi_i^2(r)\psi_j^2(r')}{|r - r'|}$$

- 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"



- No interaction:

- States quantized: $\epsilon = \frac{1}{2} k^2 \propto \frac{1}{\lambda^2} \propto N^2$

- Kinetic energy

- Each state hosts two electrons with different spin

- Two electrons: both N=1 with opposite spins

- Interaction:

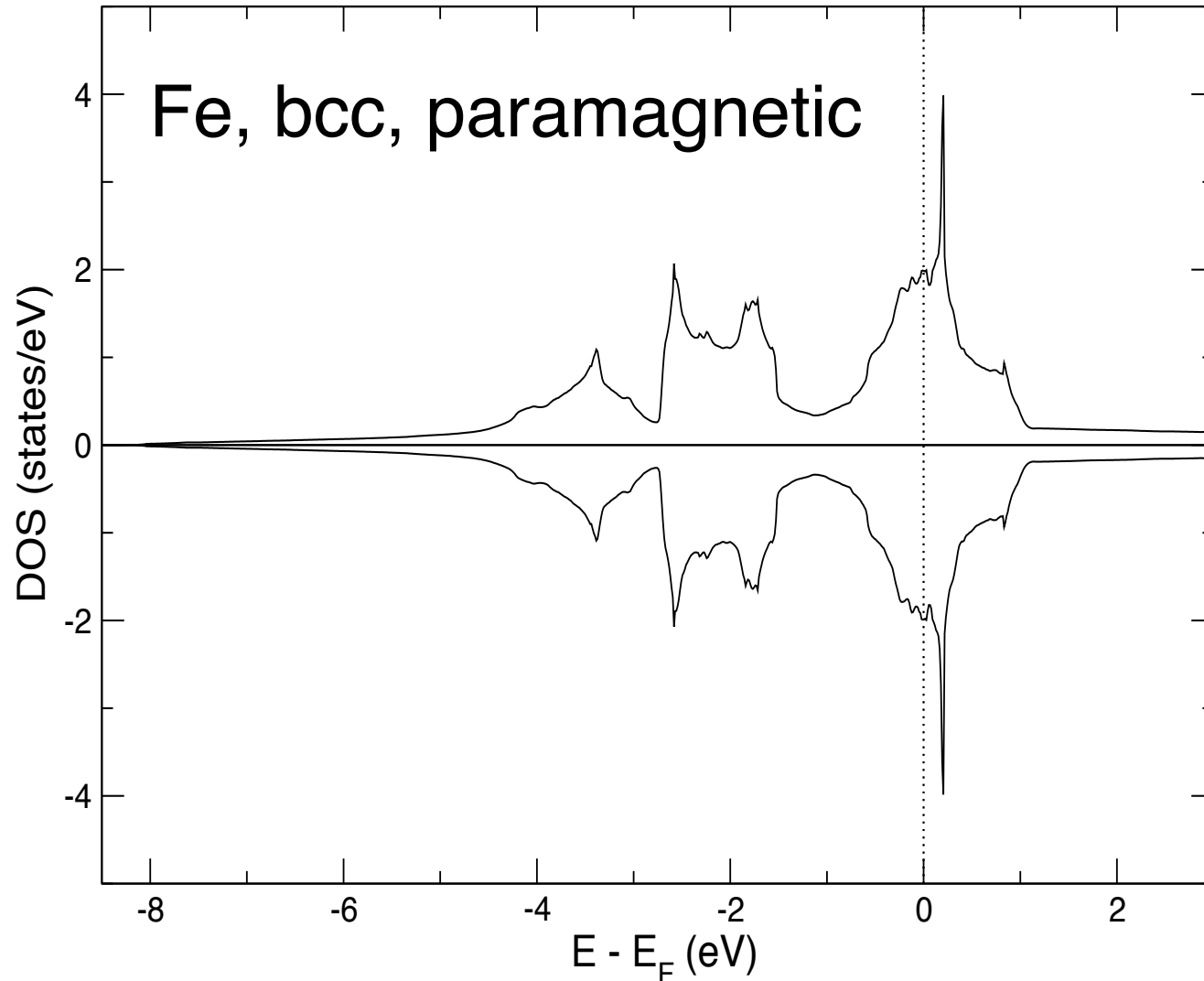
$$V_{ij} = \int \frac{\psi_i^2(r)\psi_j^2(r')}{|r - r'|}$$

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

particles in different states

electrons:

one in N=1, one in N=2 ??

