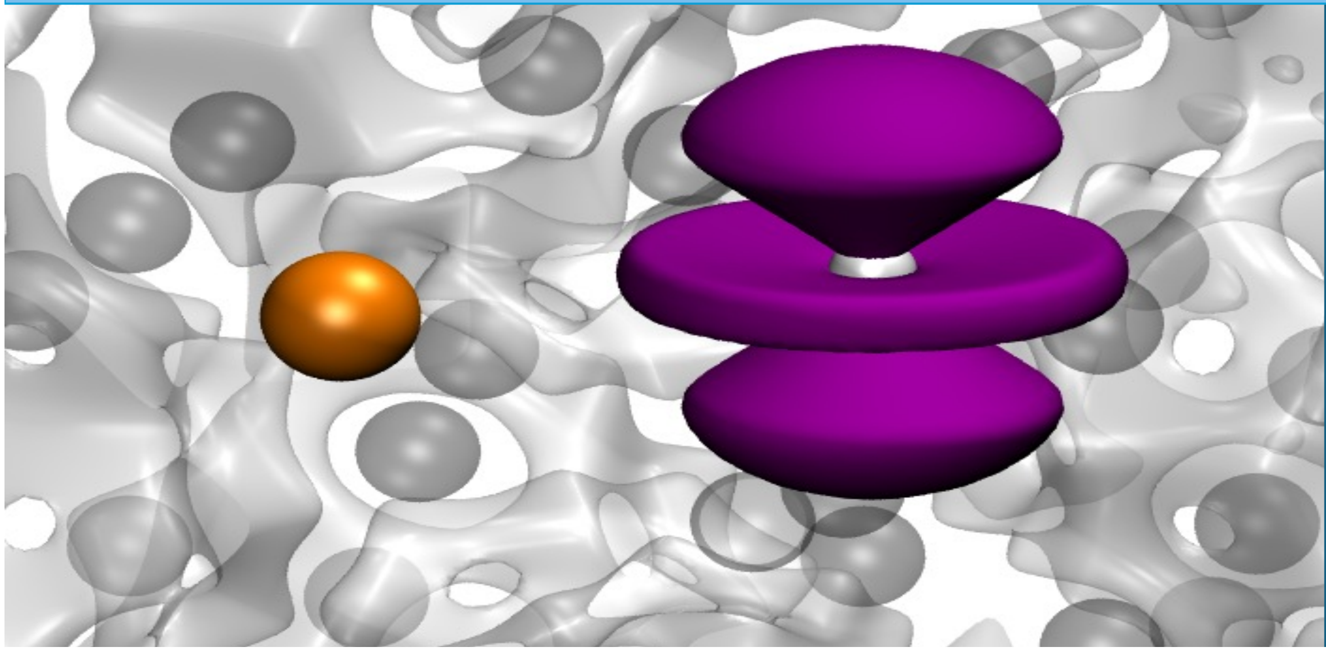
1. Atomic magnetism

2. Exchange interactions, magnetic order and structure



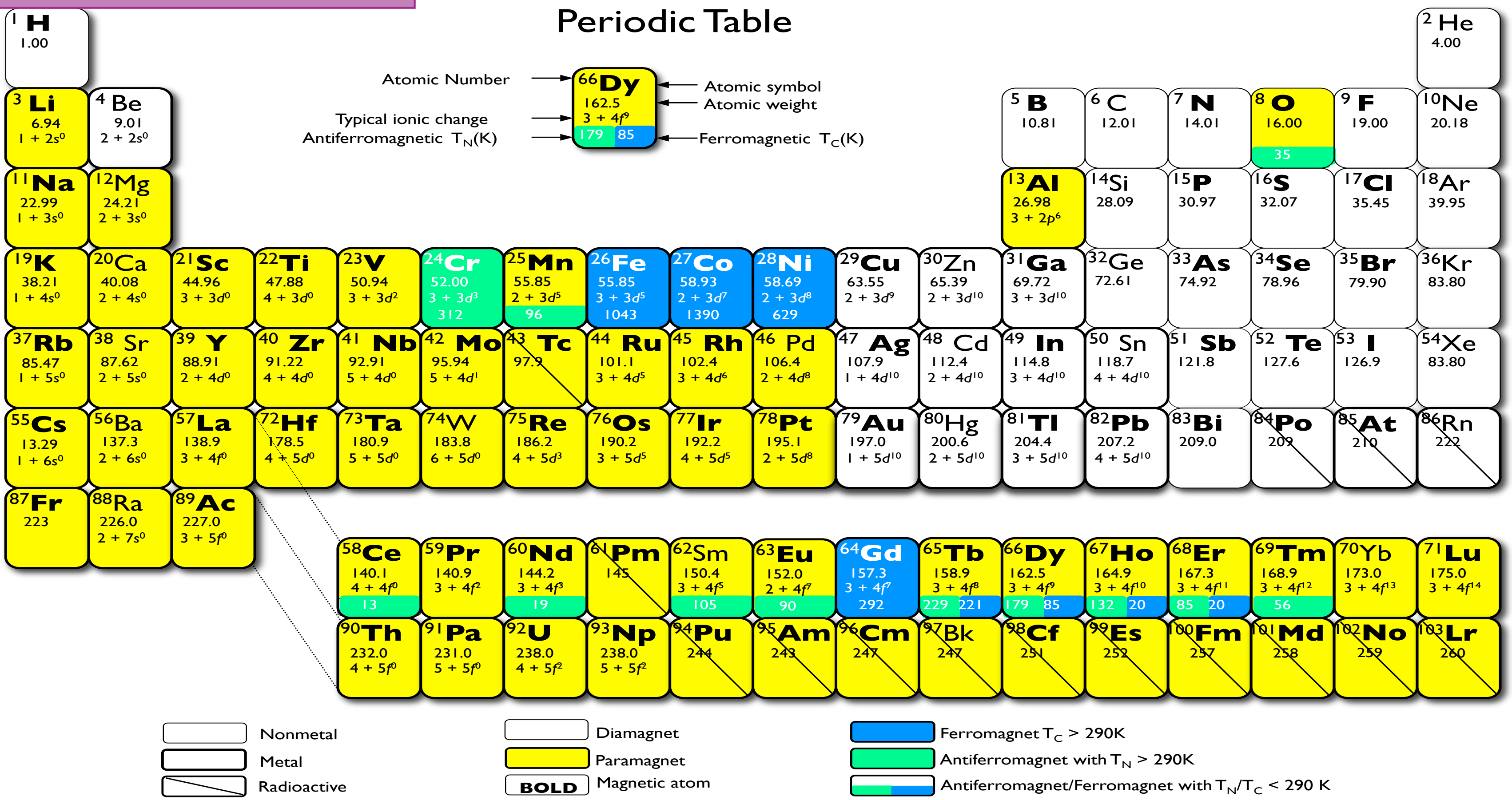
Julie Staunton

Department of Physics,

University of Warwick

European School of Magnetism 2024

J M D Coey ESM Lecture Notes 2015



Most atoms are magnetic in ground state
In condensed matter magnetic order is more elusive

Challenge for modelling materials' properties

In atoms, molecules and solids, many ($10^2 – 10^{24}$) interacting electrons and nuclei. Modelling must account for

- Kinetic energies of electrons (and nuclei)
- Electromagnetic interactions
- Indistinguishability of identical electrons, each with spin ½$\hbar$

---- > antisymmetric many electron wavefunctions

(Pauli Exclusion Principle PEP)

$$\Psi(x_1, x_2, x_3, \ldots, x_i, \ldots, x_j, \ldots) = -\,\Psi(x_1, x_2, x_3, \ldots, x_j, \ldots, x_i, \ldots)$$

Atomic Magnetism - topics

- Electron on the H-atom – revision of angular momentum in QM
- Charged particle in a magnetic field **B**
- H-atom in constant B, orbital and spin moments,
  $$\boldsymbol{\mu} = \frac{e}{2m}\,\boldsymbol{L}, \boldsymbol{\mu} = \frac{ge}{2m}\,\mathbf{S}, \text{ Total } \boldsymbol{\mu}_J = \frac{e}{2m}\,(\boldsymbol{L} + \text{g}\,\mathbf{S})$$
- Many electrons in atoms, wavefunctions in terms of antisymmetricised products of 1 – electron functions
- Hund's Rules
- Zeeman effect → paramagnetism, susceptibility χ, (diamagnetism, crystal fields)

Electron in a H-atom

- One electron and a symmetric potential, (e.g. H-atom)

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(r)\Psi(\mathbf{r},t)$$

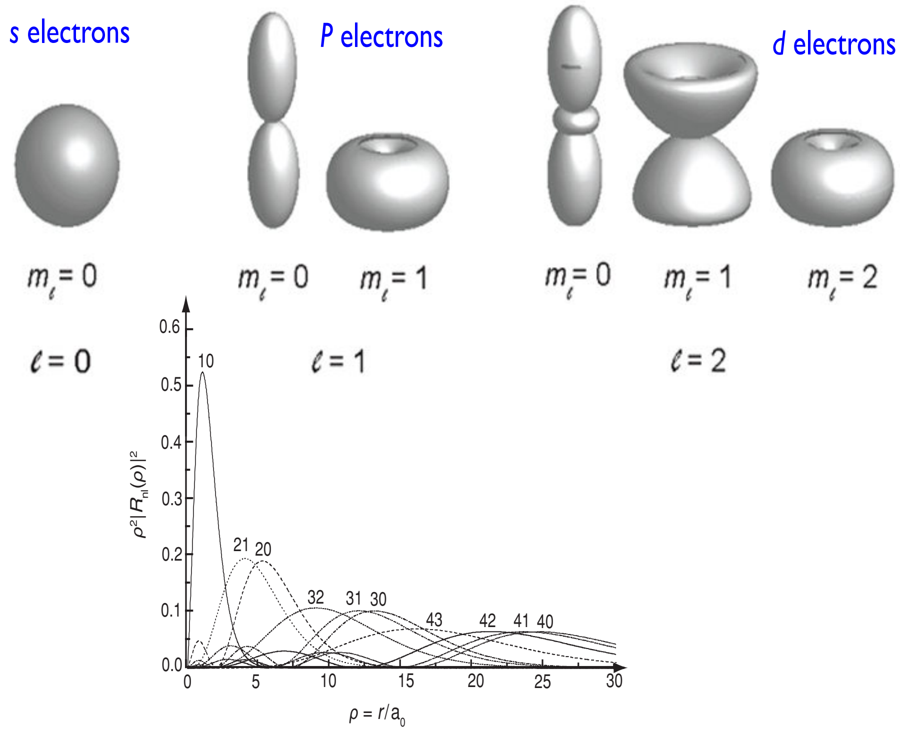
  with stationary states

$$\Psi(\mathbf{r},t) = \Phi_{n,l,m}(r,\theta,\phi)u_\sigma e^{-iE_n t/\hbar}$$

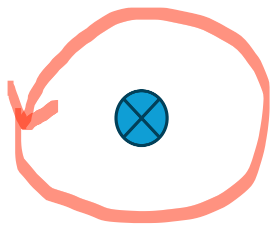
  where

$$\Phi_{n,l,m}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

  and principal, $n = 1, 2, \cdots$, angular momentum, $l = 0, 1, \cdots, n-1$ and $m = -l, -l+1, \cdots, l$ and spin, $\sigma = \uparrow, \downarrow$, quantum numbers.
- H-atom: $V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$, $E_n = -\frac{13.6}{n^2}$ eV.



