MAGNETISM BASICS

13.04.2021 I ROBIN HILGERS

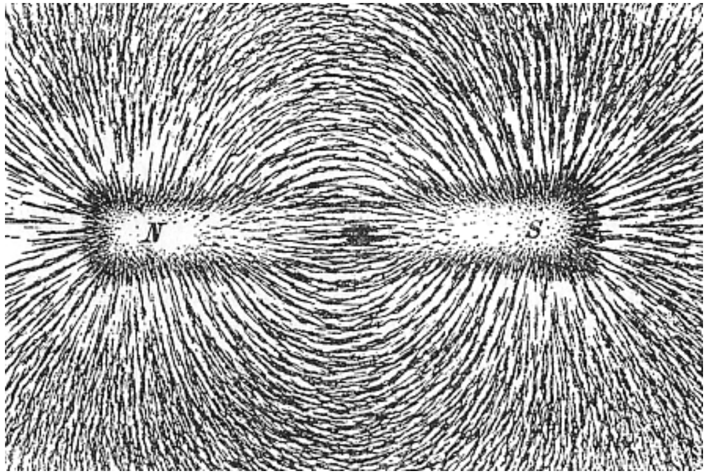
Mitglied der Helmholtz-Gemeinschaft

DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

MAGNETISM

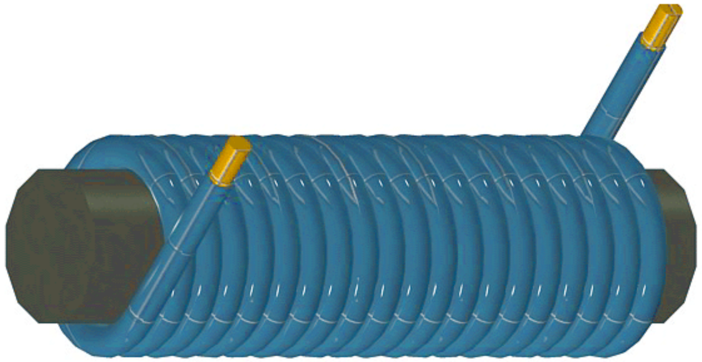
- Magnetic fields



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

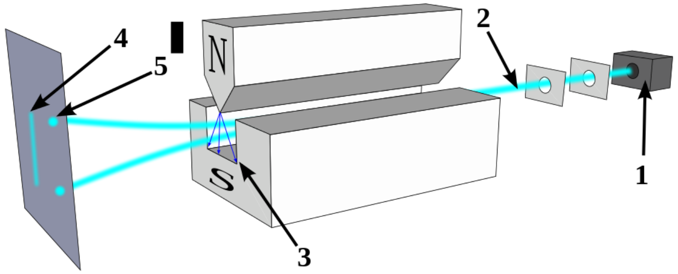
Frist source

- Electromagnetism
- Magnetic fields from electrical currents

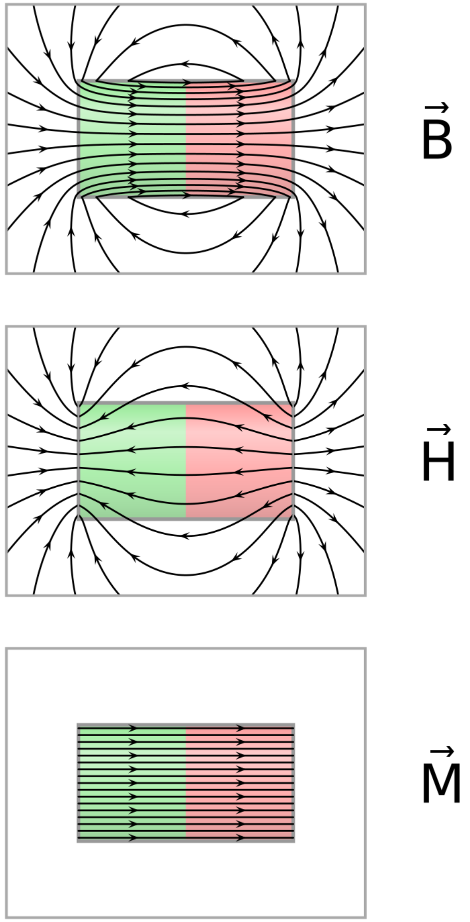


Second source:

