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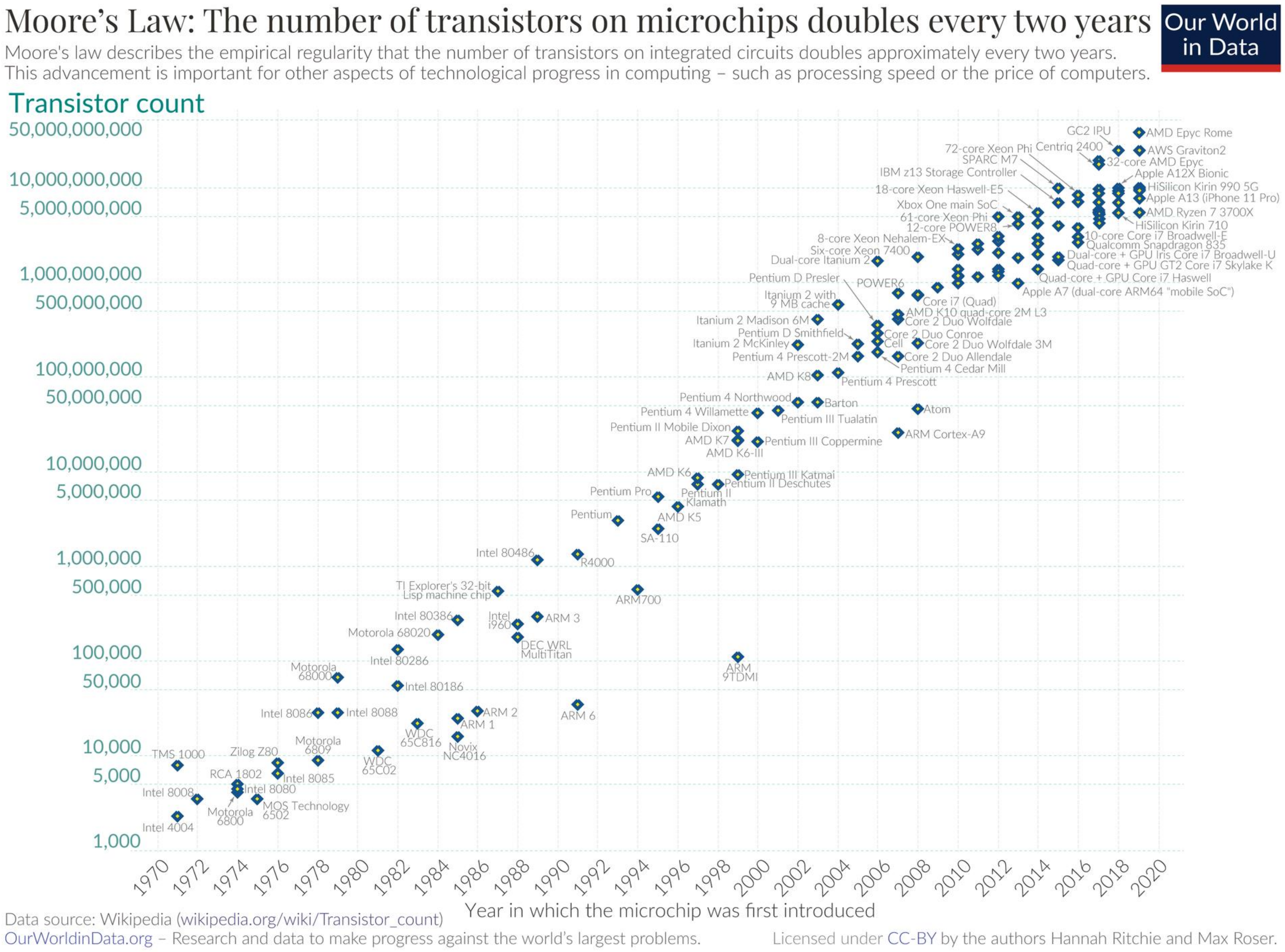
Moore's law