Charged particle in a magnetic field



Classical picture: with magnetic $\mathbf{B} = \nabla \times \mathbf{A}$ and electric fields $\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t}$, the Hamiltonian is

$$H = \frac{1}{2m}(\mathbf{p} - \mathbf{qA})^2 + \mathbf{qV}$$

with particle's motion set by

$$\frac{d\mathbf{v}}{dt} = q(\mathbf{E} + (\mathbf{v} \times \mathbf{B})).$$

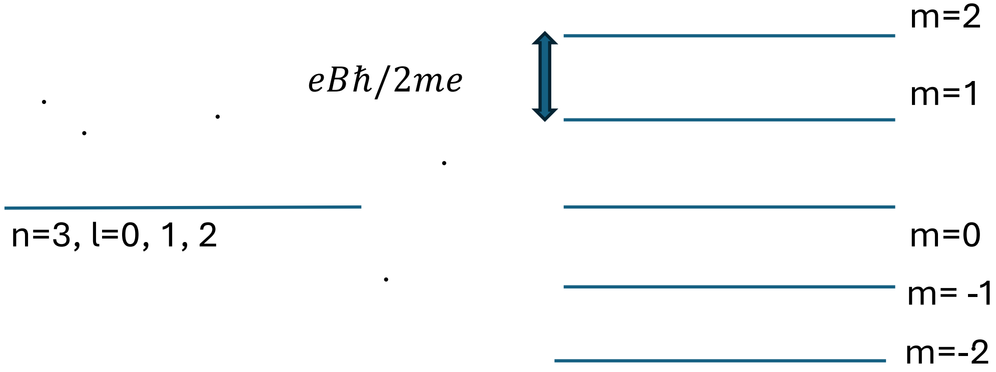
Quantum: $\hat{H}\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$ and $\mathbf{p} \to -i\hbar\nabla$.
In a constant magnetic field $\mathbf{B}$, $\mathbf{A} = -\frac{1}{2}(\mathbf{r} \times \mathbf{B})$ and the Schrodinger Eq. is

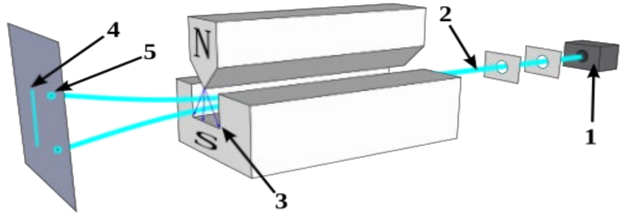
$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{q}{2m}\mathbf{B} \cdot \hat{\mathbf{L}} + \frac{q^2(\mathbf{r} \times \mathbf{B})^2}{8m} + qV\right)\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}.$$

The angular momentum $\hat{\mathbf{L}} = (\mathbf{r} \times \hat{\mathbf{p}})$ where the components follow $[\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x] = i\hbar\hat{L}_z]$ etc.
leads to an magnetic moment $\boldsymbol{\mu} = \frac{q}{2m}\hat{\mathbf{L}}$

In a weak magnetic field (Zeeman Effect) the degeneracy of the energy levels of the electron in a hydrogen atom are broken and become $E_n + m\frac{e\hbar B}{2m_e}$.

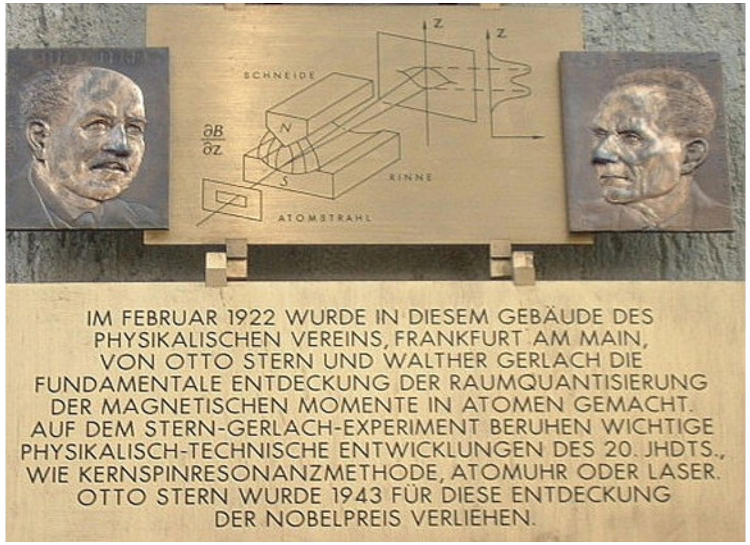
So, in a weak magnetic fields spectral lines split





but splitting is further doubled
(Stern Gerlach experiment)

→ electrons' intrinsic spin $1/2\ \hbar$
and spin magnetic moment, $\boldsymbol{\mu}_s$.



Spin, spin moments, Pauli matrices…

- An electron has spin $\frac{1}{2}\hbar$ with spin magnetic moment, $\frac{ge\hbar}{4m}\boldsymbol{\sigma} = \mu_B\boldsymbol{\sigma}$
  Interaction with magnetic field - $\mu_B\,\mathbf{B}.\boldsymbol{\sigma}$, eigenvalues $\pm\,\mu_B\,\mathrm{B}$
- Spin properties captured by 2 X 2 matrices: Pauli spin matrices,
  $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Spin angular momentum **S**= $\frac{1}{2}\hbar\,\boldsymbol{\sigma}$

Pauli-Schrodinger Eq. (omitting diamagnetic term)

$$\left(\frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{e}{2m}\mathbf{B}\cdot(\hat{\mathbf{L}} + g\hat{\mathbf{S}}) - eV(r)\right)\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}.$$

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \Psi_\uparrow(\mathbf{r},t) \\ \Psi_\downarrow(\mathbf{r},t) \end{pmatrix},$$

Relativistic QM, Dirac Eq. --- spin arises naturally and leading relativistic corrections include spin-orbit coupling $\Lambda(r)\,\boldsymbol{L}.\boldsymbol{S}$

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- Many electrons in atoms, wavefunctions in terms of antisymmetricised products of 1 – electron functions
- Hund's Rules
- Zeeman effect → paramagnetism, susceptibility χ, (diamagnetism, crystal fields)

Many electrons in atoms – spin and exchange

- Helium atom, $Z = 2$, to illustrate.
  Kinetic energy of 1st electron, its attraction to doubly charged nucleus, kinetic energy of 2nd electron, its attraction to nucleus, repulsion between the two electrons.

$$\hat{H} = \hat{H}_0 + \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$\hat{H}\Psi_\lambda = E_\lambda\Psi_\lambda,\ \Psi_\lambda(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2) = -\Psi_\lambda(\mathbf{r}_2,\sigma_2,\mathbf{r}_1,\sigma_1).$$

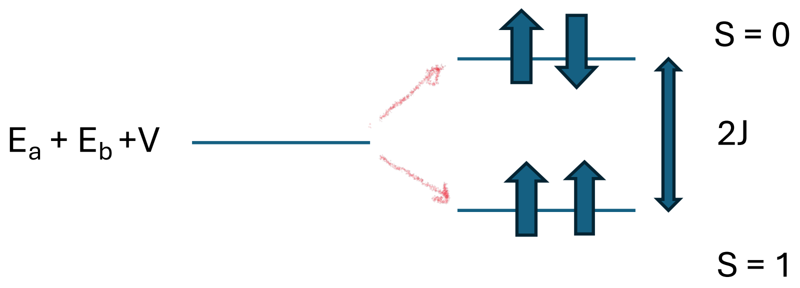
- Neglect e-e interaction and $\Psi_\lambda(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2) = \frac{1}{\sqrt{2}}(\phi_a(\mathbf{r}_1)u_{1,\sigma}\phi_b(\mathbf{r}_2)u_{2,\sigma'} - \phi_a(\mathbf{r}_2)u_{2,\sigma}\phi_b(\mathbf{r}_1)u_{1,\sigma'})$ where $a = (n, l, m)$, $b = (n', l'.m')$, $\sigma, \sigma' = \uparrow, \downarrow$ and $\phi_{a(b)}$ are one-electron hydrogenic functions for $Z = 2$.