- Intrinsic magnetic moments of elementary particles
- Spin of particles



B-FIELD AND MAGNETISATION



- 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

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

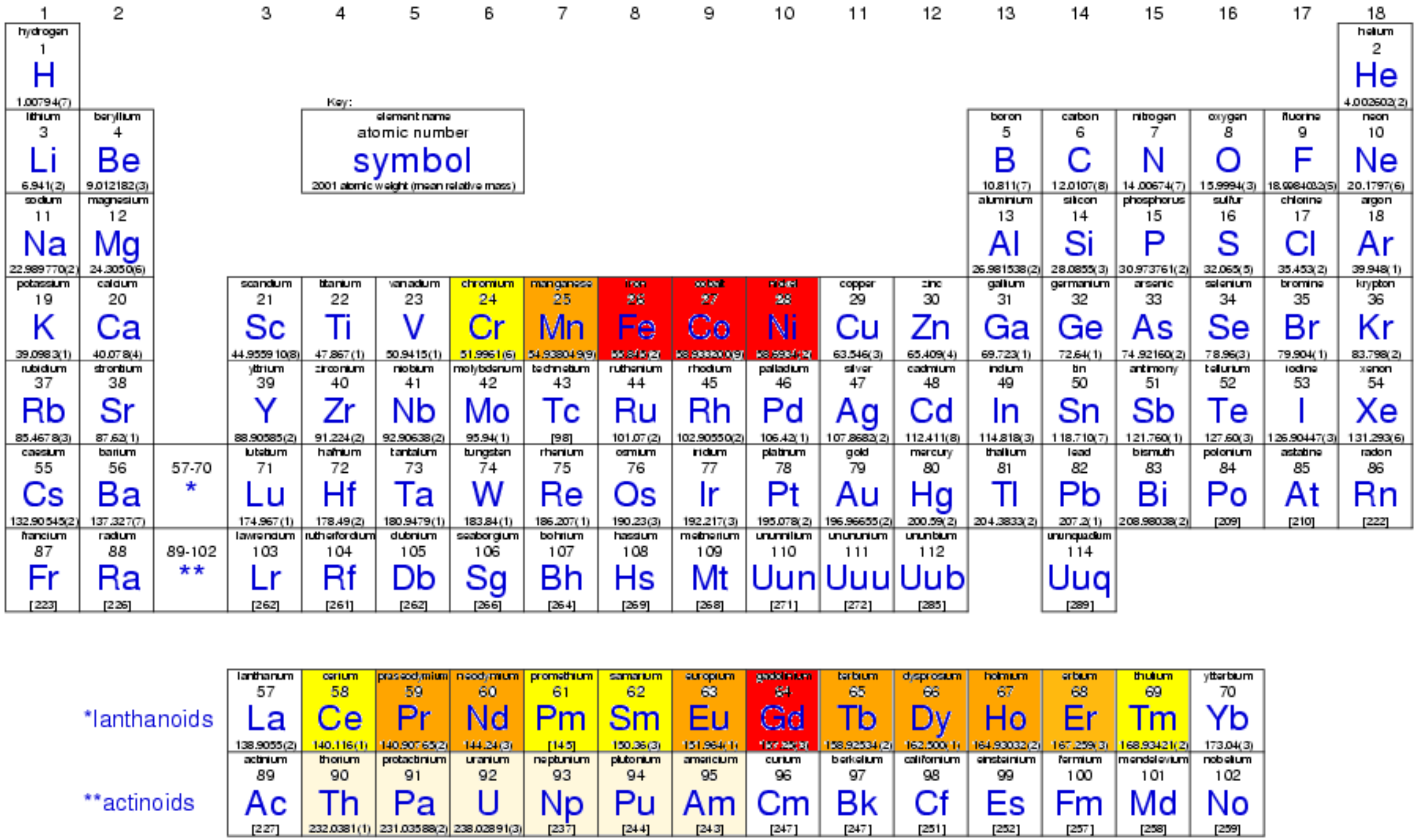
- Each electron carries a moment of approx. $-\mu_B$

- 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?