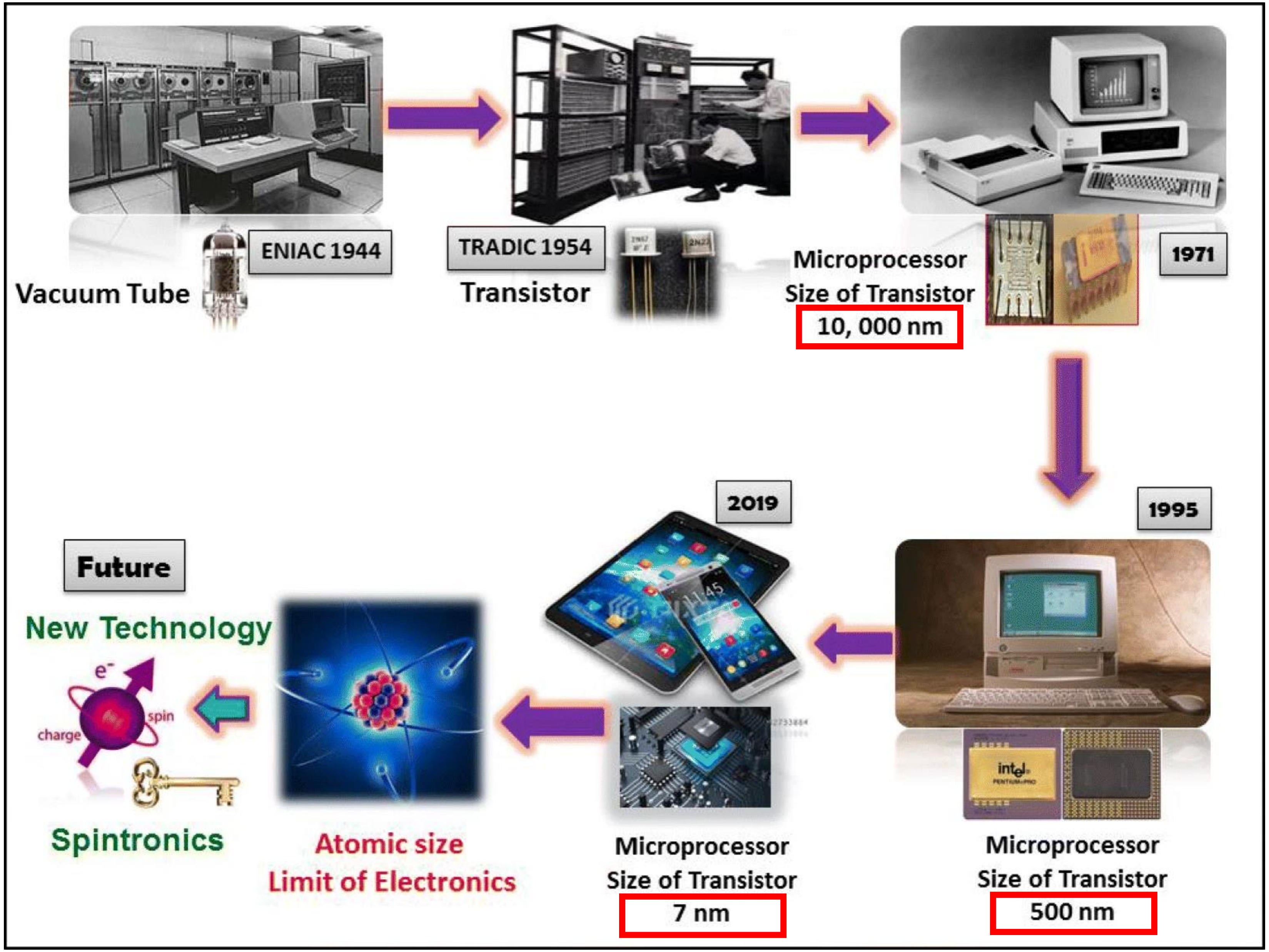
Development in electronic devices based on reducing transistor size



Evolution of transistor size

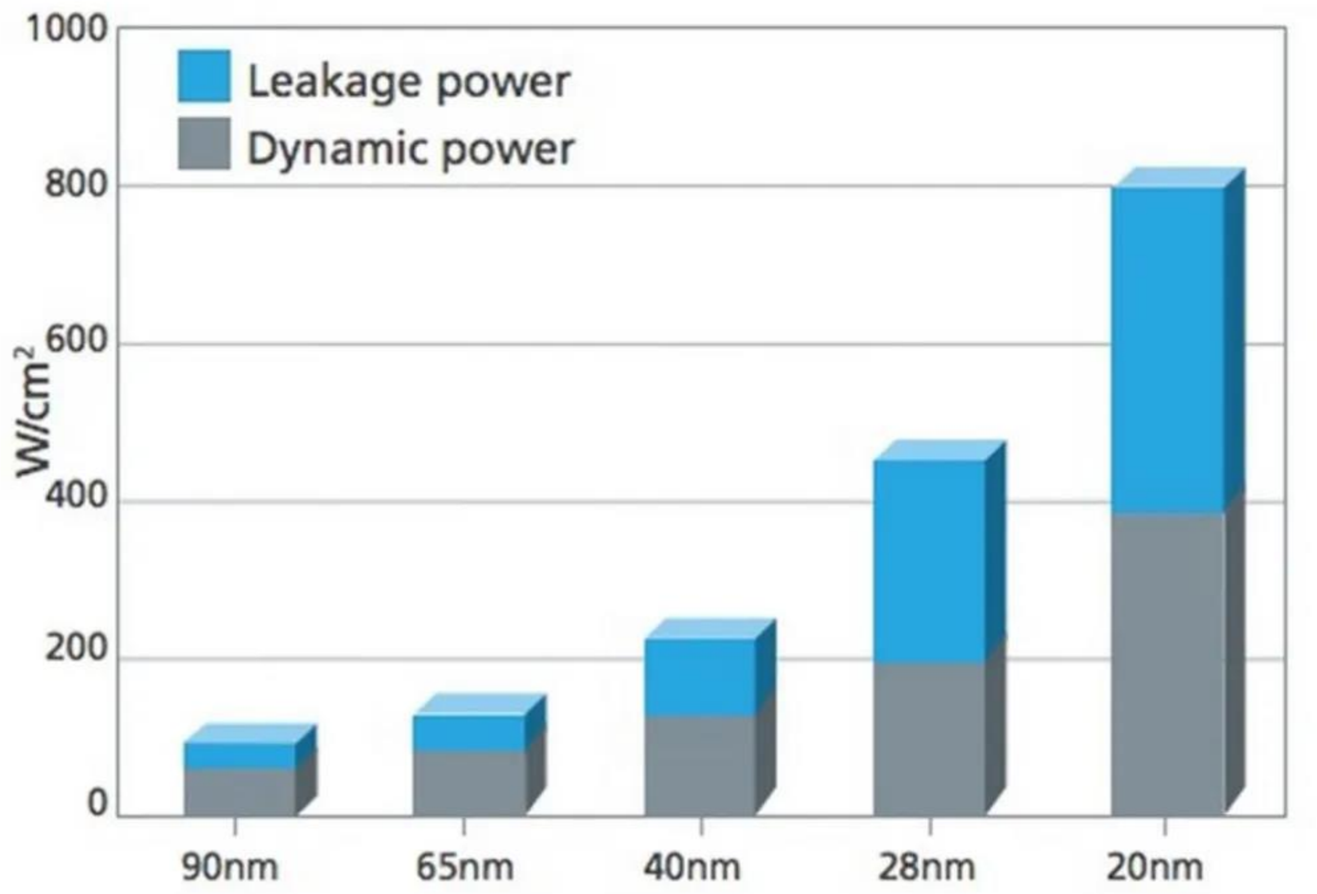
Development in electronic devices based on reducing transistor size