- Show that e-e interaction breaks degeneracy to split states into two sets: a triplet with spin $S = 1, (\uparrow\uparrow)$ and a singlet with spin $S = 0, (\uparrow\downarrow)$ and energies $E_a + E_b + (V - J)$ and $E_a + E_b + (V + J)$ respectively.
- Coulomb integral

$$V = \int\int |\phi_a(\mathbf{r}_1)|^2 V_{ee}(|\mathbf{r}_1 - \mathbf{r}_2|)|\phi_b(\mathbf{r}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2$$

and Exchange integral

$$J = \int\int \phi_a^\star(\mathbf{r}_1)\phi_b(\mathbf{r}_1)V_{ee}(|\mathbf{r}_1 - \mathbf{r}_2|)\phi_b^\star(\mathbf{r}_2)\phi_a(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2$$



Many electrons in atoms

- 2 electrons in same spatial state occupy different spin states (S=0), electrons with ‘parallel’ spins (S=1) tend to avoid each other --- spin correlation. Magnetic properties of matter.

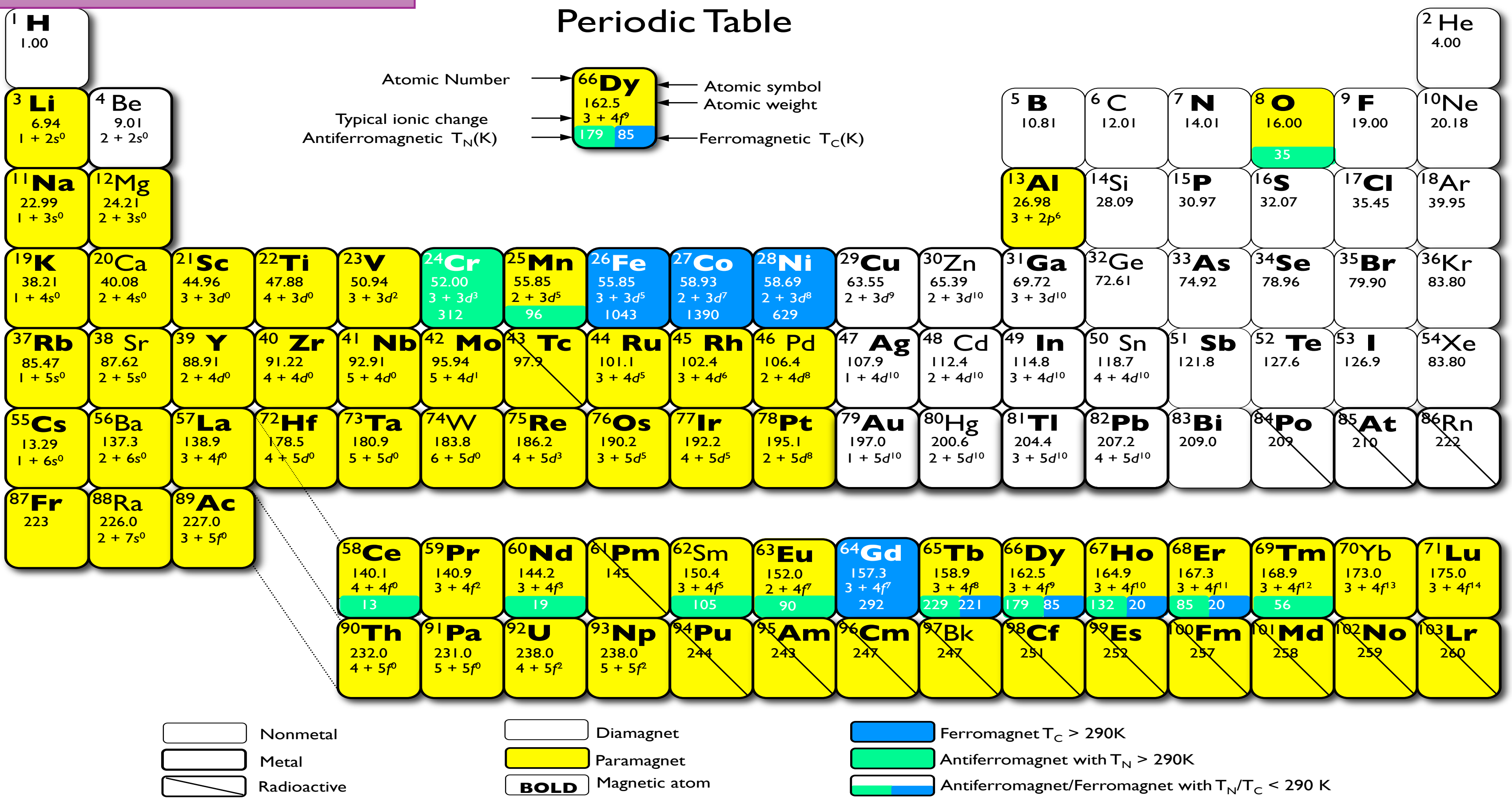
- Many electron wavefunctions as Slater determinants of 1-electron wavefunctions.

- Each electron in effective potential set up by nucleus and other electrons, l degeneracy broken.

- Products of states labelled as 1s2, 2s2, 2p6,…

- Hunds’ Rules

	n	l	m_l	m_s	No of states
1s	1	0	0	±1/2	2
2s	2	0	0	±1/2	2
2p	2	1	0,±1	±1/2	6
3s	3	0	0	±1/2	2
3p	3	1	0,±1	±1/2	6
3d	3	2	0,±1,±2	±1/2	10
4s	4	0	0	±1/2	2
4p	4	1	0,±1	±1/2	6
4d	4	2	0,±1,±2	±1/2	10
4f	4	3	0,±1,±2,±3	±1/2	14



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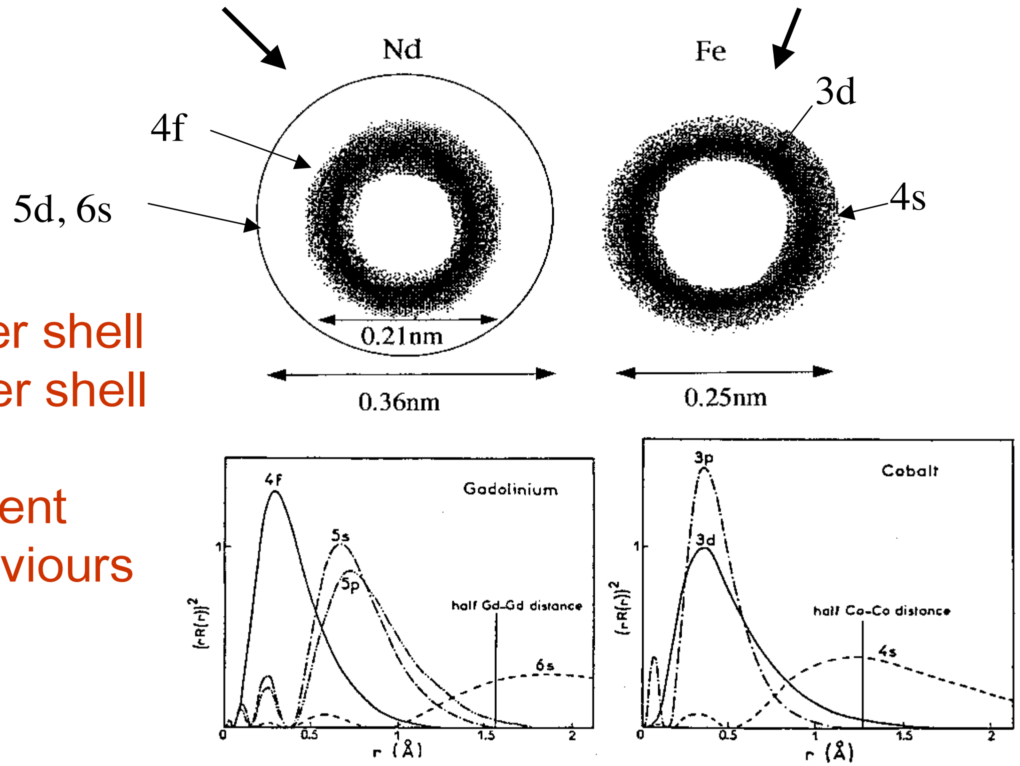
The 2 main series of magnetic elements

Rare-earth element Transition-metal element



4f electrons : inner shell
3d electrons : outer shell

leads to very different behaviours

Hunds' Rules

First add orbital **L** and spin **S** momenta of the electrons

Then couple them to give total **J = L + S**

J^2 → . $j(j+1)\hbar^2$, J_z → $m_J \hbar$, m_J = -J, -J+1, …, J

J= |L + S|, |L + S -1|, …, |L – S|

Different J-states are termed *multiplets* $^{2S+1}X_J$

X = S, P, D, F, G, … for L = 0, 1, 2, 3, 4, …

Total magnetic moment $\boldsymbol{\mu}_J = -\frac{e}{2m}(\boldsymbol{L} + g\,\mathbf{S}) = -g_J \frac{e}{2m}\mathbf{J}$

where $g_J = 3/2 + (S(S+1) - L(L+1))/2J(J+1)$

Hunds' Rules:

To determine ground state of many electron atom/ion

1. Maximise S

2. Maximise L consistent with S

3. Couple L and S to form J

- Shell < half full, J= |L – S|
- Shell > half full, J = L + S

Examples

Co^{2+} ion (Co Z = 27)

1s2, 2s2, 2p6, 3s2, 3p6, 3d7, *(4s2)*

m	-2	-1	0	1	2
	↑	↑	↑	↑	↑
	↓	↓	.	.	.