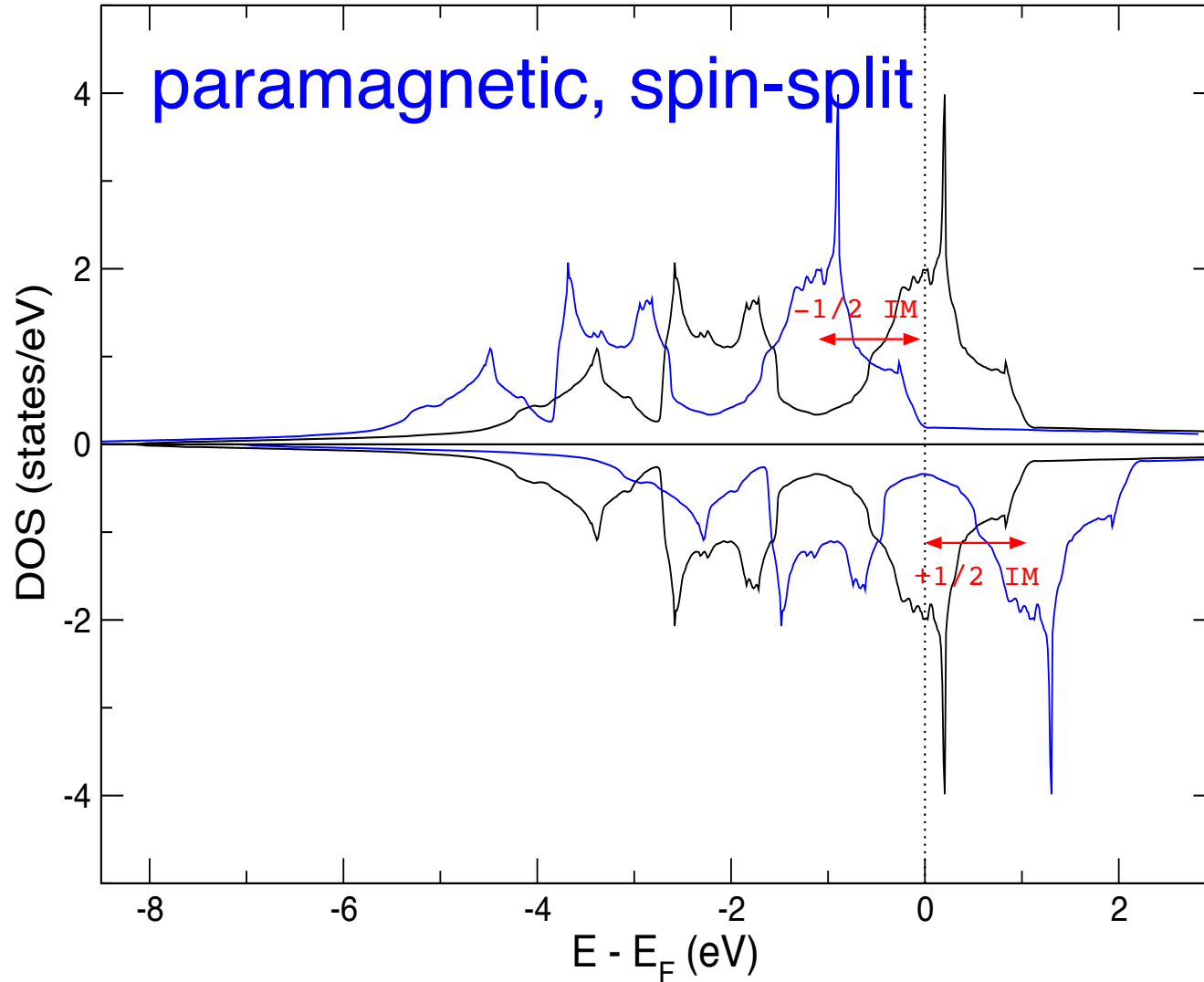


- Discrete atomic levels
- Continuous spectrum

- Magnetisation will create B-Field

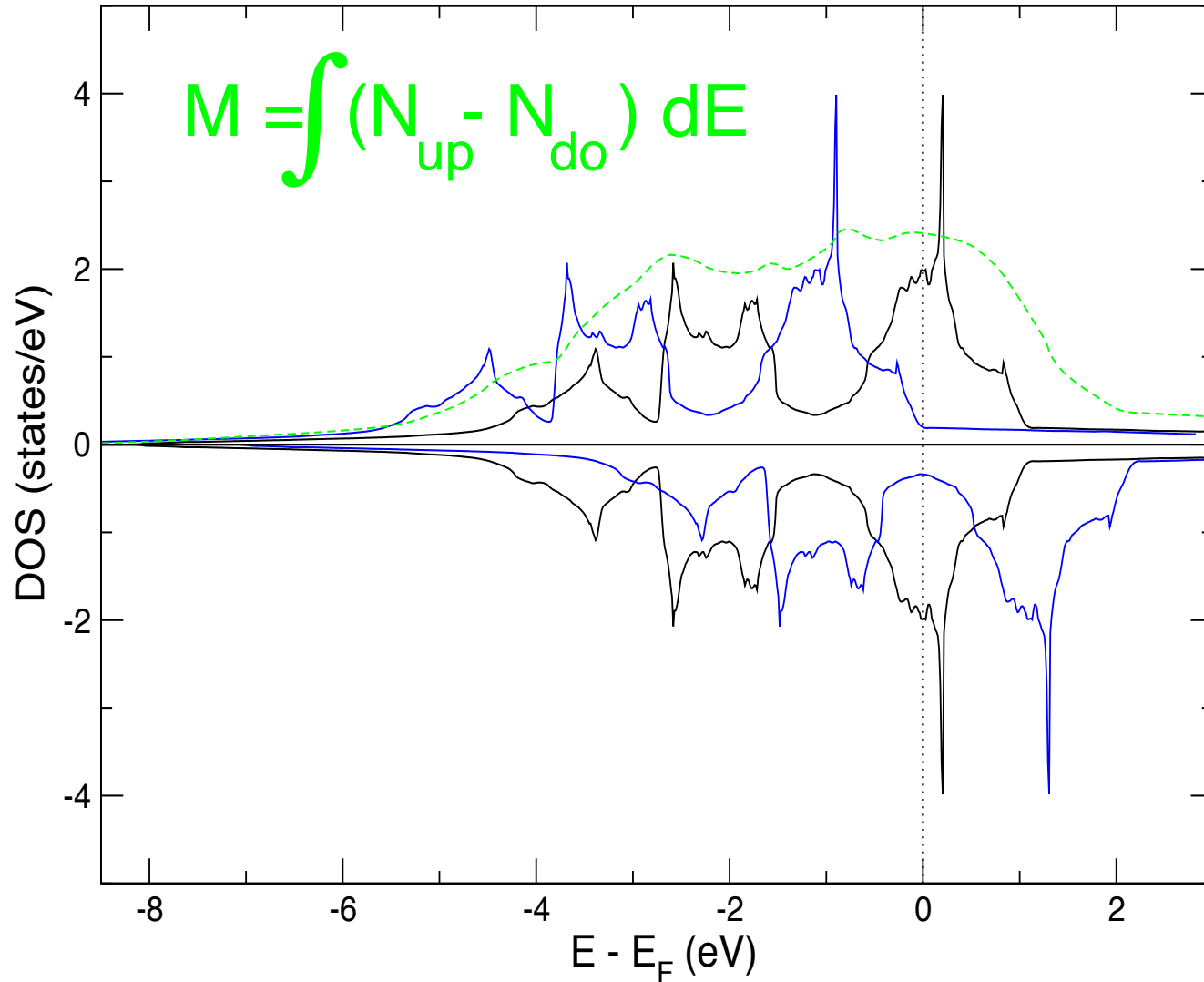
$$\vec{M} \rightarrow \vec{B}$$

$$B = I_0 * M + O(M^2)$$
$$\epsilon \approx \epsilon_0 \pm \mu_b B = \epsilon_0 \pm \frac{1}{2} IM$$