Leakage current due to quantum tunneling at the nanometric scale: loss of information



S. M. Yakout; Journal of Superconductivity and Novel Magnetism (2020) 33:2557–2580

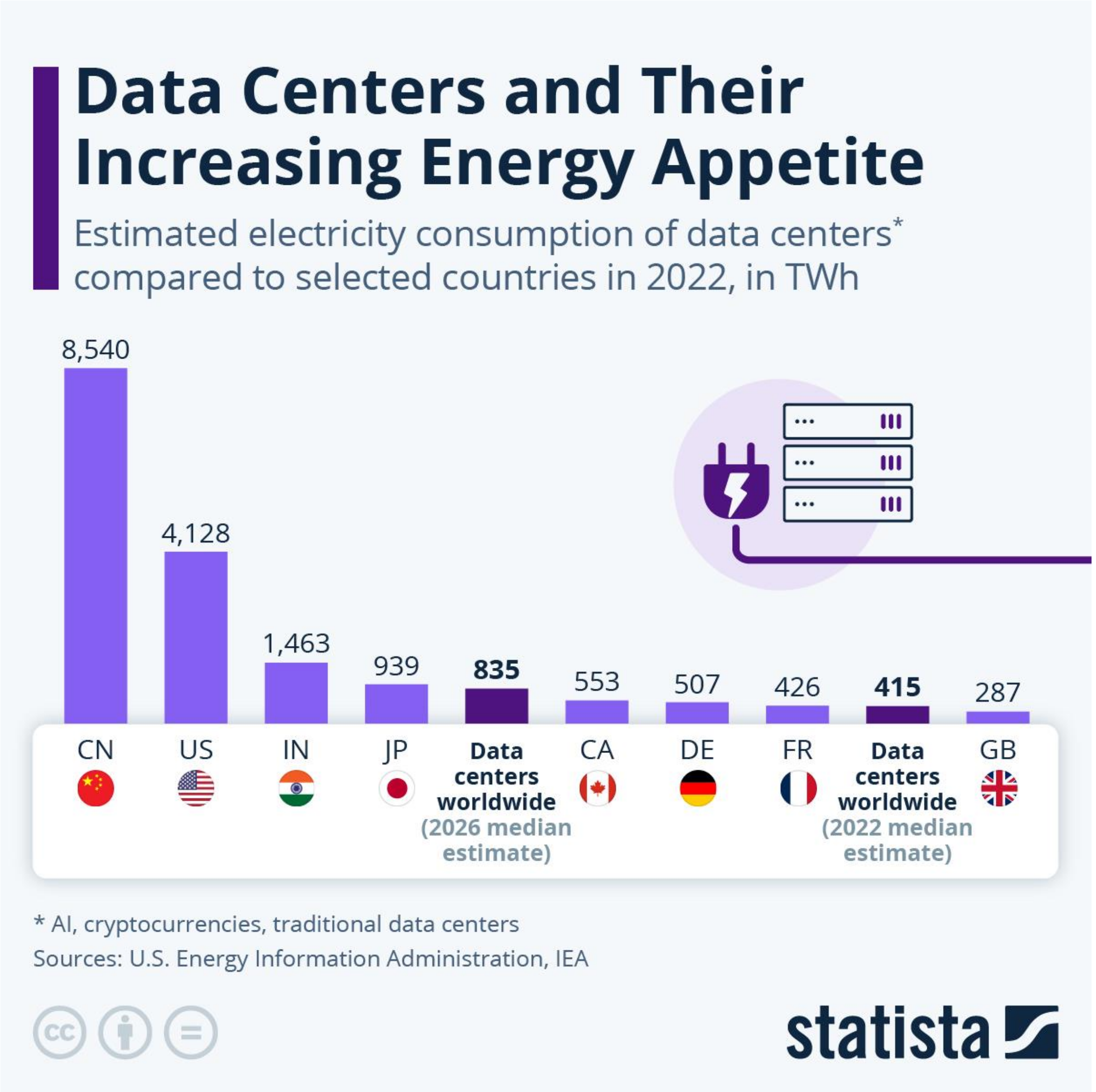
Microprocessor power consumption



https://semiengineering.com/as-nodes-advance-so-must-power-analysis/