MAX DRIVING THE EXASCALE TRANSITION

http://www.webelements.com/



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ATOMIC MAGNETISM

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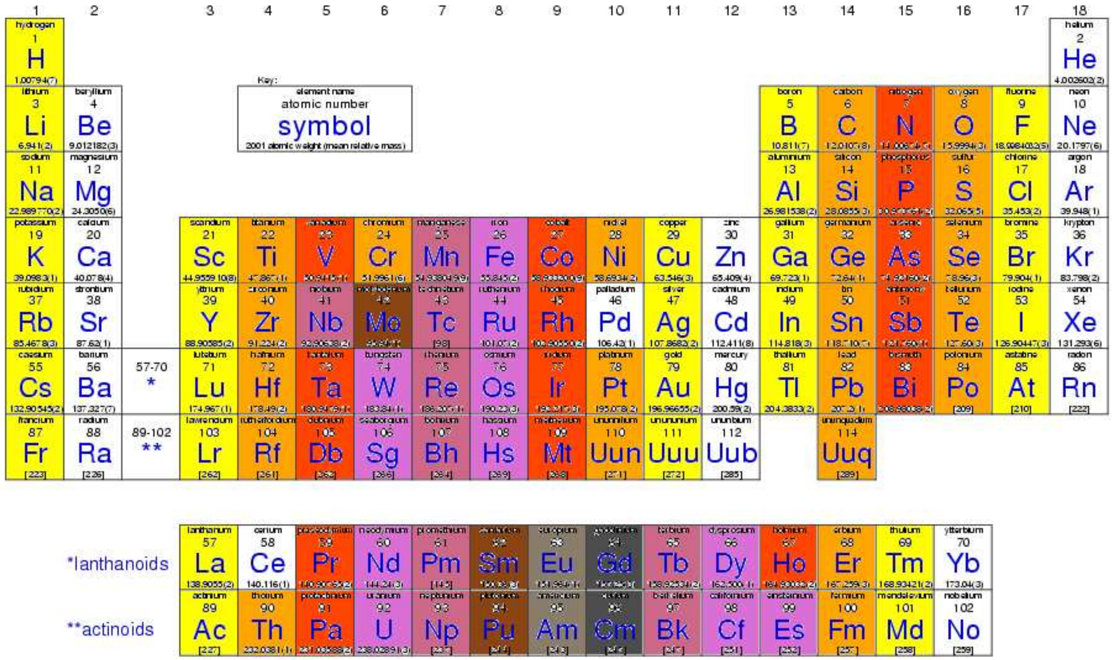
Isolated atoms:

- 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!

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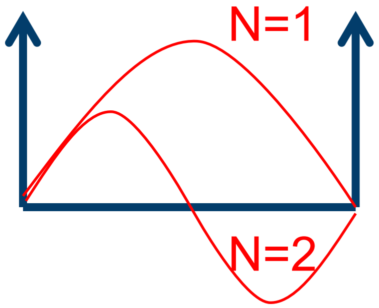
WHAT DRIVES MAGNETISM?

DRIVING THE EXASCALE TRANSITION

- 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:

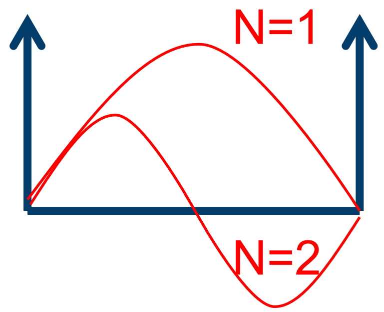
$$V_{ij} = \int \frac{\psi_i^2(r)\psi_j^2(r')}{|r - r'|}$$

- 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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  - Kinetic energy
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    different spin
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    both N=1 with opposite s

- Interaction:

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

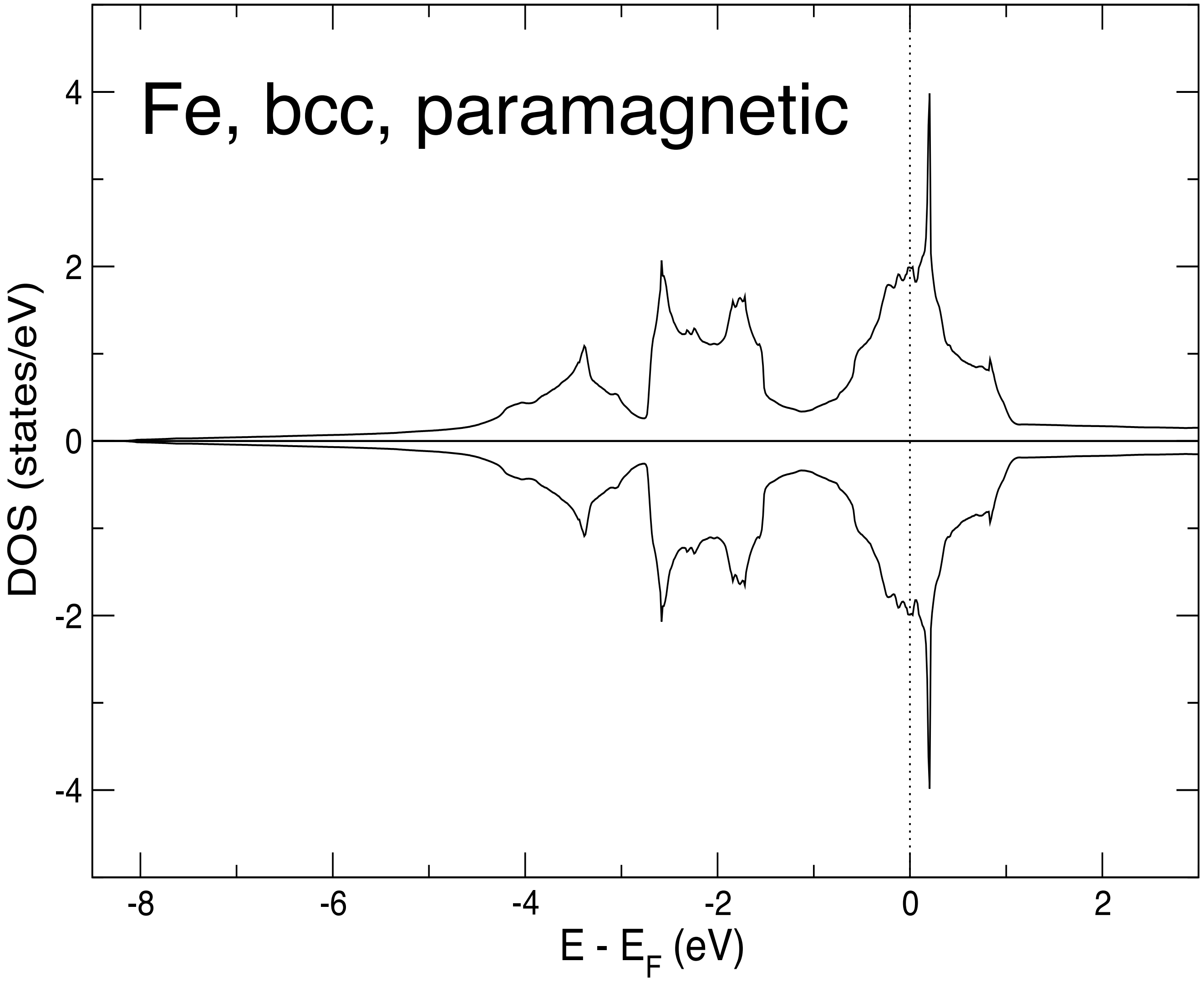
oarticles in different states

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

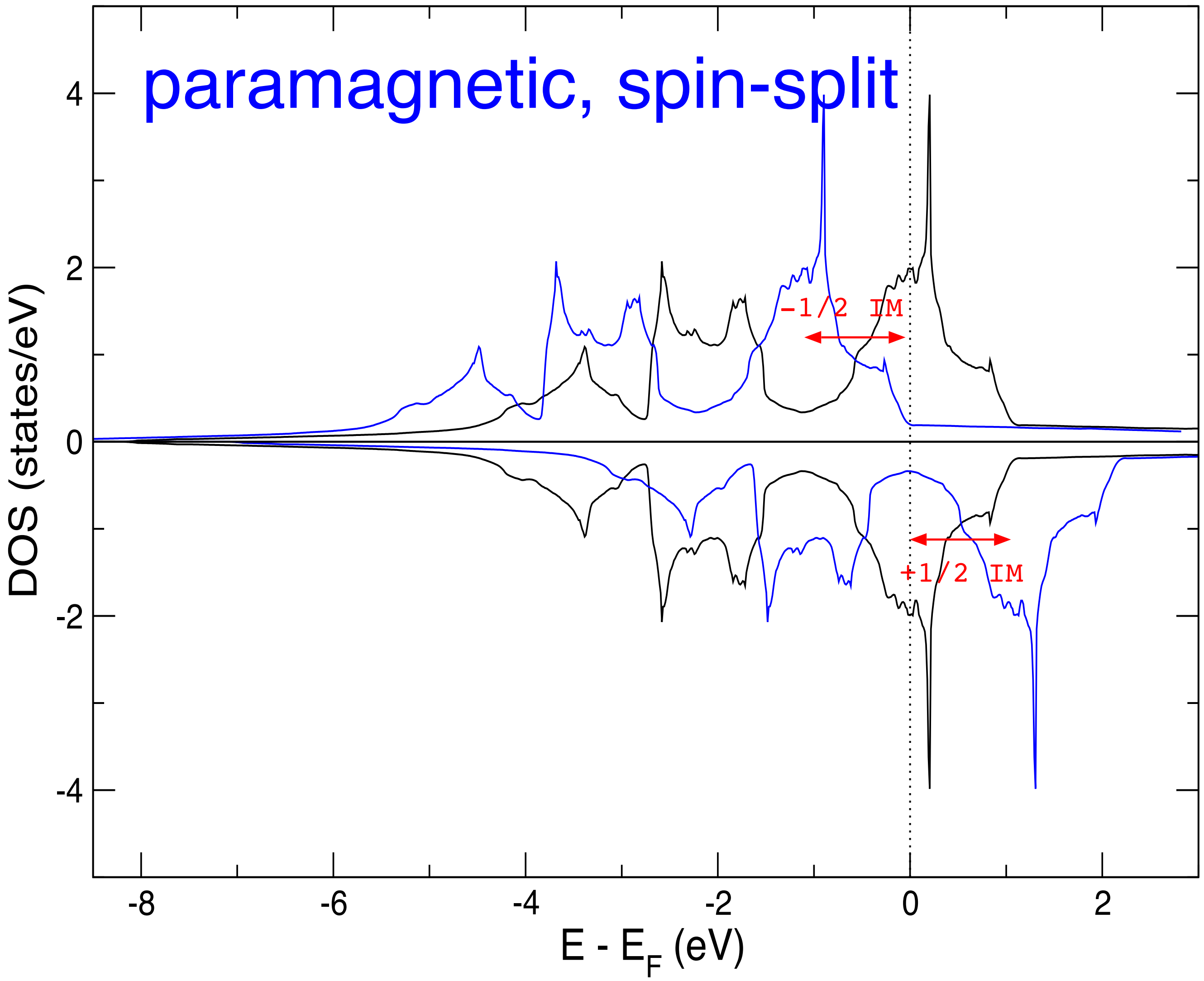