- Discrete atomic levels
- Continuous spectrum
- Magnetisation will create B-Field
- B-Field will split energy levels

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

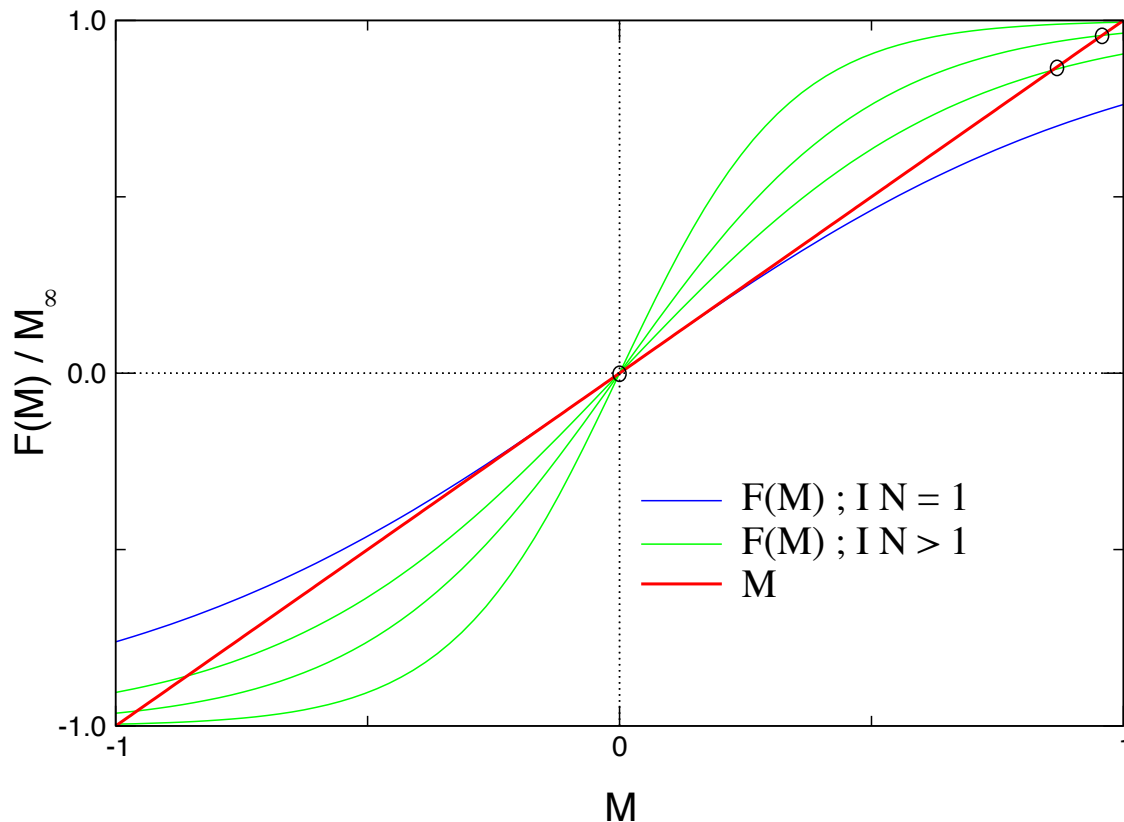


- Discrete atomic levels
- Continuous spectrum
- Magnetisation will create B-Field
- B-Field will split energy levels
- Split will lead to magnetisation