Clothes iron: 10 W/cm^2
Power: 2kW
Surface: 200 cm^2

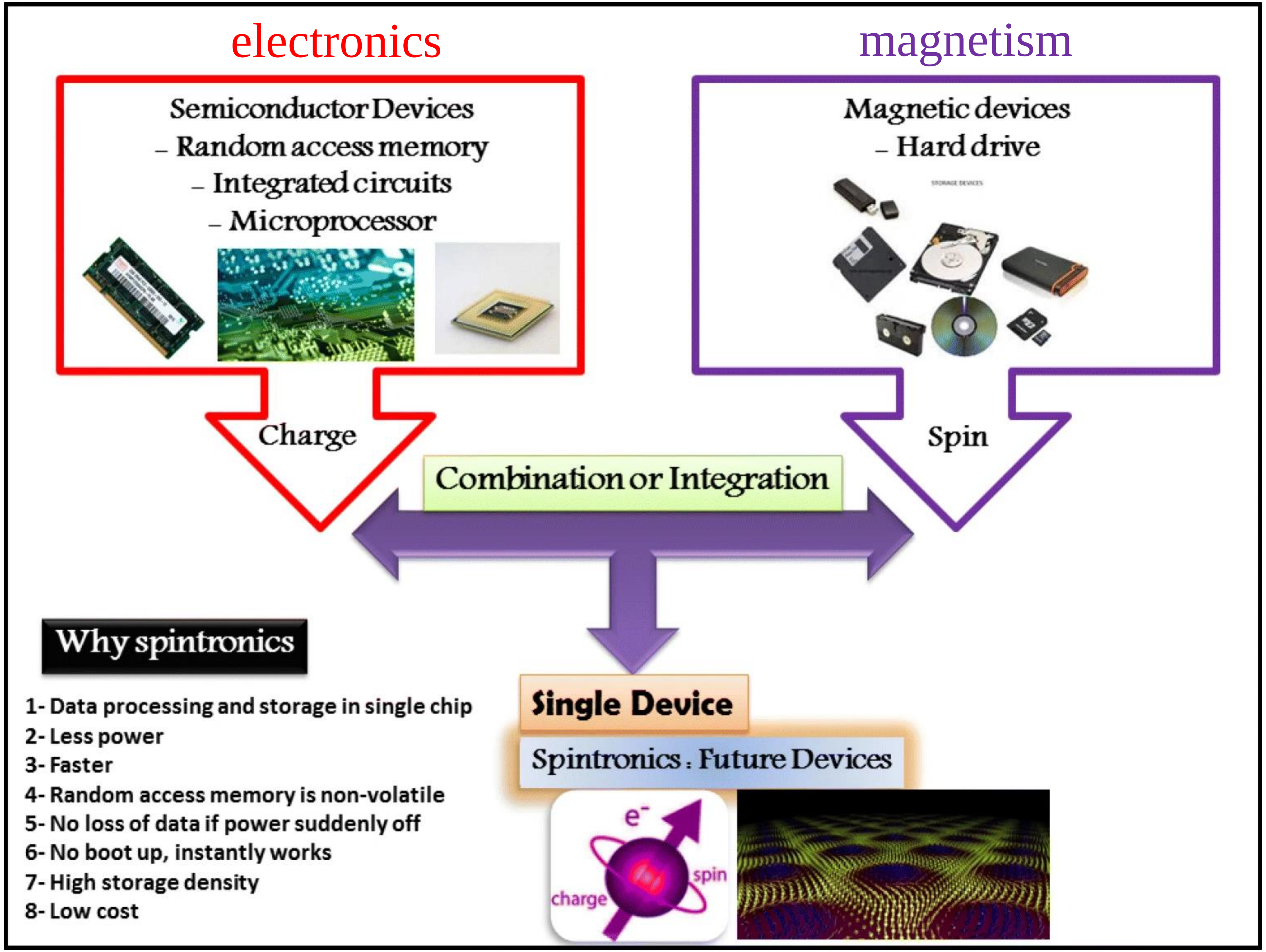
Data center power consumption



Combining electron charge and spin: Spintronics

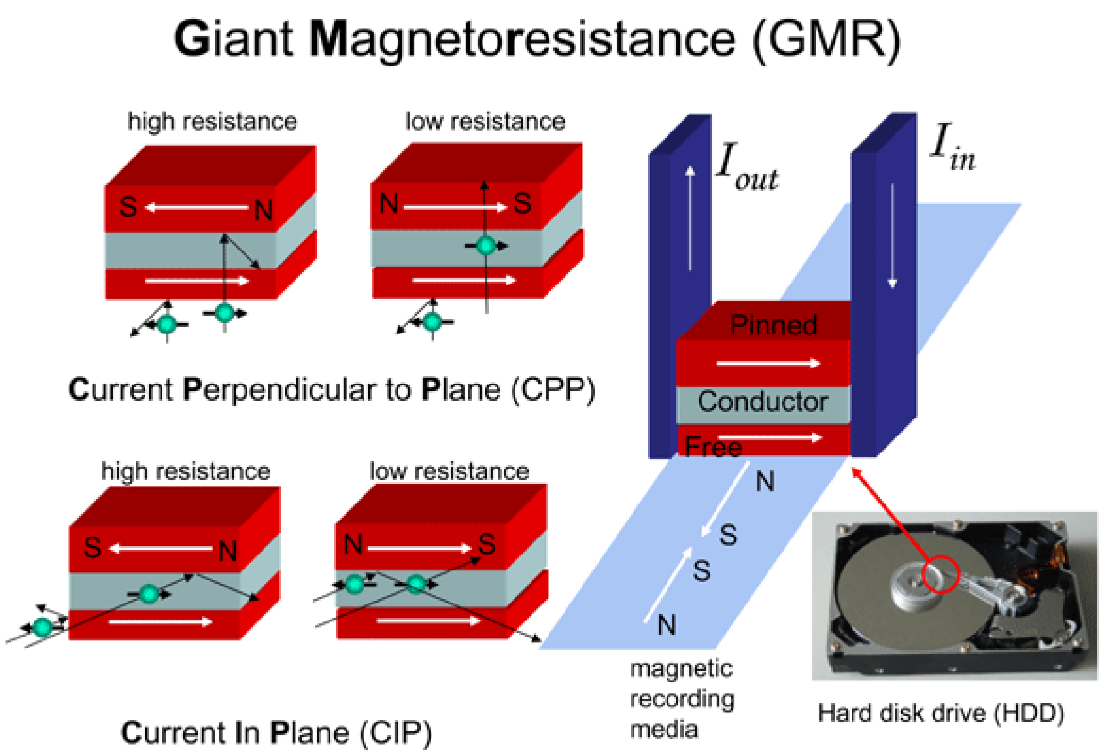
Need of new technology allowing simultaneously:

1) **Reduced memory size**
2) **Reduced power consumption**



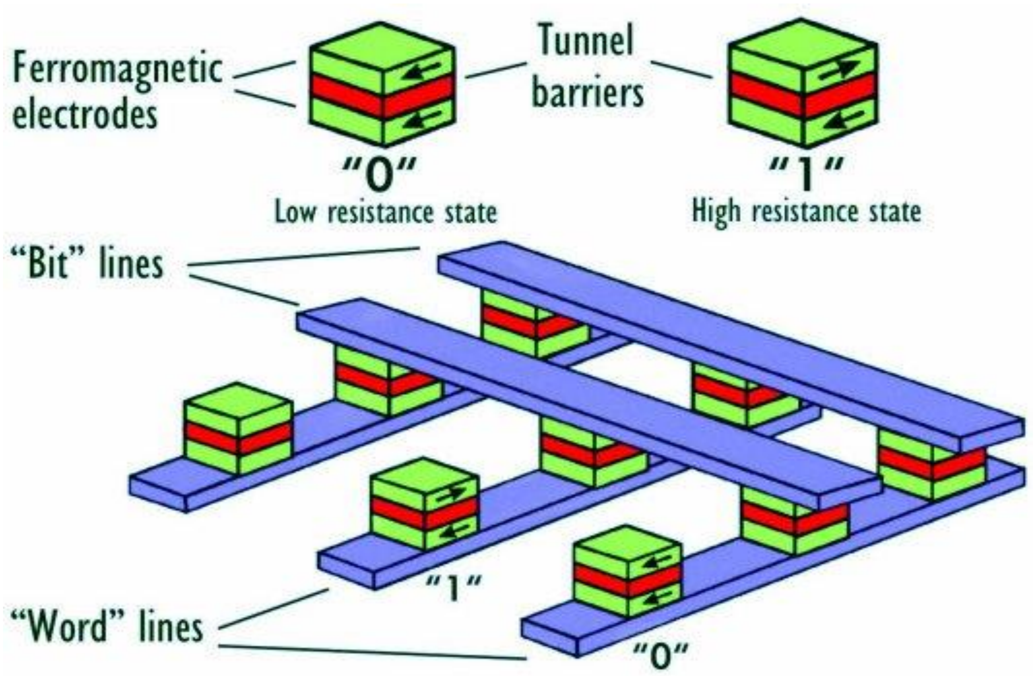
S. M. Yakout; Journal of Superconductivity and Novel Magnetism (2020) 33:2557–2580

Reading head in HDD



Spin valve

MRAM: Magnetic Random Access Memory



Spin valve + spin torque

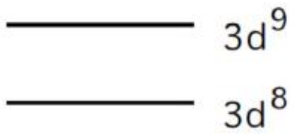
Magnetism in materials: localized *vs* delocalized spins

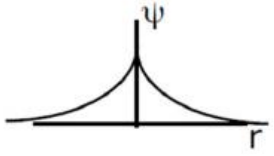
LOCALIZED MAGNETISM

Integral number of 3d or 4f electrons on the ion core; Integral number of unpaired spins; Discreet energy levels.

with

Ni^{2+} $3d^8$ $m = 2\ \mu_B$





$\psi \approx \exp(-r/a_0)$

Boltzmann statistics

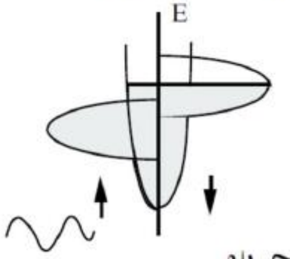
DELOCALIZED MAGNETISM

Nonintegral number of unpaired spins per atom.

Spin-polarized energy bands

strong correlations.

Ni $3d^{9.4}4s^{0.6}$ $m = 0.6\ \mu_B$



$\psi \approx \exp(-i\mathbf{k}.\mathbf{r})$

Fermi-Dirac statistics

4f metals	*localized electrons*
4f compounds	*localized electrons*
3d compounds	*localized/delocalized electrons*
3d metals	*delocalized electrons.*

Above the Curie temperature, neither localized nor delocalized moments disappear, they just become disordered in a paramagnetic state when $T > T_C$.

Ref: J.M.D. Coey, *Magnetism and magnetic materials* (Cambridge).