$$\vec{M} \rightarrow \vec{B}$$

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

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

ITINERANT MAGNETS

DRIVING THE EXASCALE TRANSITION



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

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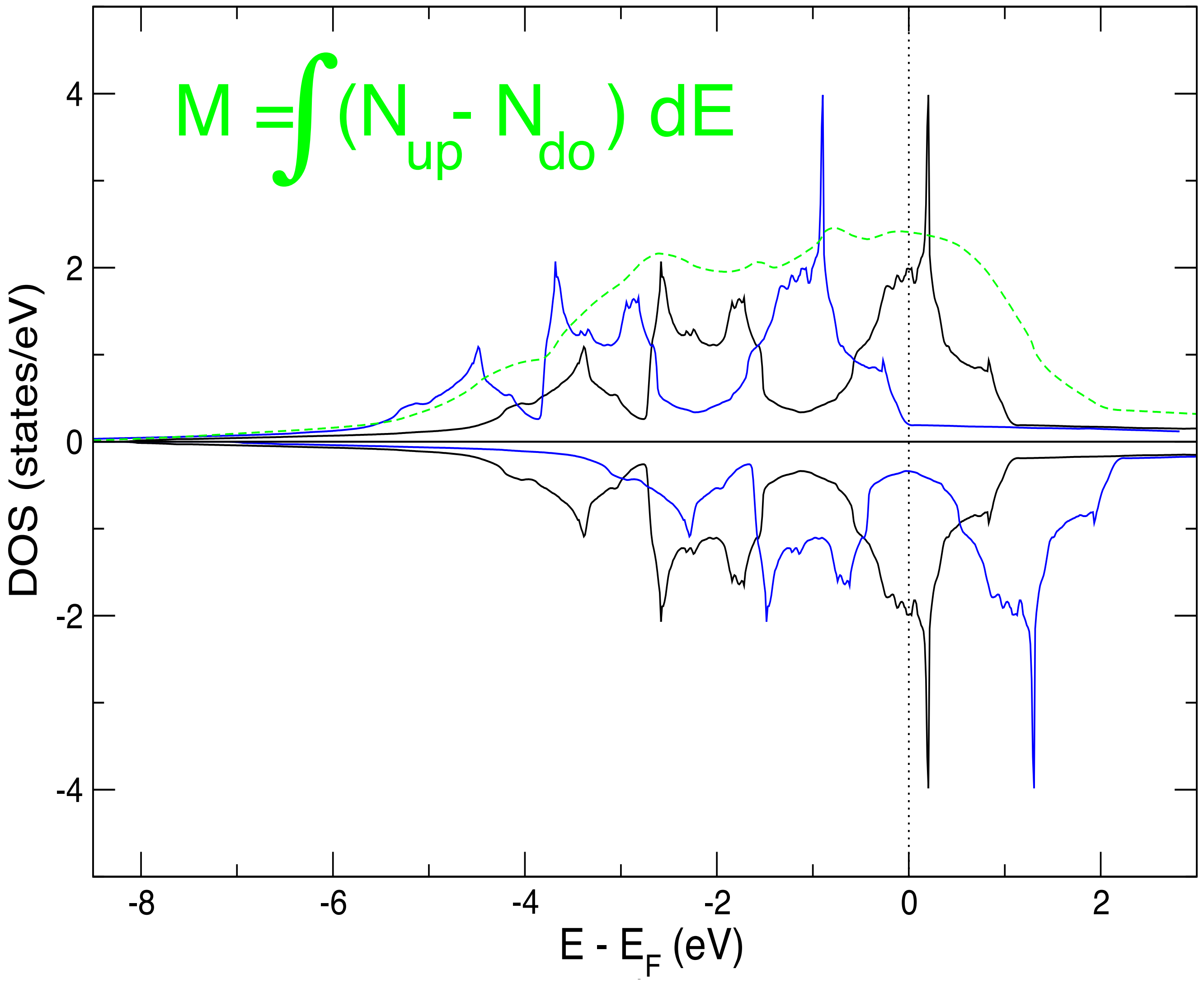
ITINERANT MAGNETS



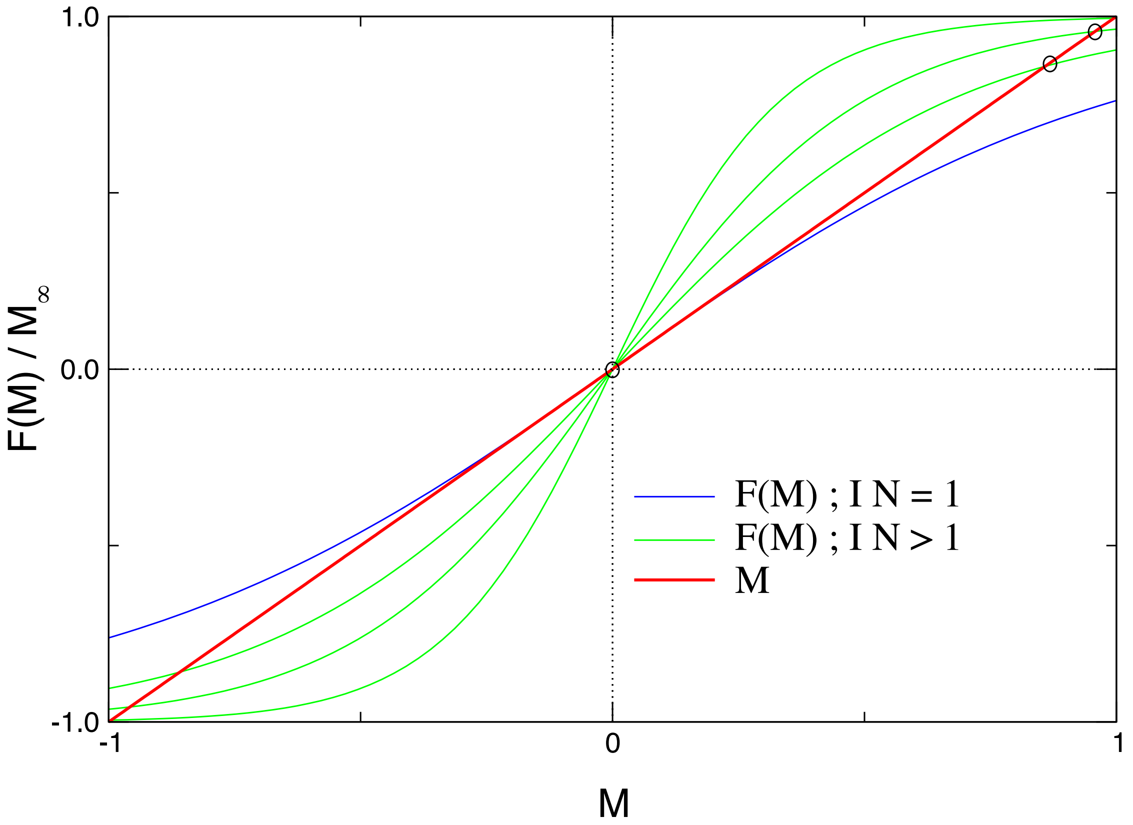
- ~~Discrete atomic levels~~
- Continuous spectrum