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

STONER CRITERION

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

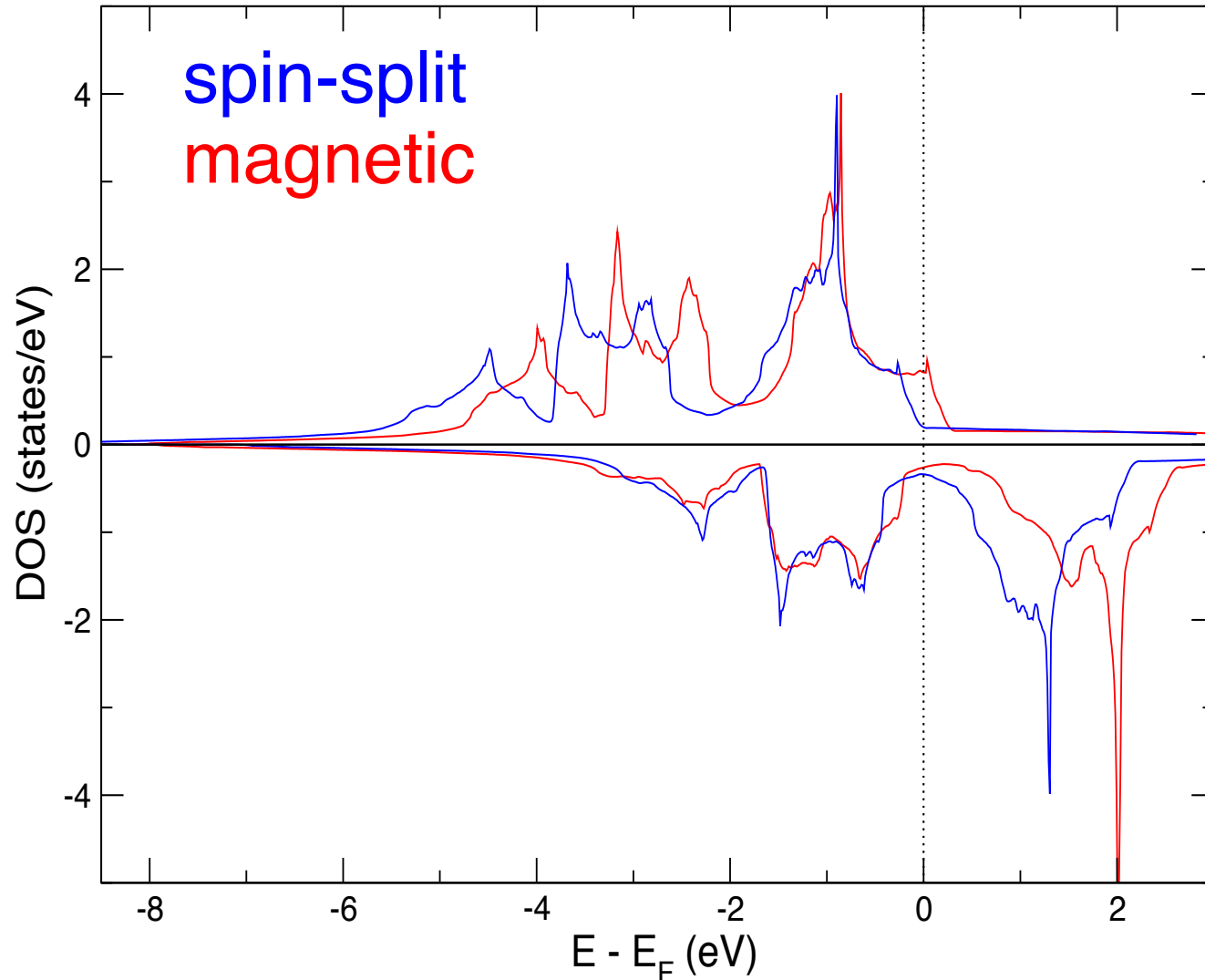


- Different possible solutions

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

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

$$I = 0.4 - 0.5eV$$



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

- Reminder the "D" in DFT:

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

- Potential is a functional of the density as well:

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

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

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

- Does it work?

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

- (Spin-)Magnetisation obtained in DFT

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

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	
$M_{\text{tot.}}$	experiment	2.22	1.71	0.61	7.63

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

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

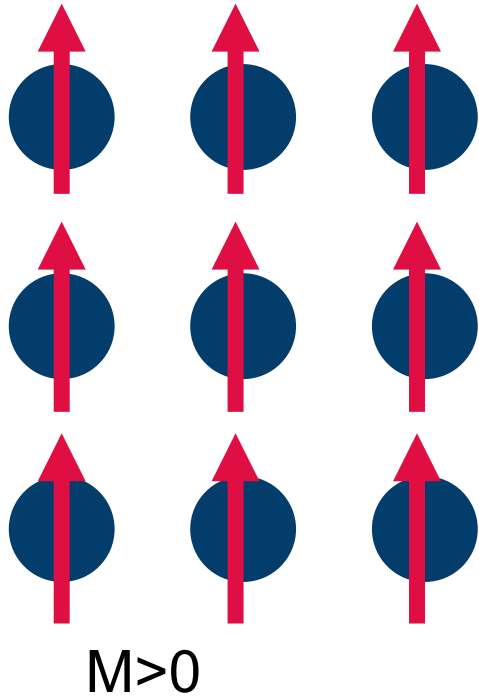
At a certain atom ν , the orbital moment M_{ν}^{orb} is:

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

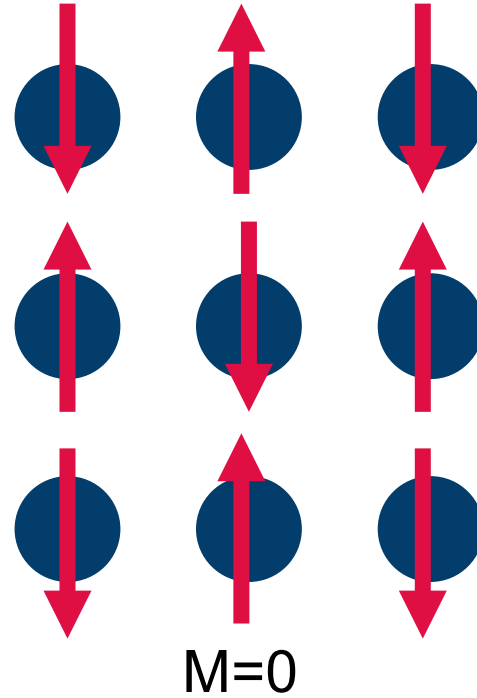
Property	source	Fe (bcc)	Co (fcc)	Ni (fcc)
M_{orb}	LSDA	0.05	0.08	0.05
M_{orb}	experiment	0.09	0.16	0.05