Complementary magnetism courses during Spring semester

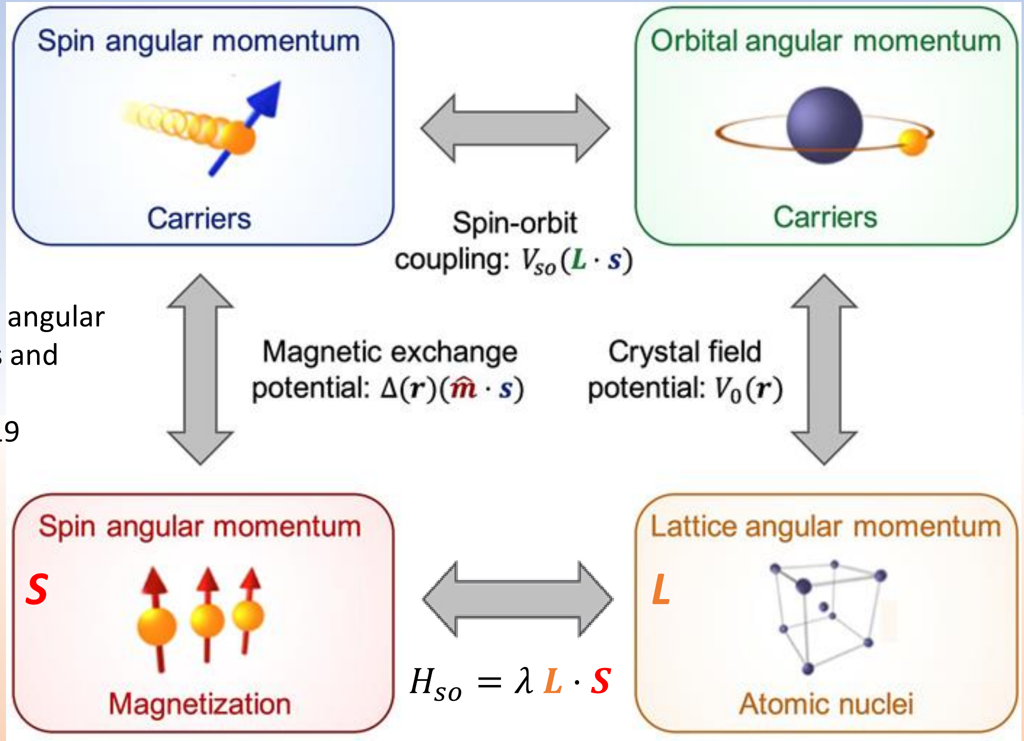
Spintronics: development of devices using electron spin as an additional degree of freedom to boost performance. The course provides the basis necessary to understand and describe spin dynamics in solids and nanostructures.

Spintronics: basics and applications

PHYS-510 / 4 credits Thursday 08:15-12:00

Stefano Rusponi, Marina Pivetta

Schematic of different angular momentum reservoirs and their interactions doi:10.1063/5.0024019



Magnetism in materials

PHYS-491 / 4 credits Tuesday 15:15-19:00

Ivica Zivkovic

Introduction to magnetism in materials: spin and orbital degrees of freedom, interactions between moments and some typical ordering patterns, selected experimental techniques and their application in current research

Content

1) Spin dynamics in solids and nanostructures
- Basics: isolated atoms, crystal field, magnetic anisotropy energy, exchange energy
- Continuum approximation: Landau-Lifshitz-Gilbert (LLG) equation and explanation of its microscopic origin
- Magnetization dynamics induced by magnetic field and temperature
- Bit reversal: coherent *vs* incoherent reversal
- Designing and writing the recording media in HDD

2) Spin transfer torque (STT)
- Giant (GMR) and tunnel (TMR) magnetoresistance, magnetic tunnel junctions (MTJ)
- Writing by means of spin-polarized currents: Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation
- GMR/TMR for reading heads in HDD, and for MRAM operation

3) Spin orbitronics
- Spin-orbit interaction
- Spin-orbit torque (SOT) in bulk (Dresselhaus effect) and at interfaces (Rashba-Edelstein effect)
- SOT- MTJ *vs.* STT- MTJ: opportunities and challenges for devices
- SOT in exotic materials: oxides and 2D dichalcogenides

4) From the continuum approximation to quantum description
- Single atom magnets and single ion molecular magnets
- Quantum tunneling of magnetization
- Demagnetization induced by spin-phonon and spin-electron scattering
- Writing and reading single atom magnets with spin-polarized currents: spin polarized scanning tunneling microscopy (SP-STM)

Spin-orbit coupling (SOC): a perturbation but….

Atomic moment

Magnetization easy axis

DMI exchange

Magnetocrystalline anisotropy Energy (MCA)

Spin-orbit:

$$\Delta E_{SO} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

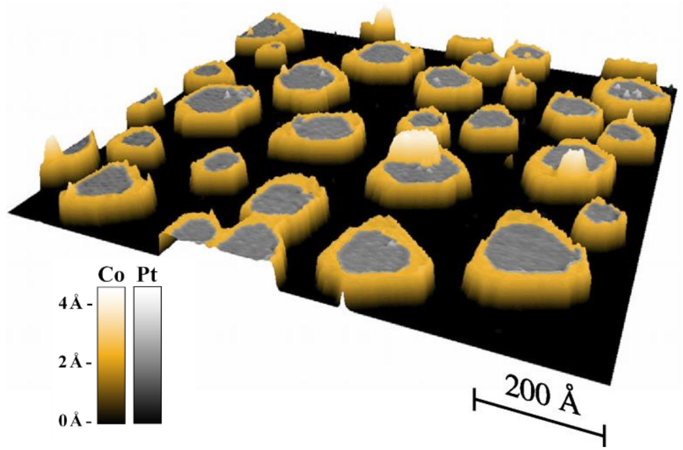
Rashba effect

Exchange of energy and moment between spin and lattice

Spin-orbit torque (SOT)