Maximising S = 3/2
Maximising L = 3
J = L + S = 9/2

$^4F_{9/2}$

Sm^{3+} ion (Sm Z = 62)

[Xe], 4f5, (6s2, 5d1)

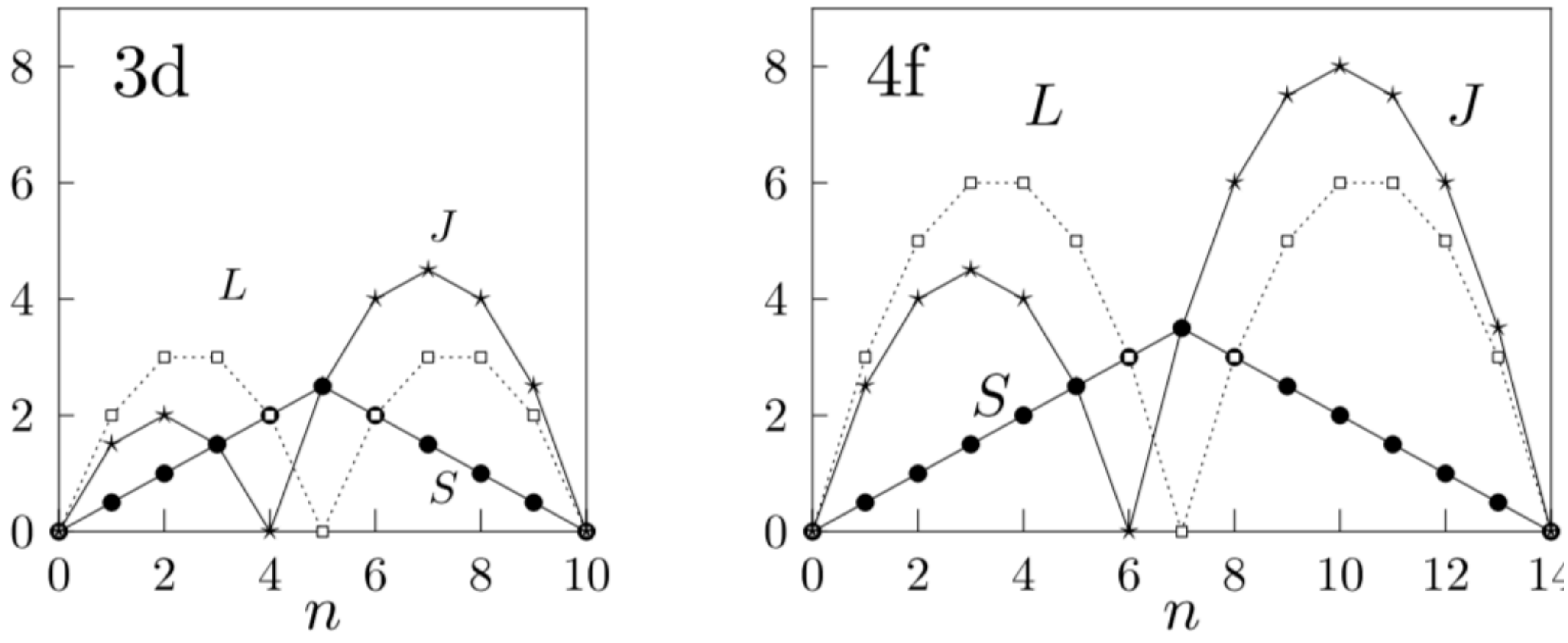
m	-3	-2	-1	0	1	2	3
	.	.	↑	↑	↑	↑	↑
	.	.	.	.	.	.	.

Maximising S = 5/2
Maximising L = 5
J = |L – S| = 5/2

$^6H_{5/2}$

Try Mn^{2+} (Mn Z=25) and Ho^{3+} (Ho Z=67) ions

Mn^{2+} :S=5/2, L=0, J= 5/2, $^6S_{5/2}$.
Ho^{3+} :S=2,L=6, J=8, $^5I_8$



S. J. Blundell, Magnetism in Condensed Matter (OUP, 2001)

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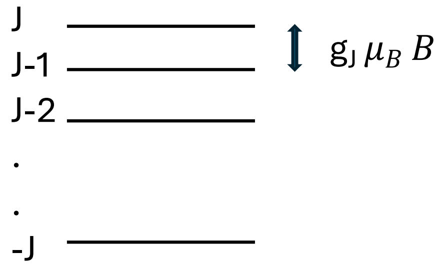
- Zeeman effect → paramagnetism, susceptibility χ, (diamagnetism, crystal fields)

Zeeman effect, χ, paramagnetism

- What is the change to magnetization M to N atoms in volume V by applying a magnetic field B?
- Energy levels are split into 2J+1
- Partition function Z, Free Energy, magnetisation M



$$Z = \sum_i e^{-E_i/k_BT} = \sum_{m_J=-J}^{m_J=J} e^{\frac{-m_J\, g_J\, \mu_B\, B}{k_BT}}.$$

$$F = -(N/V)\, k_BT\, \ln Z,$$

$$M = -\frac{\partial F}{\partial B}$$

Paramagnetism weak, positive, T-dependent

(stronger than T-independent diamagnetism).

$$\chi = \frac{M}{H} = \frac{\mu_0 M}{B} = (N/V)\frac{\mu_{eff}^2}{3k_BT}$$

$$\mu_{eff} = g_J \mu_B \sqrt(J(J+1))$$

Workings, saturation magnetization, M_s, Brillouin function $B_J(y)$…

$$Z = \sum_i e^{-E_i/k_BT} = \sum_{m_J=-J}^{m_J=J} e^{\frac{-m_J g_J \mu_B B}{k_BT}}.$$

$$F = -(N/V)\, k_BT\, \ln Z,$$

$$M = -\frac{\partial F}{\partial B}$$

$$M = M_S\, \mathcal{B}_J\left(\frac{J\, g_J \mu_B B}{k_BT}\right)$$

$$M_S = (N/V)\, g_J\, \mu_B\, J$$

$$\mathcal{B}_J\,(y) = \frac{(2J+1)}{2J}\coth\left(\frac{(2J+1)}{2J}\, y\right) - \frac{1}{2J}\coth\left(\frac{y}{2J}\right)$$

$$J \to \infty, \mathcal{B}\,(y) = \coth(y) - \frac{1}{y}.$$

$$J = \frac{1}{2}, \mathcal{B}_{1/2}\,(y) = \tanh(y)$$

$$y \to 0, \mathcal{B}_J\,(y) = \frac{(J+1)y}{3J}$$

$$\chi = \frac{M}{H} = \frac{\mu_0 M}{B} = (N/V)\frac{\mu_{eff}^2}{3k_BT}$$

$$\mu_{eff} = g_J \mu_B \sqrt{(}J(J+1))$$

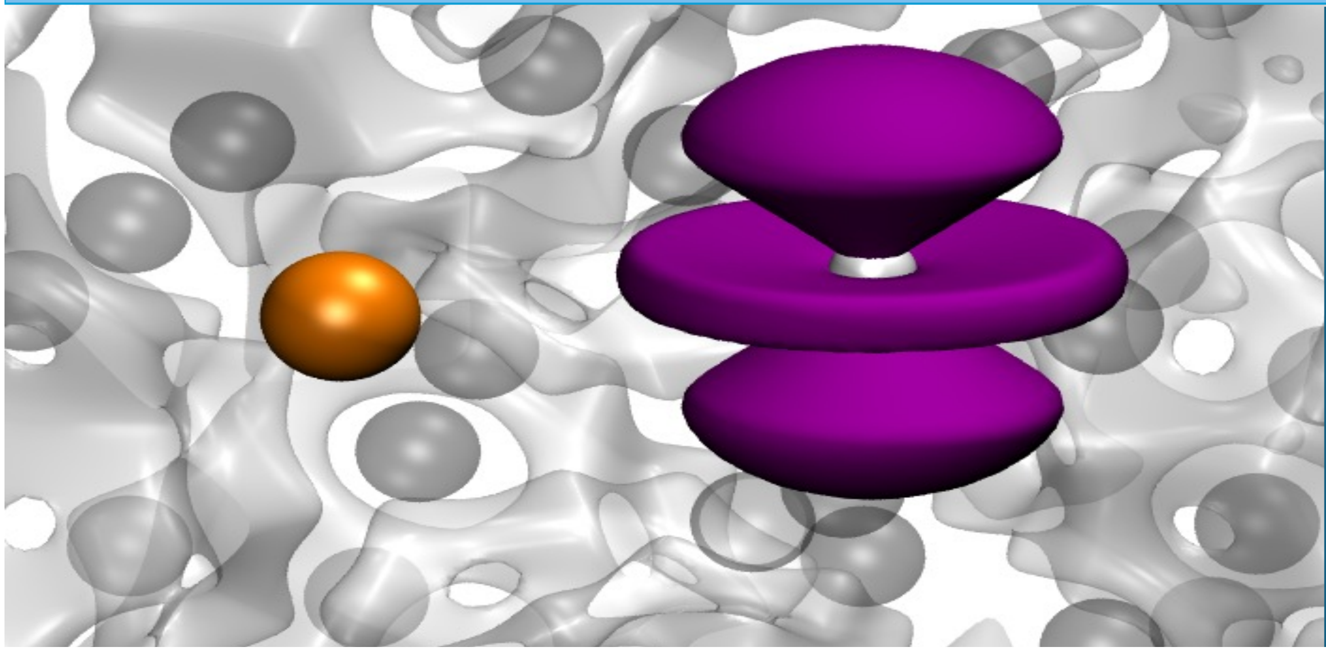
Supporting material

- S. J Blundell, “*Magnetism in Condensed Matter*”, O. U. P. (2001).
- N. W. Ashcroft and N. D. Mermin, “*Solid State Physics*”, Cengage, (2021).
- J. M. D. Coey, ”*Magnetism and Magnetic Materials*”, C. U. P. (2010).
- J. Kübler, “*Theory of Itinerant Electron Magnetism*”, O. U. P. , (2021)

Lecture notes from past ESMs by e.g.
S. Blundell, J. M. D. Coey, D. Givord, I. Mertig, W. Wulfhekel,…..

1. Atomic magnetism

2. Exchange interactions, magnetic order and structure



Julie Staunton
Department of Physics,
University of Warwick

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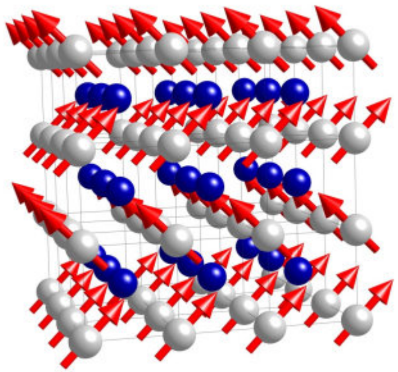
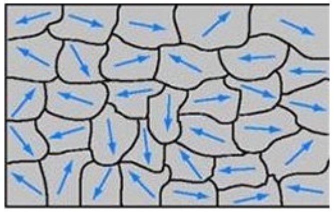
Exchange interactions, magnetic order and structure - topics

- Dipolar interactions between moments, $\boldsymbol{\mu}_i$'s

- Exchange interactions
  - Direct exchange
  - Superexchange
  - Indirect exchange
- Itinerant electrons --- $\boldsymbol{\mu}_i$'s ?