- 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

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



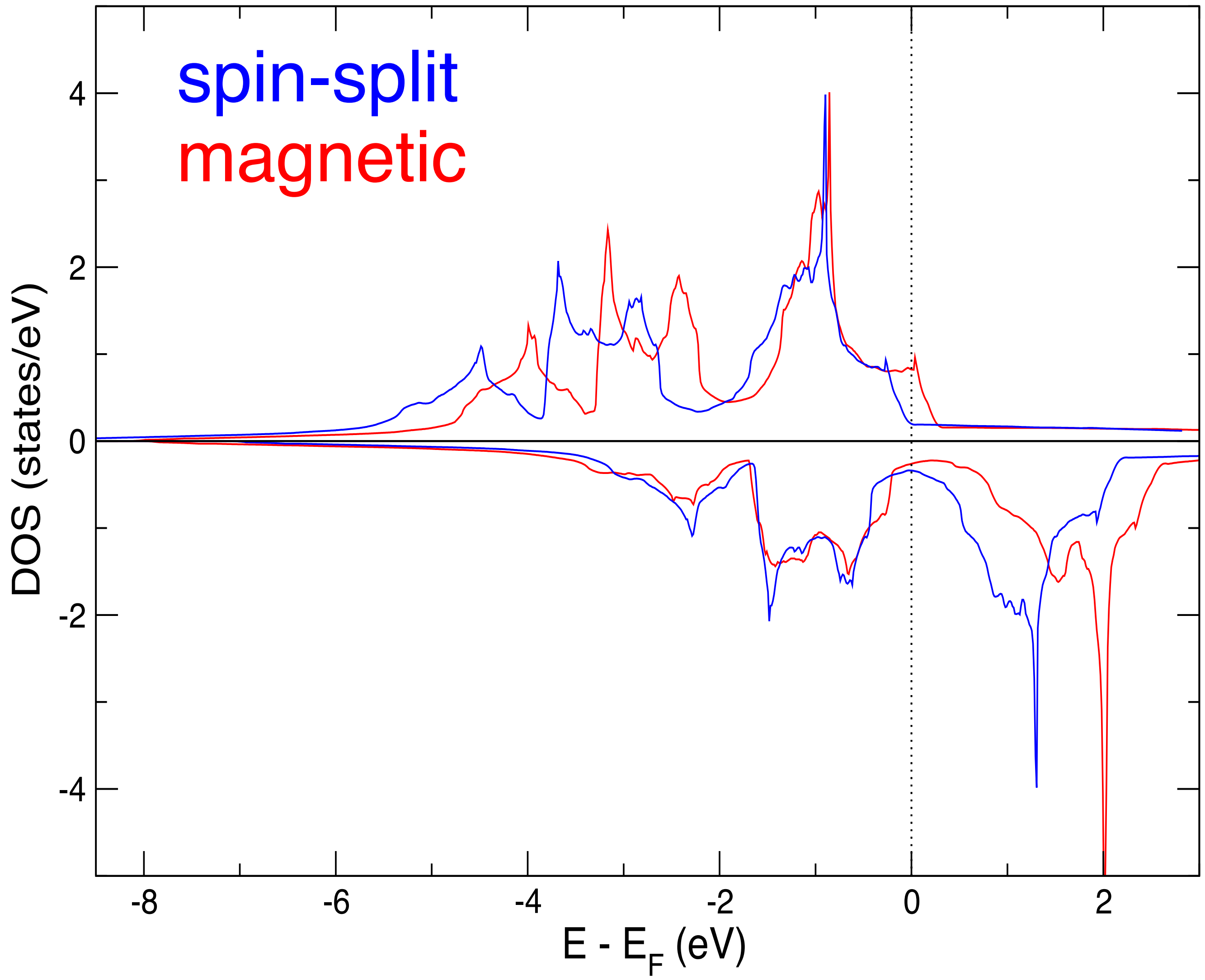
- ~~Different possible solutions~~

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

- 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

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

MAGNETISM IN DFT