MAGNETIC ORDER

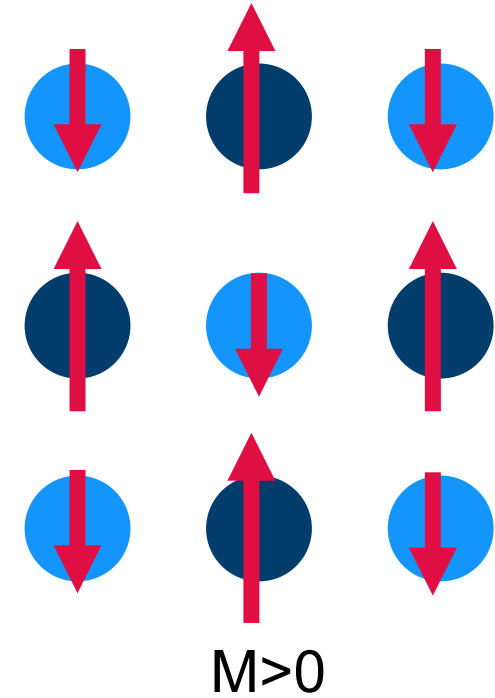
Ferromagnets



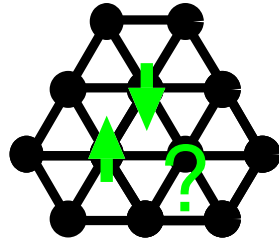
Anti-Ferromagnets



Ferrimagnets

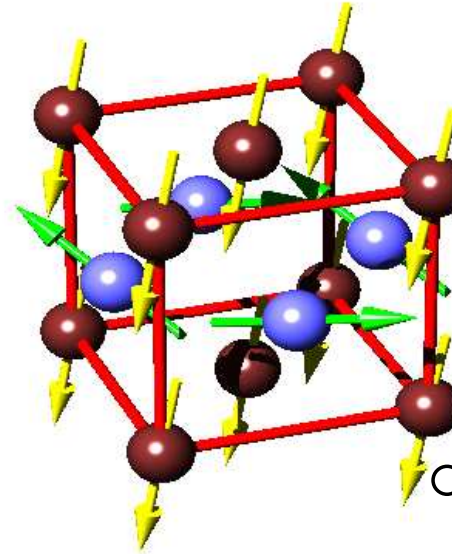


COLLINEAR VS NON-COLLINEAR

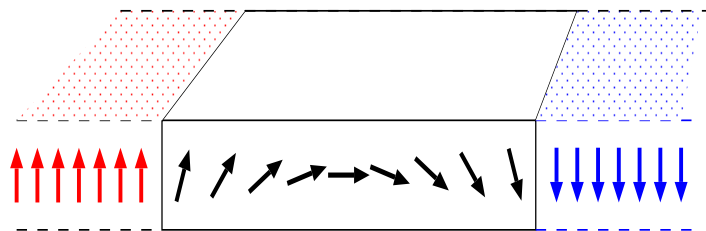


frustrated antiferromagnets
[e.g. Cr/Cu(111)]

ferro/antiferro
alloys
[e.g. FeMn]

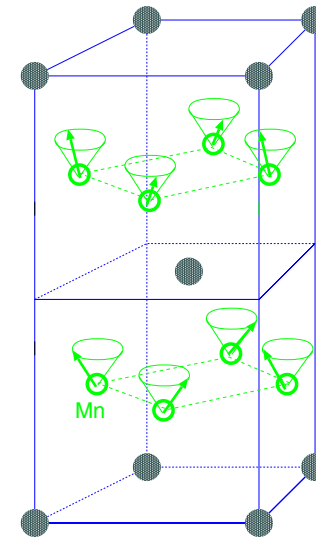


non-collinear
magnetic systems



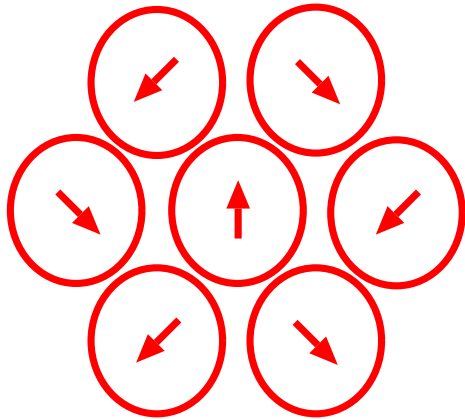
domain walls in thin films
[e.g. Fe/W(110)]

incommensurate
spin spirals
[e.g. fcc Fe,
bcc Eu,
LaMn₂Ge₂]

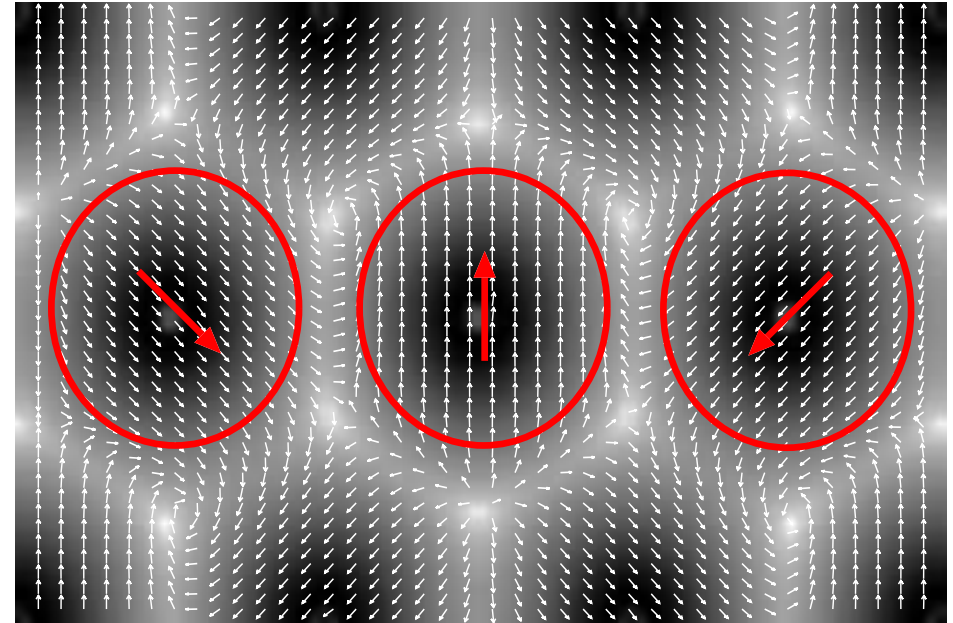


Cr monolayer on Cu(111): Néel structure
Inside the red spheres:

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

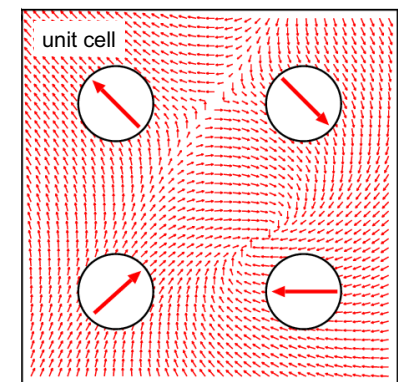


Néel structure



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:
- Wave function consists of two component spinor
- Hamiltonian becomes 2x2 matrix in spin
- Density: $n = \sum |\psi|^2$