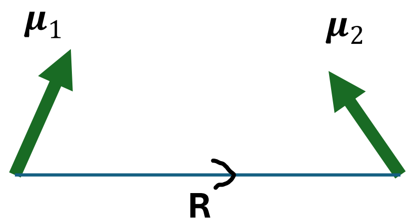


- "Spin" models for magnetism over longer length scales - mean field approximation
- Magnetic order, T_c, T_N. Magnetic phases



Dipolar Interactions

$E_{dd} \sim (\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - 3(\boldsymbol{\mu}_1 . \boldsymbol{R})(\boldsymbol{\mu}_2 . \boldsymbol{R}))/R^3$



$E_{dd} \sim 10^{-5}$ eV

Dipoles order at v. low T but magnetic ordering temperatures can be much higher e.g
Tc of Fe ~ 1000K, Gd ~ 290K, $Nd_2Fe_{14}B$ ~ 700K
T_N of antiferromagnetic MnO ~ 120K.

Need another physical mechanism

Spin and Exchange effects from many electrons spread over several atoms are principal causes of magnetic order in condensed matter

Challenge for modelling materials' properties

- Kinetic energies of electrons (and nuclei)
- Electromagnetic interactions
- Indistinguishability of identical electrons, each with spin ½$\hbar$

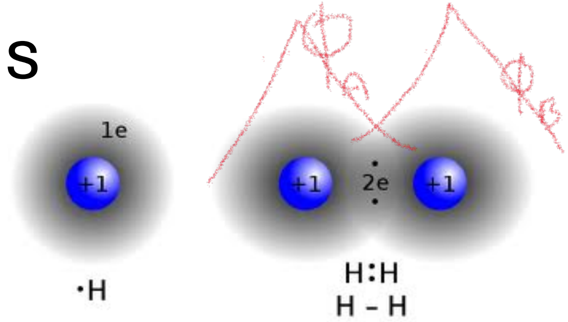
  ---- > antisymmetric many electron wavefunctions (PEP)

$$\Psi(x_1, x_2, x_3, \dots, x_i, \dots, x_j, \dots) = -\Psi(x_1, x_2, x_3, \dots, x_j, \dots, x_i, \dots)$$

- Many electron states in terms of products of 1-electron states in effective potentials (HF, DFT, etc.)
- Exchange and spin effects

Exchange interactions

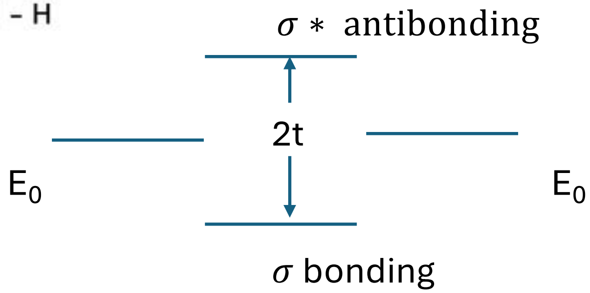
Hydrogen molecule illustration



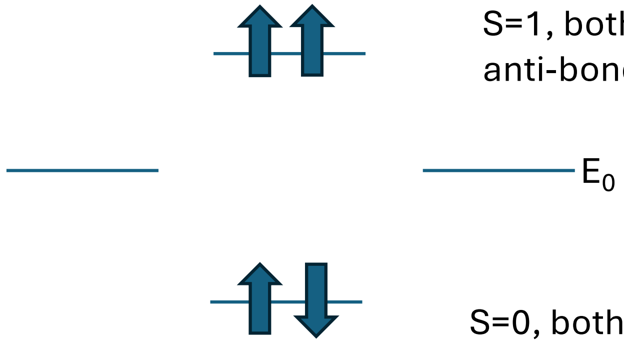
H_2^+ ion first, **single electron**

$$\hat{H} = \frac{\hat{p}^2}{2m} + V_A + V_B, \quad \hat{H}_A = \frac{\hat{p}^2}{2m} + V_A, \quad \hat{H}_A \phi_A(\mathbf{r}) = E_0 \phi_A(\mathbf{r}).$$

$$\Psi(\mathbf{r}) = c_A \phi_A(\mathbf{r}) + c_B \phi_B(\mathbf{r}), t = \int \phi_B^*(\mathbf{r}) \hat{H} \phi_A(\mathbf{r}) d\mathbf{r}, \quad S = \int \phi_B^*(\mathbf{r}) \phi_A(\mathbf{r}) d\mathbf{r}$$

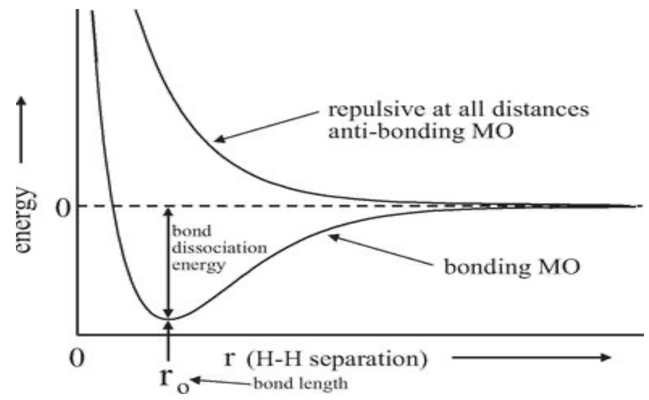


2 electrons in the H_2 molecule



S=1, both electrons in antisymmetric anti-bonding state

S=0, both electrons in symmetric bonding state



Direct exchange

General aspect of 2 electrons –
spins combine to form either an S =0 singlet state (↑↓)
or an S=1 triplet state (↑↑).
Difference in energy - exchange 2J,

$$J = \int \int \phi_a^*(\mathbf{r}_1)\, \phi_b(\mathbf{r}_1)\, V_{ee}(|\mathbf{r}_1 - \mathbf{r}_2|)\, \phi_b^*(\mathbf{r}_2)\, \phi_a(\mathbf{r}_2)\, d\mathbf{r}_1 d\mathbf{r}_2$$

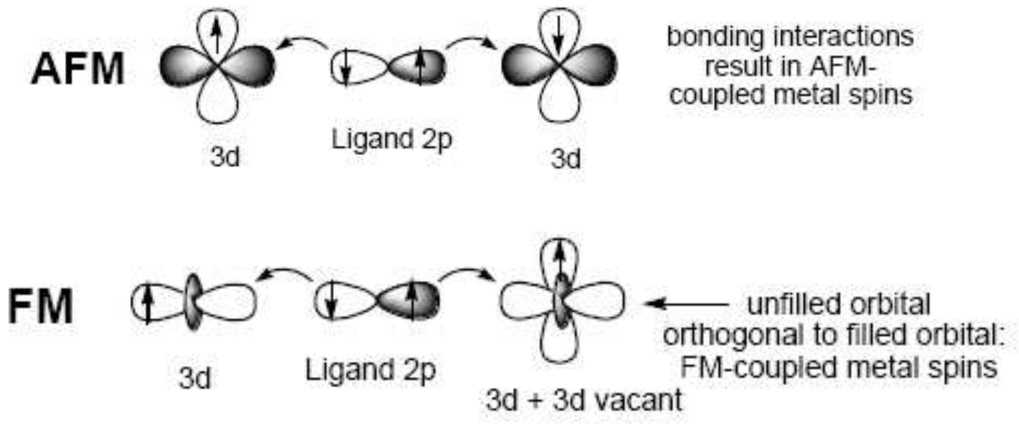
Motivates Heisenberg model

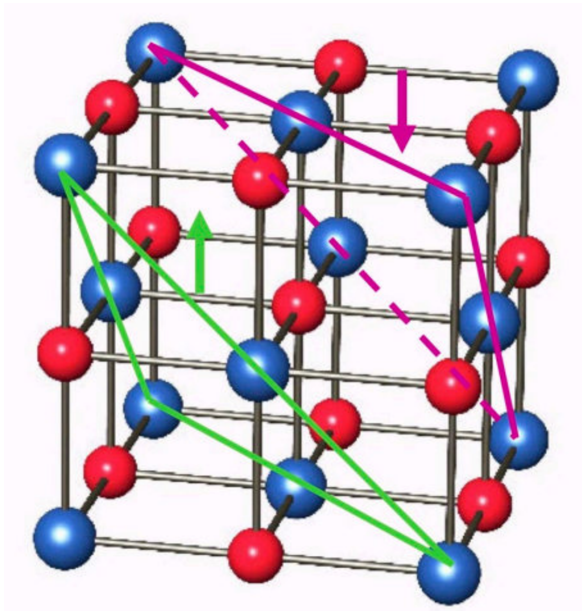
$$H = - \sum J_{ij}\ \mathbf{S}_i \cdot \mathbf{S}_j$$