- 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 $\mathbf{L} = \vec{r} \times \vec{v}$:

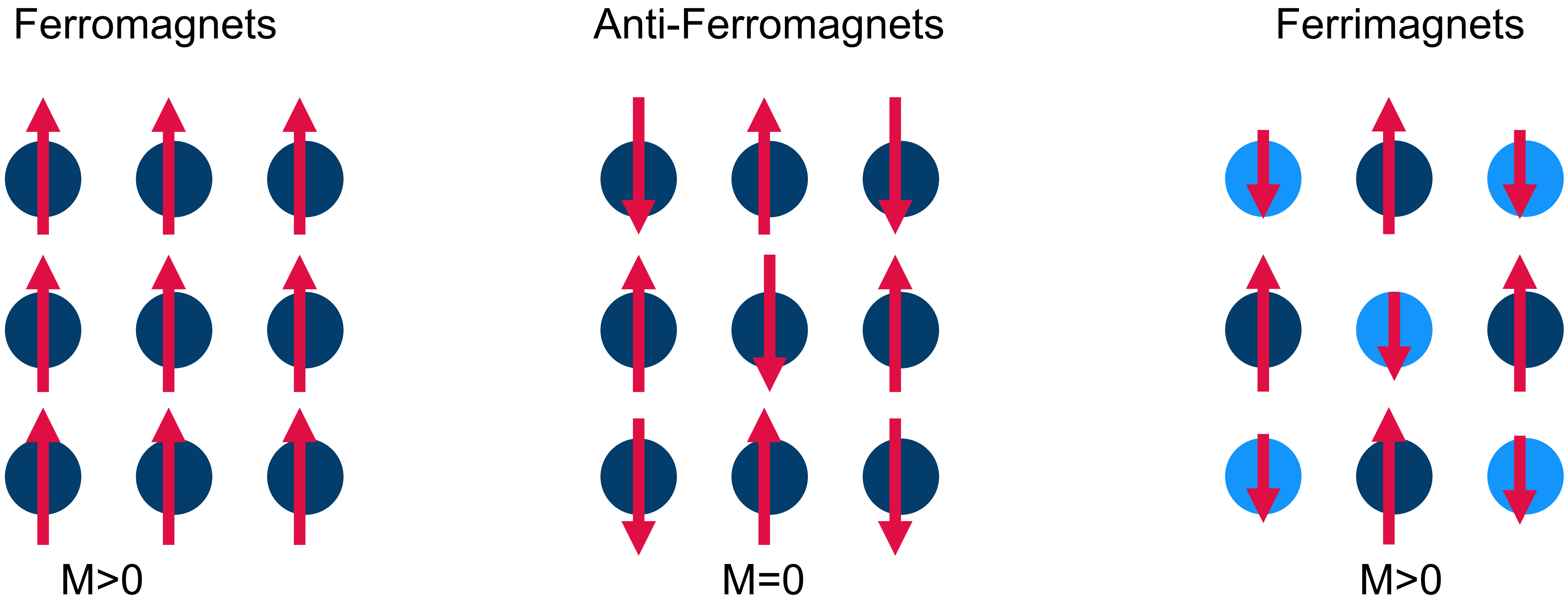
$$\vec{m}^{\mathrm{orb}}(\vec{r}) = -\mu_{\mathrm{B}} \sum_i \langle \phi_i | \vec{r} \times \vec{v} | \phi_i \rangle .$$

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



OUTLOOK

Non-collinear magnetism:

- Magnetic moments directions aside from collinear up and down
- Spin-Spirals
- Local moments