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

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

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

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

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 :

$$(H_0 + v) \phi_i = \epsilon_i \phi_i$$

$$\begin{aligned} (H_0 + v + B^\uparrow) \phi_i^\uparrow &= \epsilon_i^\uparrow \phi_i^\uparrow \\ (H_0 + v + B^\downarrow) \phi_i^\downarrow &= \epsilon_i^\downarrow \phi_i^\downarrow \end{aligned}$$

$$\left(H_0 + \begin{array}{c|c} V_{\uparrow\uparrow} & V_{\uparrow\downarrow} \\ \hline V_{\downarrow\uparrow} & V_{\downarrow\downarrow} \end{array} \right) \begin{pmatrix} \phi_i^\uparrow \\ \phi_i^\downarrow \end{pmatrix} = \epsilon_i \begin{pmatrix} \phi_i^\uparrow \\ \phi_i^\downarrow \end{pmatrix}$$

Inversion sy. :

real-symmetric

real-symmetric

complex-hermitian

Unit cell :

small

large

large

irreducible BZ :

small

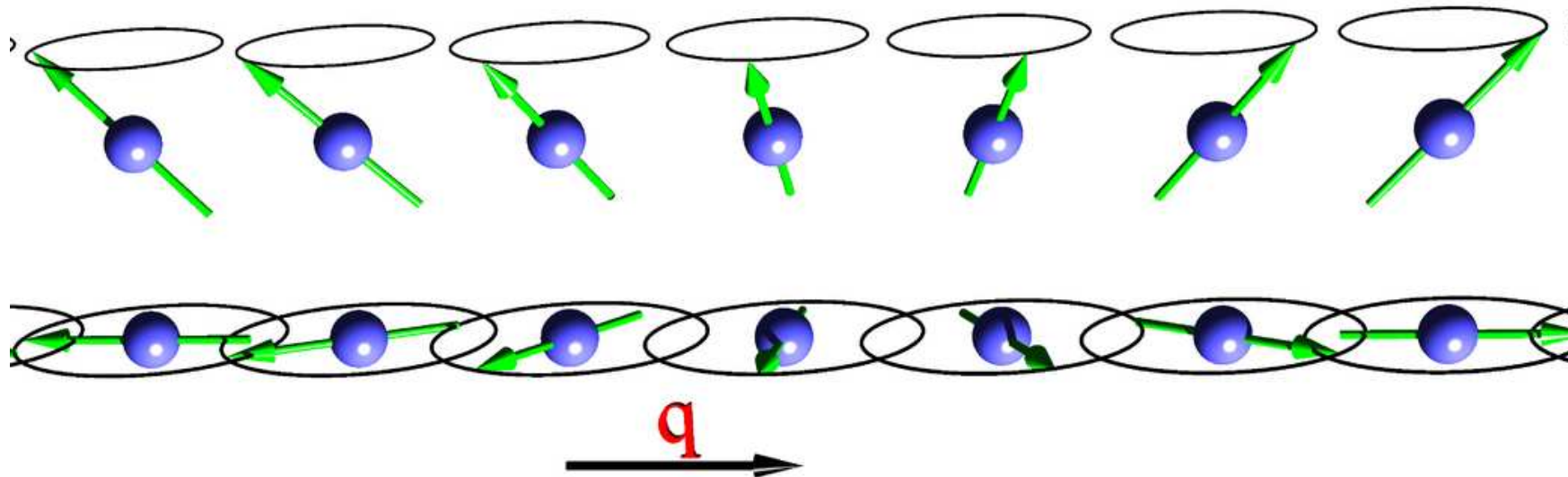
small

large

SPIN SPIRALS

- Special non-collinear state

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



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

Bloch theorem

generalised Bloch theorem

translation \vec{R}_n

translation + spin rotation U_φ

$$U_\varphi = \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0 \\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix}; \varphi = \vec{q} \cdot \vec{R}_n$$

$$\mathcal{T}_n \Psi_{\vec{k}}(\vec{r}) = \Psi_{\vec{k}}(\vec{r} + \vec{R}_n) = e^{i\vec{k} \cdot \vec{R}_n} \Psi_{\vec{k}}$$

$$\mathcal{T}_n \Phi_{\vec{k}}(\vec{r}) = U_\varphi \Phi_{\vec{k}}(\vec{r} + \vec{R}_n) = e^{i\vec{k} \cdot \vec{R}_n} \Phi_{\vec{k}}(\vec{r})$$

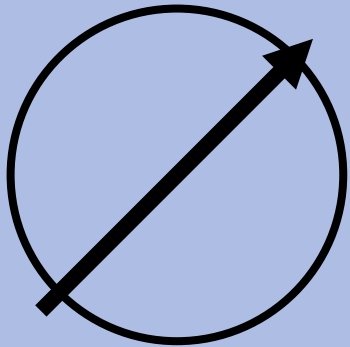
$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u(\vec{r})$$

$$\Phi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \begin{pmatrix} e^{-\frac{i\vec{q} \cdot \vec{r}}{2}} u_\uparrow(\vec{r}) \\ e^{\frac{i\vec{q} \cdot \vec{r}}{2}} u_\downarrow(\vec{r}) \end{pmatrix}$$

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

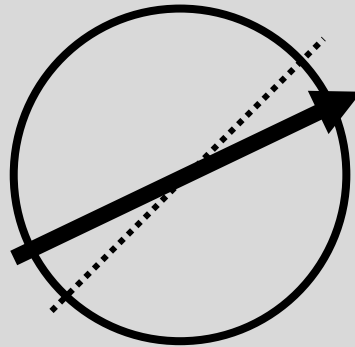
MAGNETIC MOMENTS DIRECTION

Input magnetisation:



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

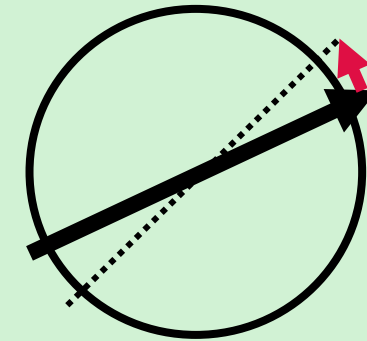
Output magnetisation:



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

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

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" .../>
```

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

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

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" .../>
```