between pairs of spins

Important when metal atoms like Fe, Mn, Co, Ni are close together

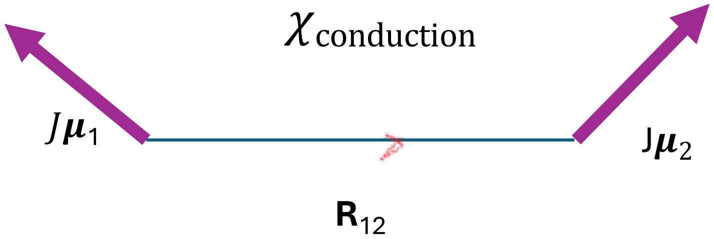
Superexchange



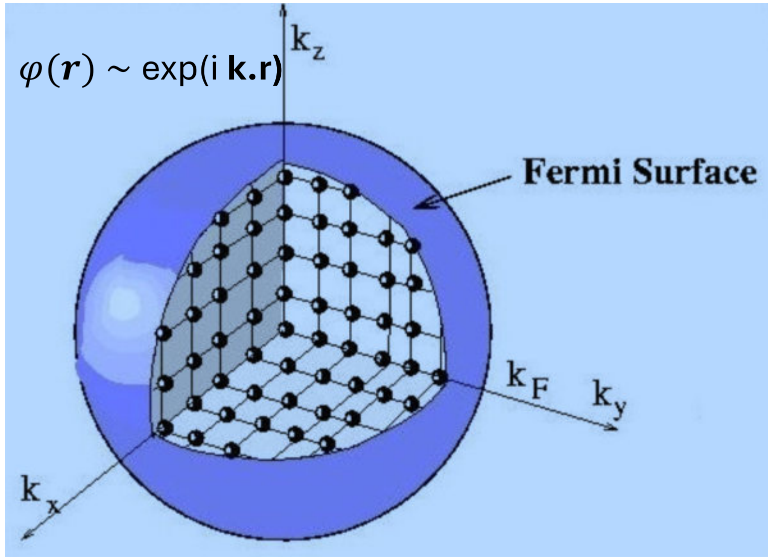


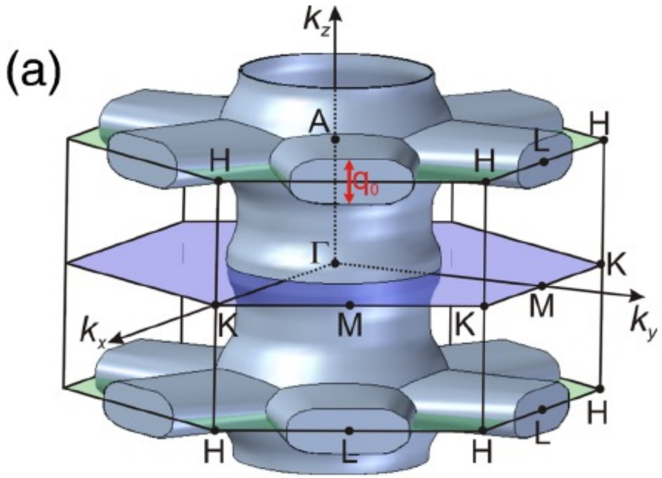
Most often antiferromagnetic, prevalent in transition metal oxides MnO etc.

Indirect exchange

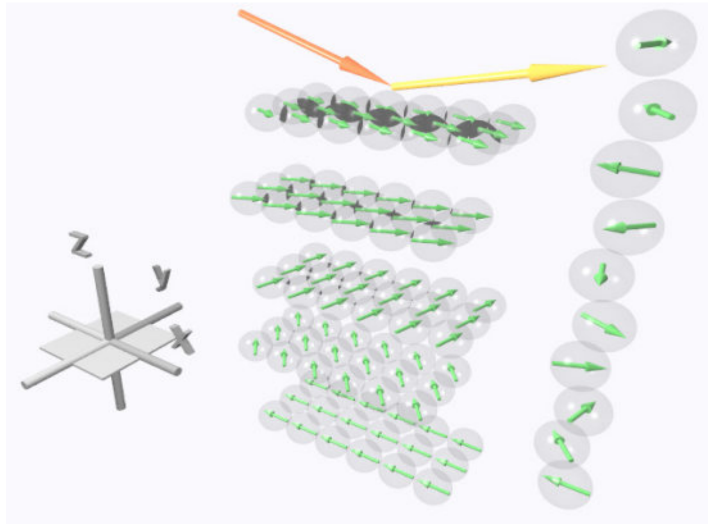


$$J_{RKKY} \sim J^2 \boldsymbol{\mu}_1 . \boldsymbol{\mu}_2 \, \chi_{cond} \, (R_{12}) \propto \frac{\cos(2\, kF\, R_{12})}{R_{12}{}^3}$$





Interaction between 2 partially-filled f-shells in lanthanides via their effect on the conduction electrons, [Xe] $4f^n$ 6s2 5d1



Exchange interactions, magnetic order and structure - topics

- Dipolar interactions between moments, $\boldsymbol{\mu}_i$'s

- Exchange interactions
  - Direct exchange
  - Superexchange
  - Indirect exchange
- Itinerant electrons --- $\boldsymbol{\mu}_i$'s ?

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Itinerant and localised electrons

Rare earths in solids are described in terms of both localised atomic orbitals (partially filled f-shells) and delocalised Bloch waves of the conduction electrons

Localisation

Degree of electron localisation causes magnetism in solids or not.

- Simple metals and semi-conductors – non-magnetic
- Rare earth atoms have atomically localised magnetic moments
- Transition metals have partially filled d-shells, weakly localised electrons subject to itinerant exchange interactions.

Stoner model paradigm (rigorously with DFT)

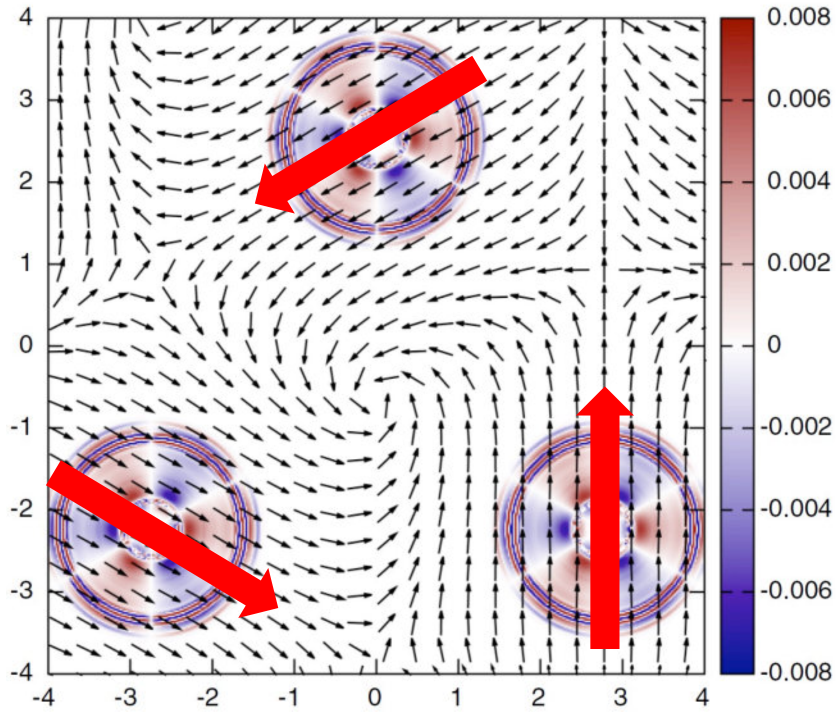
Itinerant electrons and the Stoner model

$$\left(\frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{ge}{2m}\mathbf{B}^{eff.}(\mathbf{r}) \cdot \hat{\mathbf{S}} + V^{eff.}(\mathbf{r})\right)\Phi_n(\mathbf{r}) = E_n\Phi_n(\mathbf{r}),$$

$$n(\mathbf{r}) = \sum_n^{E_F} \Phi_n^*(\mathbf{r})\Phi_n(\mathbf{r}), \mathbf{M}(\mathbf{r}) = \sum_n^{E_F} \Phi_n^*(\mathbf{r})\hat{\mathbf{S}}\Phi_n(\mathbf{r})$$

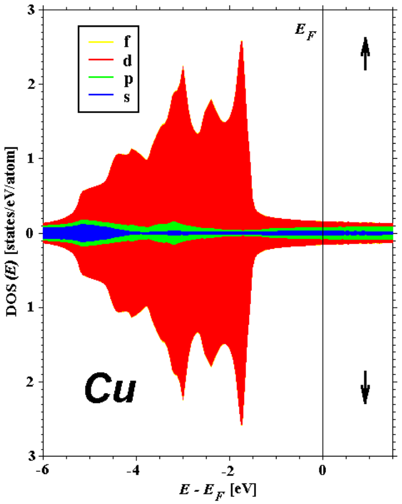
$V_{eff.}$ and $B_{eff.}$ depend on charge and spin densities n(r) and M(r). A ferromagnetic metal sustains a finite spin density M and the electronic band structure is spin-polarised.

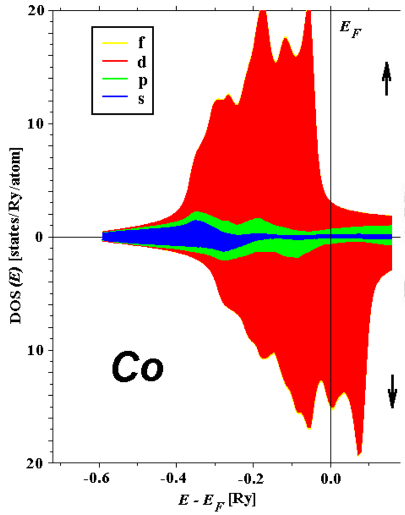
Local magnetic moments are identified in regions around the atoms. These are the 'spins' for describing magnetic order in itinerant electron magnets with orientations {$\mathbf{e}_i$}