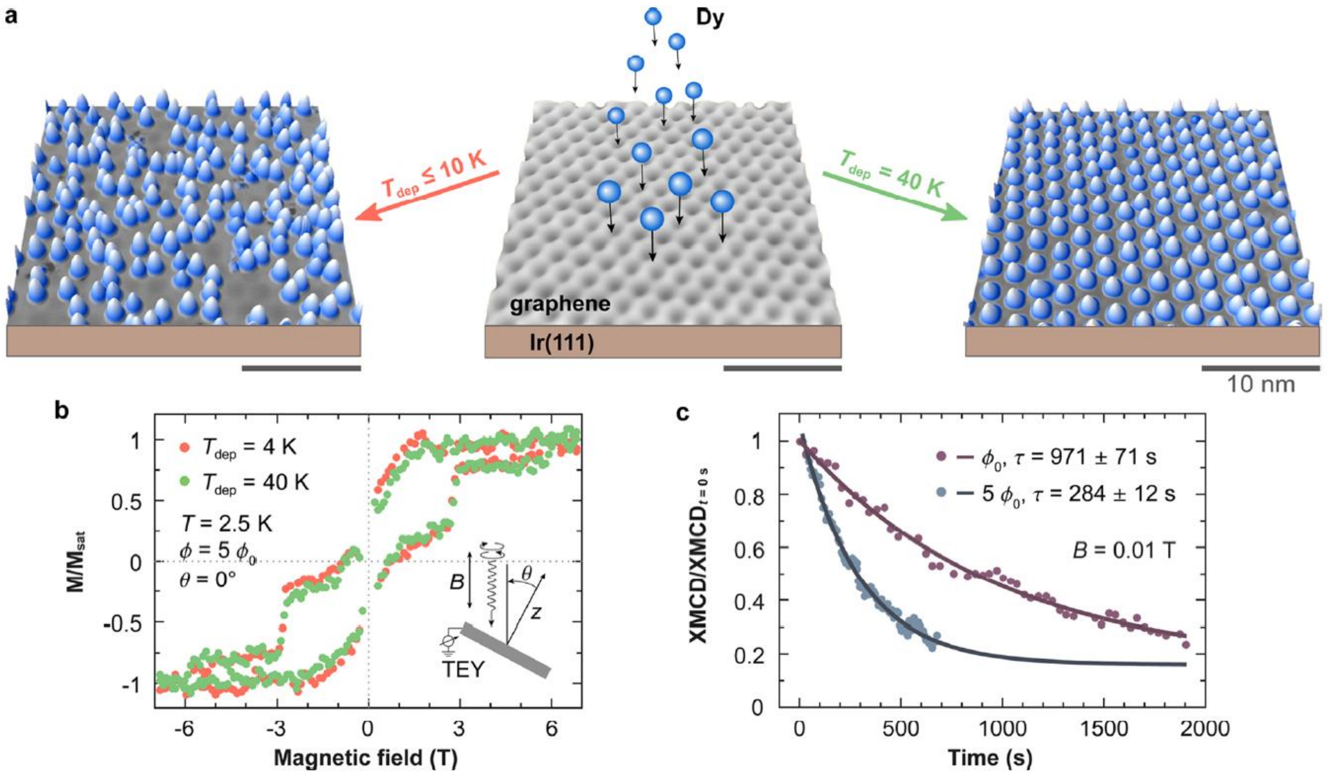
Growth and study of nanostructure magnetic properties

2D clusters: Pt core and Co shell



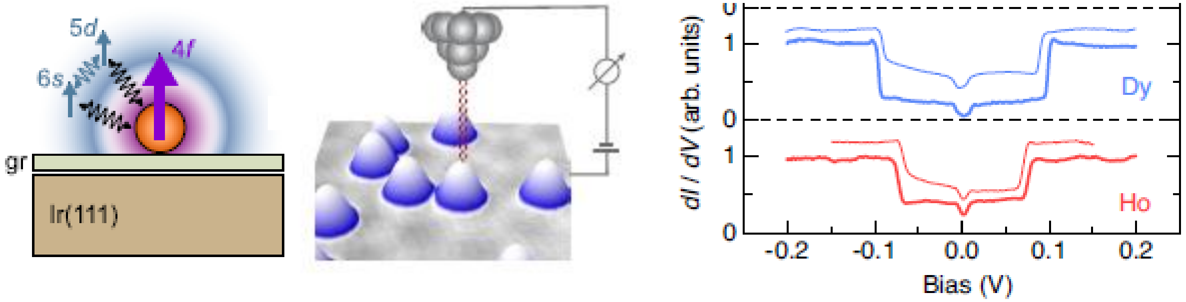
S. Rusponi *et al.*, Nature Mat. **2**, 546 (2003).

Superlattice of single atom magnets



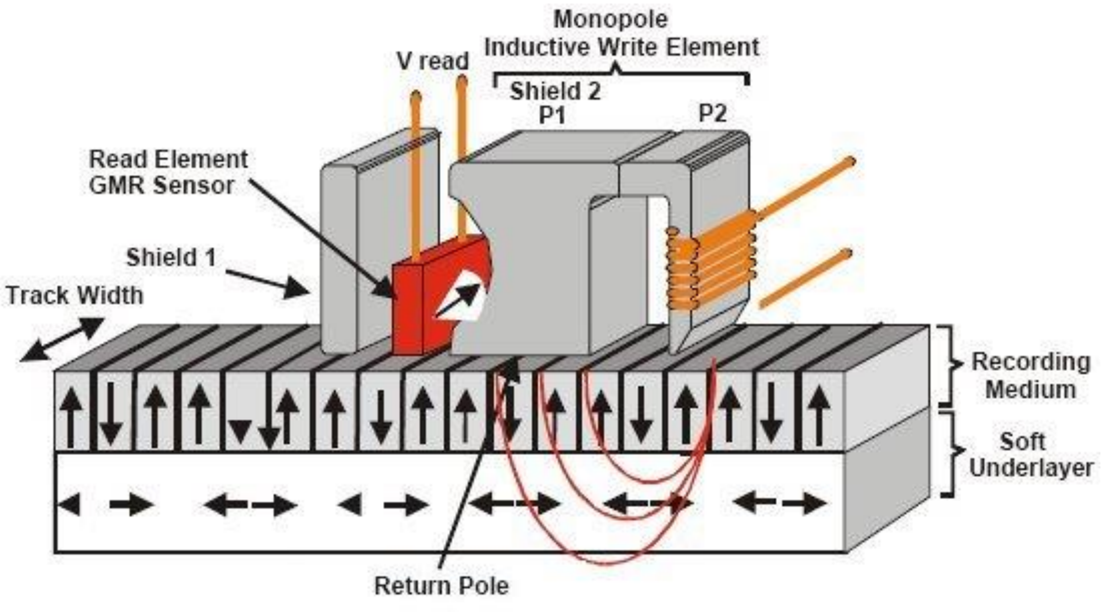
R. Baltic *et al.*, Nano Letters **16**, 7610 (2016).