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

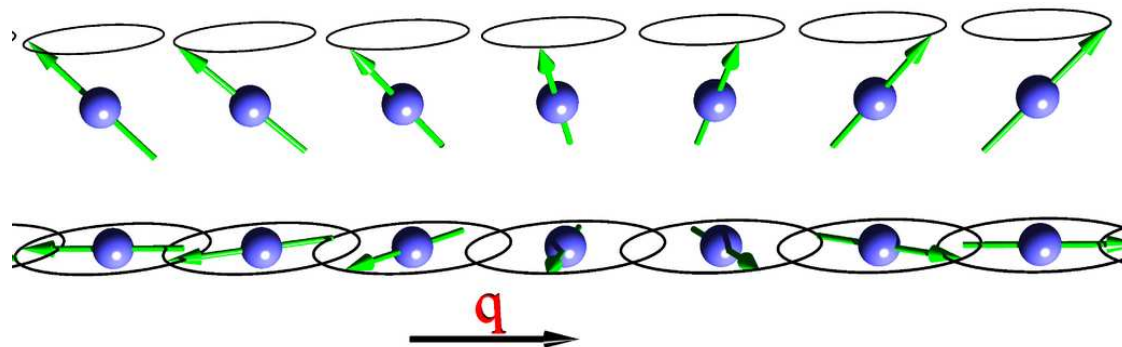
Simplify $H = - \sum_{nn'} J_{nn'} \vec{S}_n \cdot \vec{S}_{n'}$ by Fourier-transformation:

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

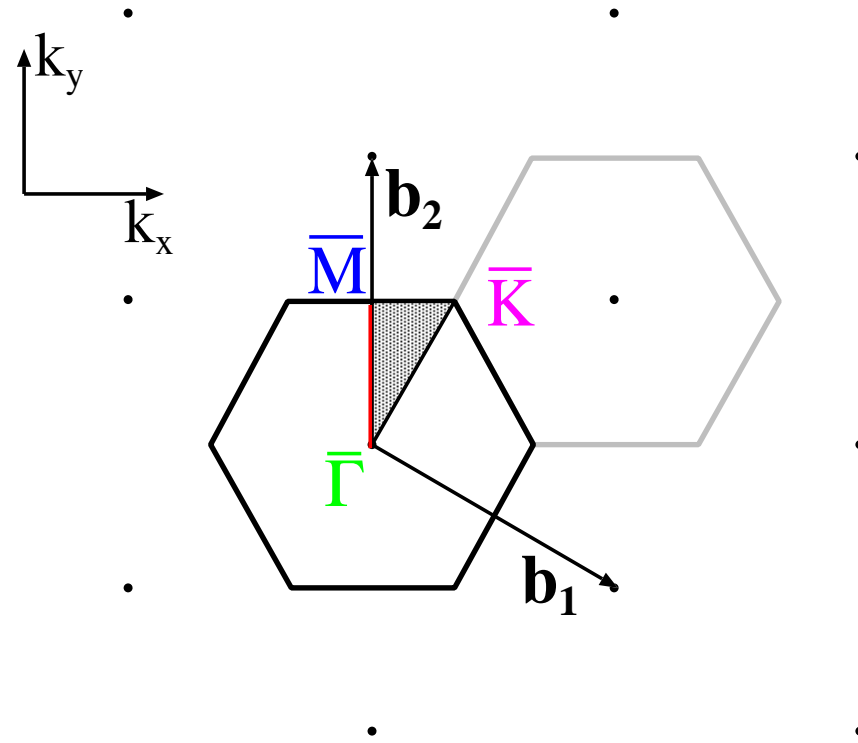
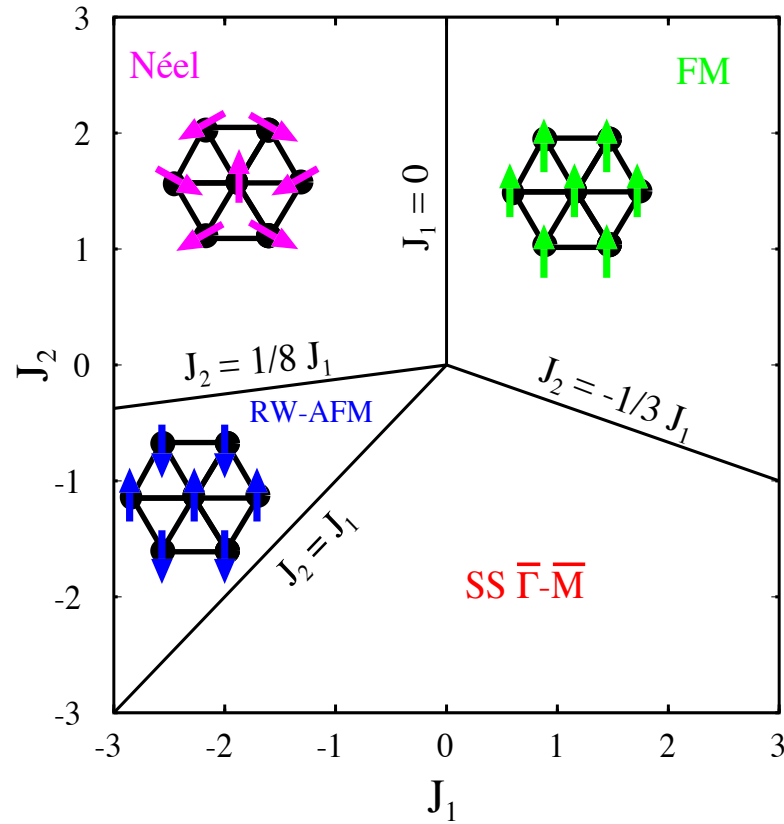
leads to