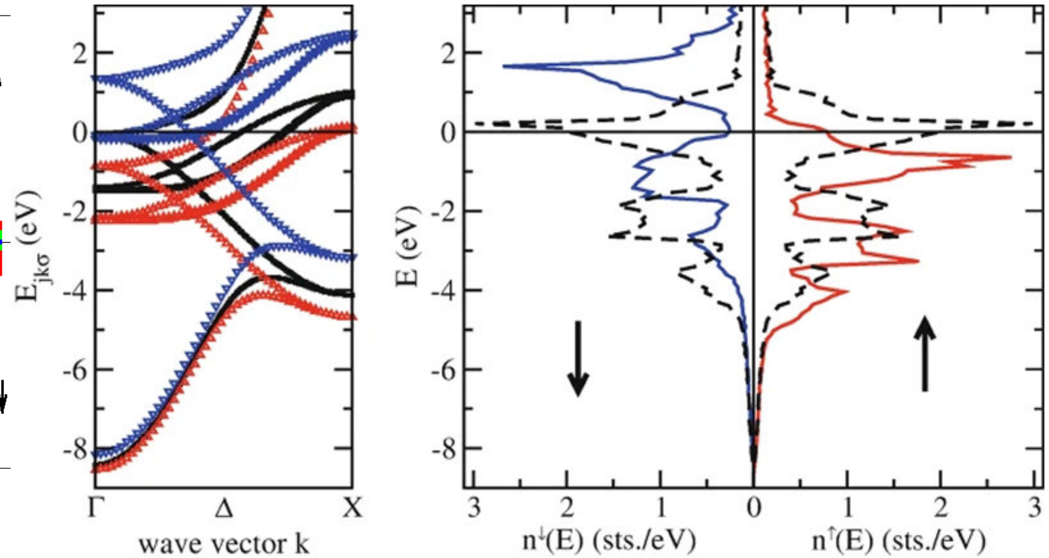


I. Mertig ESM 2017 lecture notes

Spin-polarised density of states of the electrons





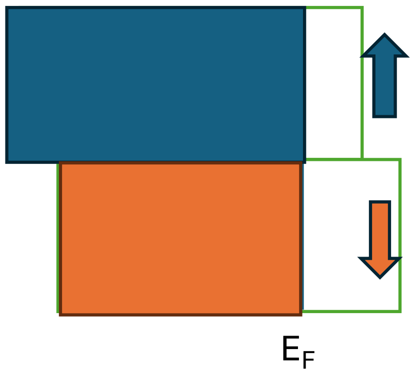


D(E), d.o.s.

$D^{\uparrow(\downarrow)}(E) = D(E \pm I\,M/2)$

$M = N^{\uparrow} - N^{\downarrow}$

Ferromag. if $(I\,D(E_F)) > 1$
Stoner criterion

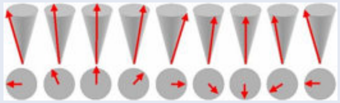


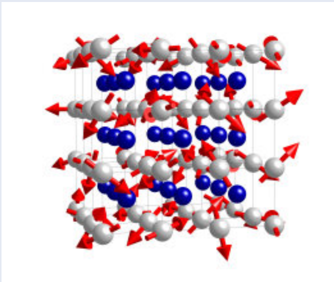
b.c.c. **Fe** non-magnetic and
ferromagnetic bands and density of states

Fluctuating local moments and itinerant electrons

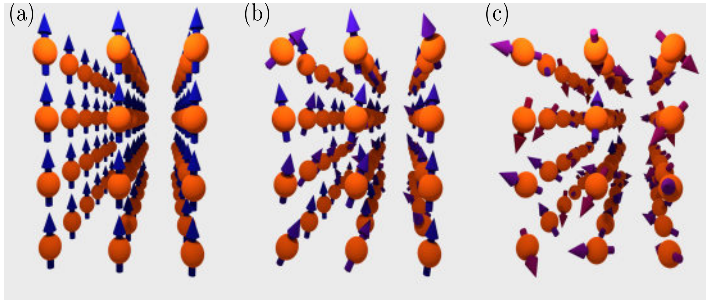
Slow nuclei vibrations about nearly fixed crystal lattice positions surrounded by electron glue with fast and slow fluctuations ···

Spin waves at low T coalesce into 'local moments' at higher T -

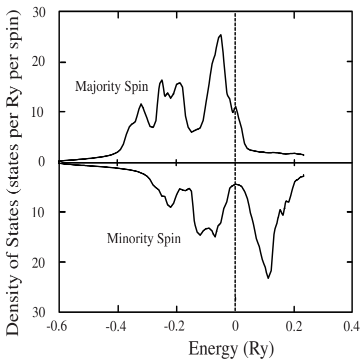




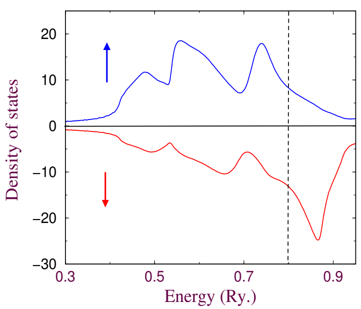
local polarisation of electronic spin density around an atom changes orientation slowly on time scale of other electronic behaviours, $\{\hat{e}_i\}$. Energies $\mathcal{H}\{\hat{e}_i\}$.



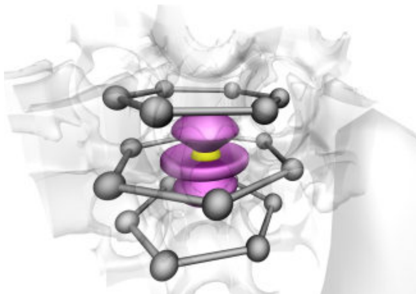
'Spins' from collective behaviour of the electrons for further atomistic modelling

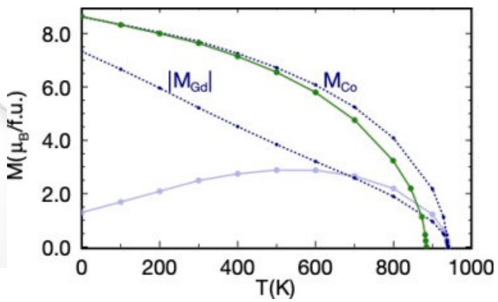


Iron above the Curie temperature



Localised and itinerant magnetism





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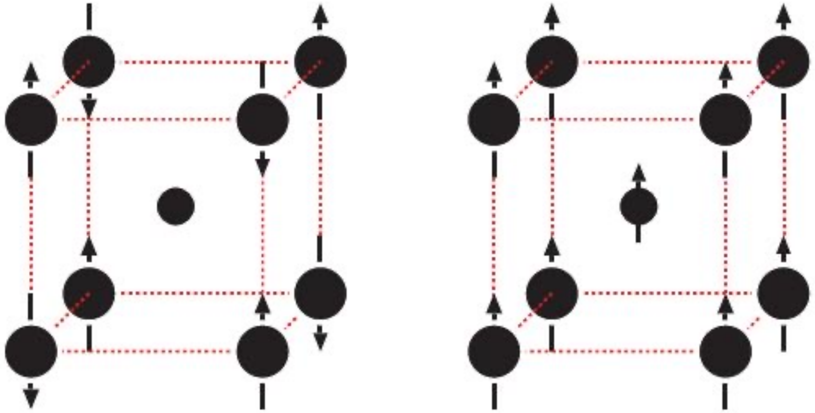
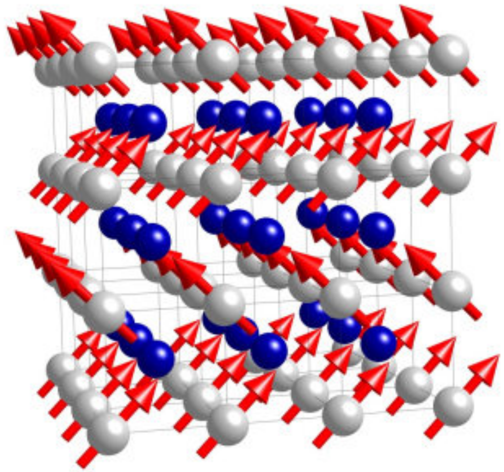
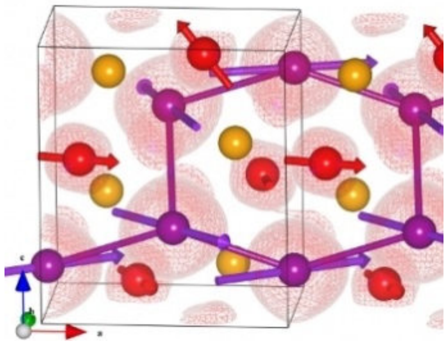
Spin models, magnetic ordering and structure







$$\hat{H}\{\mathbf{S}_i\}$$

$$\hat{H} = -\frac{1}{2}\sum_i \sum_j J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + \cdots + g\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{B}$$

Mean field approximation

A very useful inequality,
the Feynman – Peierls' Inequality

$$F \leq F_0 + \langle \hat{H} - \hat{H}_0 \rangle_0 = \mathcal{F}, \quad \hat{H}_0 = \sum_i \mathbf{S}_i \cdot \mathbf{h}_i.$$

$$\frac{\partial \mathcal{F}}{\partial \mathbf{h}_i} = 0 \cdots \mathbf{h}_i = \frac{\partial \Omega}{\partial \mathbf{m}_i}, \quad \mathbf{m}_i = \langle \mathbf{S}_i \rangle_0, \quad \Omega = \langle \hat{H} \rangle_0.$$

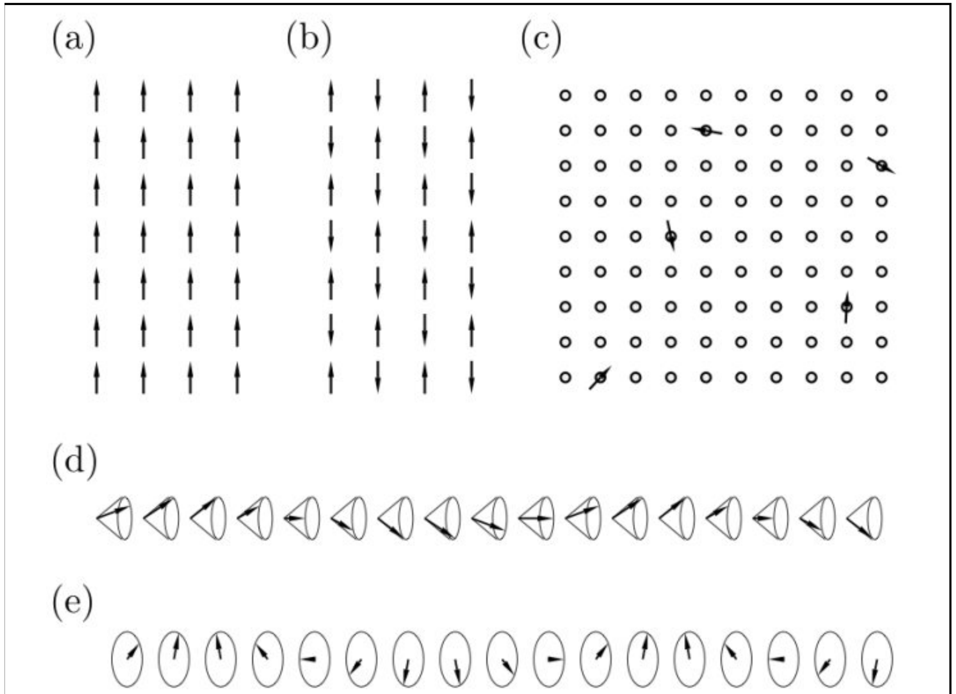
$$\mathbf{h}_i = g\mu_B \mathbf{B} - \sum_j J_{ij} \mathbf{m}_j + \cdots, \quad \mathbf{m}_i = \mathcal{B}_S \left(\frac{S\, h_i}{k_B T} \right) \frac{\mathbf{h}_i}{|\mathbf{h}_i|}.$$

Weiss field

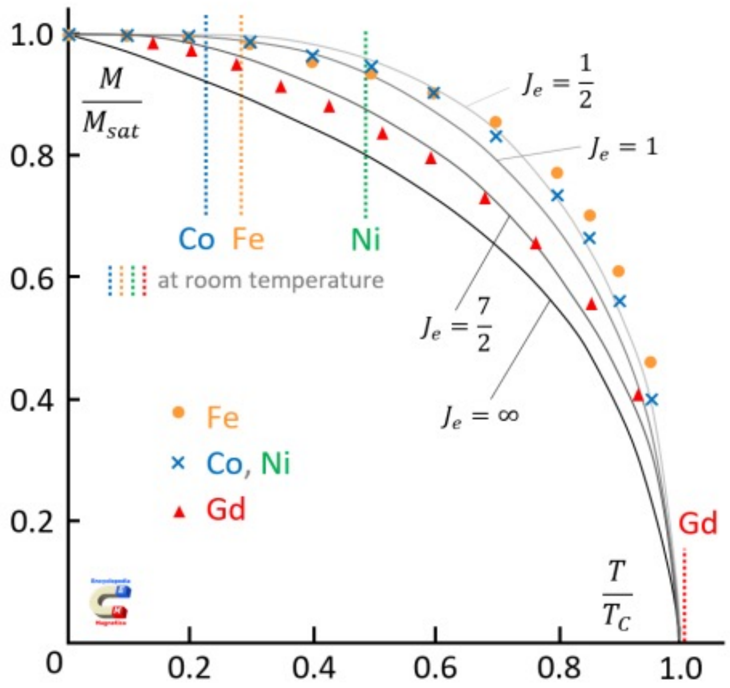
Brillouin function again

For ferromagnetic order, $m_1 = m_2 = m_3 \ldots\ldots = m$,
antiferromagnetic, e.g. m_i's $m_1 = -m_2 = m_3 = -m_4 \ldots\ldots$

$$\boldsymbol{m}(\boldsymbol{R}) = m_{\boldsymbol{Q}} \left(\cos(\boldsymbol{Q}.\boldsymbol{R}) \sin a, \sin(\boldsymbol{Q}.\boldsymbol{R}) \sin a, \cos a \right)$$



S. J. Blundell, Magnetism in Condensed Matter (OUP, 2001)

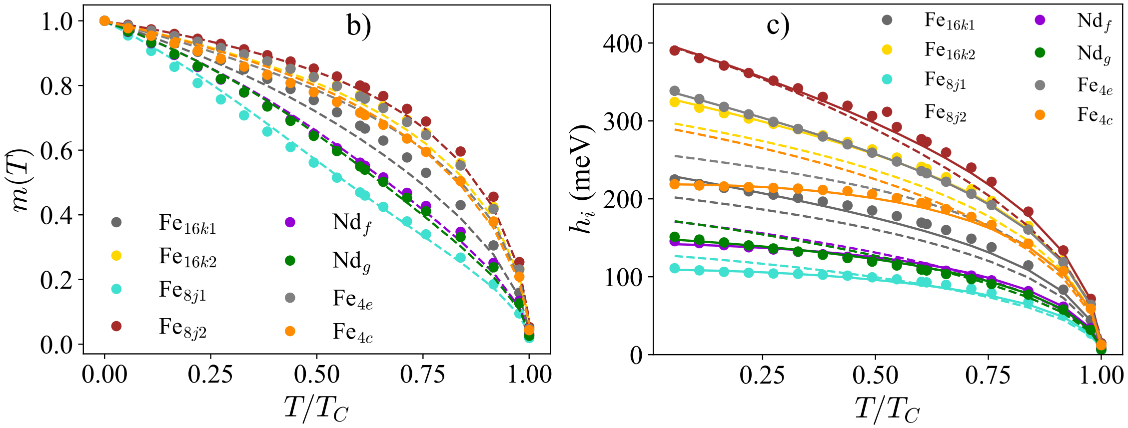


$$k_B T_C = \frac{(S+1)J(0)}{3S},$$

$$J(\mathbf{Q}) = \frac{1}{N}\sum_j J_{ij}\cos(\mathbf{Q}\cdot\mathbf{R}_{ij})$$

$$k_B T_N = \frac{(S+1)J(\mathbf{Q}_{max})}{3S}$$

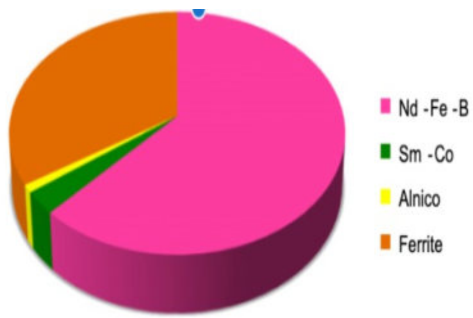
Example of Nd2Fe14B – the ubiquitous magnet

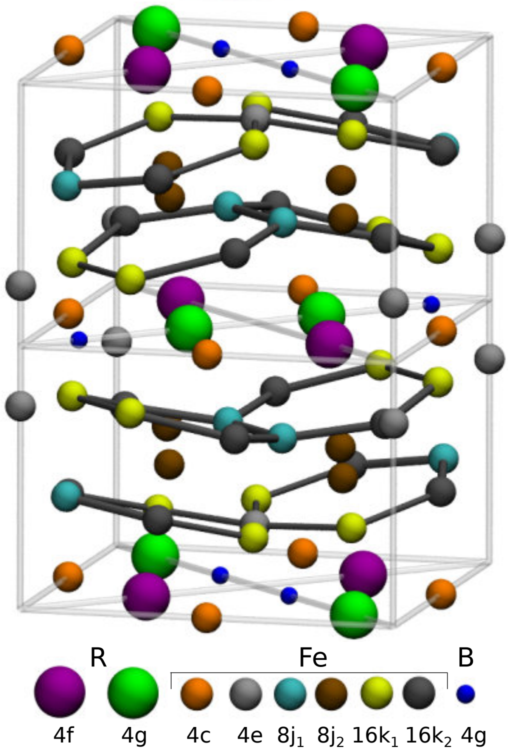


J. Bouaziz et al. PRB 107, L020401,(2023).

$$\bar{\Omega} = -\frac{1}{2}\sum_{ij}\mathcal{J}_{ij}\boldsymbol{m}_i \cdot \boldsymbol{m}_j - \frac{1}{4}\sum_{i}\mathcal{B}_I(\boldsymbol{m}_i \cdot \boldsymbol{M})^2$$

Pairwise exchange J_{ij} and higher order B_I parameters produced for further atomistic spin modelling.





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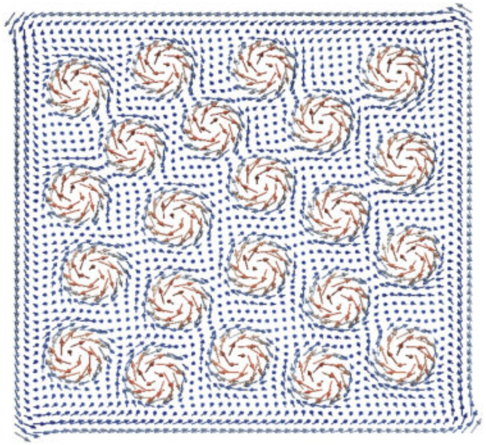

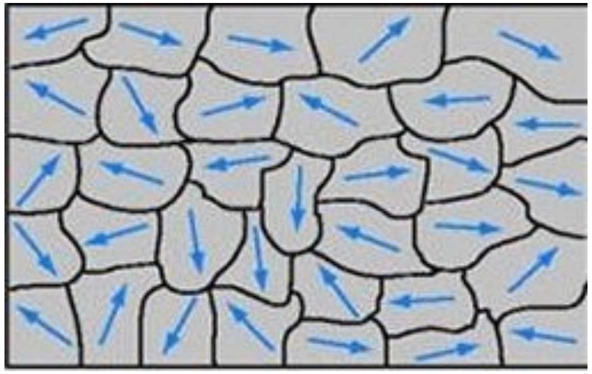

Supporting material

- S. J Blundell, “*Magnetism in Condensed Matter*”, O. U. P. (2001).
- N. W. Ashcroft and N. D. Mermin, “*Solid State Physics*”, Cengage, (2021).
- J. M. D. Coey, ”*Magnetism and Magnetic Materials*”, C. U. P. (2010).
- J. Kübler, “*Theory of Itinerant Electron Magnetism*”, O. U. P. , (2021)

Lecture notes from past ESMs by e.g.
S. Blundell, J. M. D. Coey, D. Givord, I. Mertig, W. Wulfhekel,.....