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

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



SPIN SPIRALS



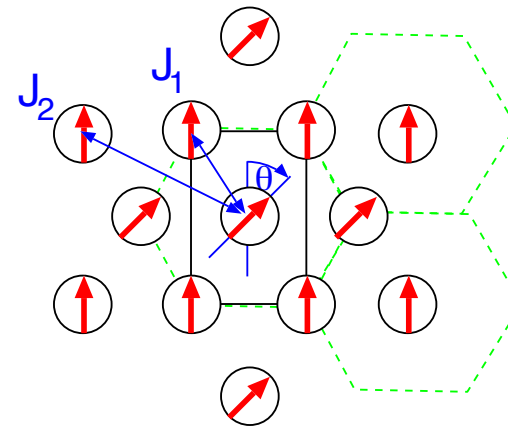
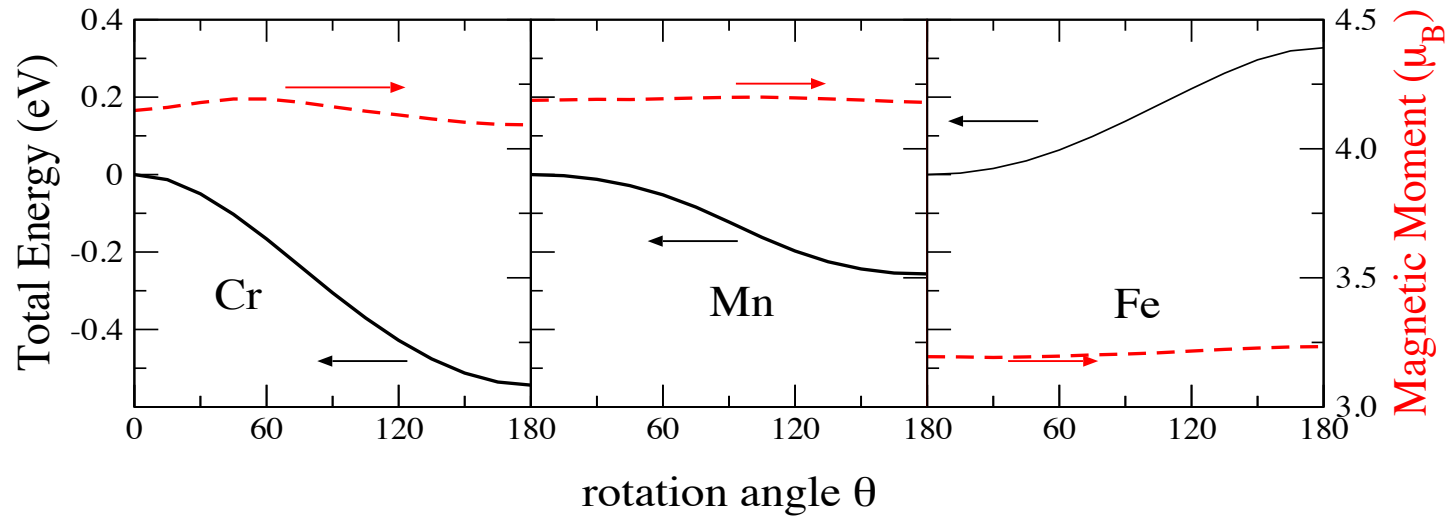
Ferromagnetic state: $\vec{q} = (0, 0)$

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:

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

- ➊ (+) no self-consistency required
- ➋ (−) perturbation has to be small

USING MODEL TO DETERMINE TC

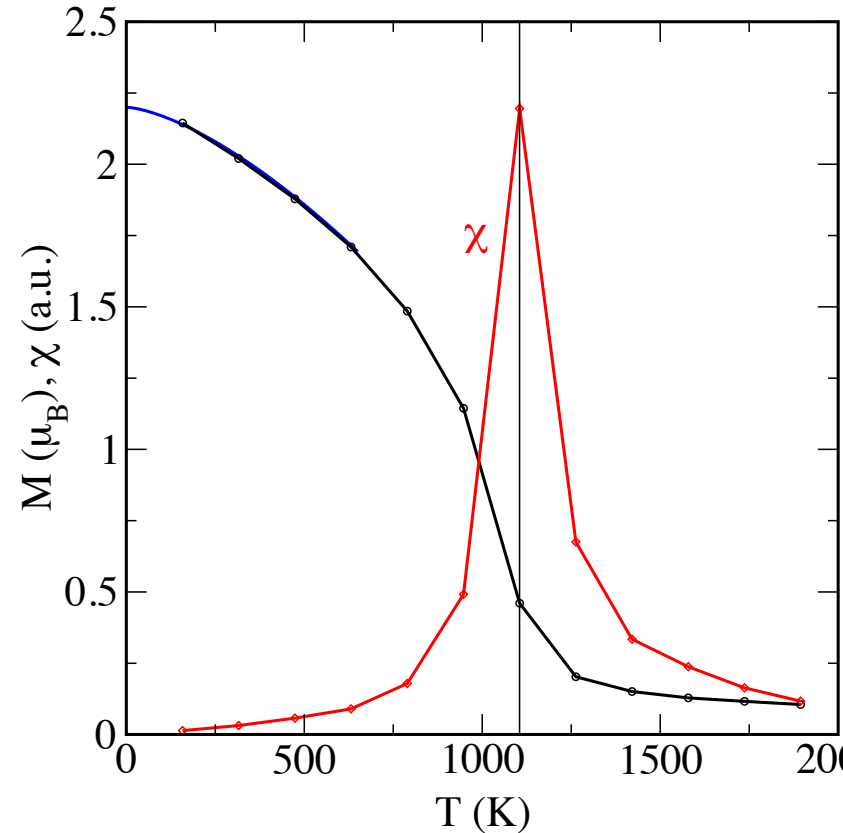
From $J_{nn'}$ one can:

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

to estimate T_C .

In all cases:

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



$$k_B T_C^{\text{MFA}} = \frac{2}{3} J_0 \quad k_B T_C^{\text{RPA}} = \frac{2}{3} \left(\sum_{\vec{q}} \frac{1}{J(\vec{q})} \right)^{-1}$$

Heisenberg model:

- magnetic exchange
- Interaction 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:

Spin-moment

Magnetic Order

Spin-Spirals

Collinear Magnetism

Orbital-moment

Exchange interaction

Non-collinear magnetism

Heisenberg model