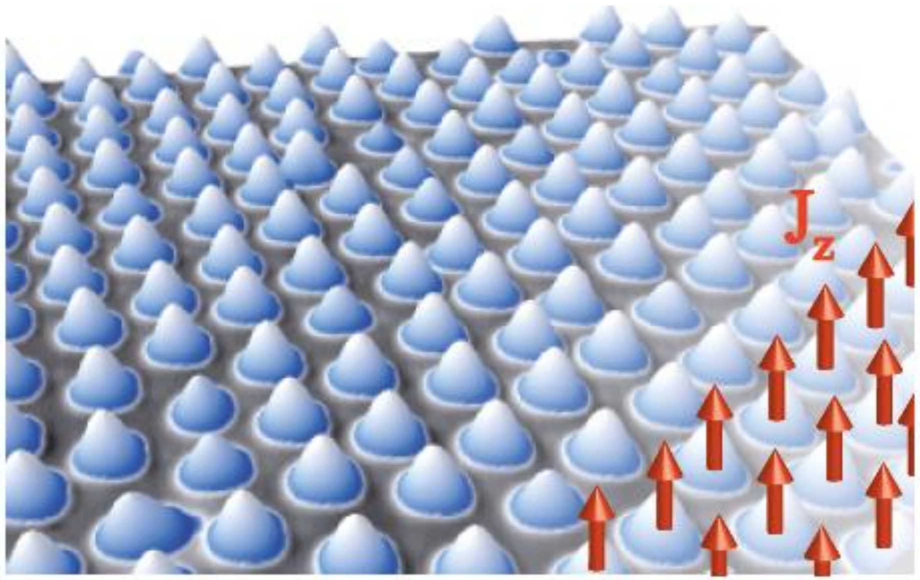
Intra-Atomic Exchange Energy in Rare-Earth Adatoms



M. Pivetta *et al.*, Phys. Rev. X 10, 031054 (2020)

Growth and study of nanostructure magnetic properties





One atom is the smallest magnet:
Ideal binary system for “classic” magnetic storage but also for quantum applications

Bibliography

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[Bel89] -> G. M. Bell, and D. A. Lavis, *Statistical mechanics of lattice models* (Ellis Horwood limited 1989)

[Plu01] -> M.L. Plumer, J. van Ek, and D. Weller, *The physics of ultra-high-density magnetic recording* (Springer 2001)

Analytical solution for hydrogen and hydrogenic atoms (one electron)

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi - \frac{Ze^2}{4\pi\varepsilon_0 r}\psi = E\psi \qquad \frac{1}{\mu} = \frac{1}{m_\mathrm{e}} + \frac{1}{m_\mathrm{N}}$$

Schrödinger equation for the motion of one electron relative to the nucleus
Z: atomic number

→ variable separation, radial and angular parts of wavefunctions: $\Psi_{nlm} = R_{nl}(r)Y_l^m$

$n = 1, 2, 3, 4 \ldots$ principal quantum number; average distance of an electron from the nucleus; energy of the electron: $E_n \propto -{Z^2}/{n^2}$

$l = 0, 1, \ldots n-1$ orbital quantum number;
magnitude of the angular moment of the electron: $|\boldsymbol{l}| = \sqrt{l(l+1)}\hbar$

$m = l, l-1, \ldots, -l$ magnetic quantum number; $(2l+1)$ values; $l_z = m\hbar$ is the component of the angular momentum with respect to an applied magnetic field, usually along z
Orbital magnetic moment: $\boldsymbol{\mu}_l = -\frac{\mu_B}{\hbar}\boldsymbol{l}$ $\left(\mu_B = \frac{e\hbar}{2m_e} = 0.058\ \mathrm{meV/T}\text{ is the Bohr magneton}\right)$
Orbital magnetic moment along quantization axis : $\mu_{l_z} = -\frac{\mu_B}{\hbar} l_z$

electron configurations, identified by the **shell**: $n = 1 \quad 2 \quad 3 \quad 4 \ldots$ (K L M N …) and the **subshell**: $l = 0 \quad 1 \quad 2 \quad 3 \ldots$ (s p d f …)

$n =$	1	2	3	4	…
	K	L	M	N	…
$l =$	0	1	2	3	…
	s	p	d	f	…

Hydrogenic radial wavefunctions

$$R_{n,l}(r) = N_{n,l}\rho^l L_{n+1}^{2l+1}(\rho)\mathrm{e}^{-\rho/2}$$

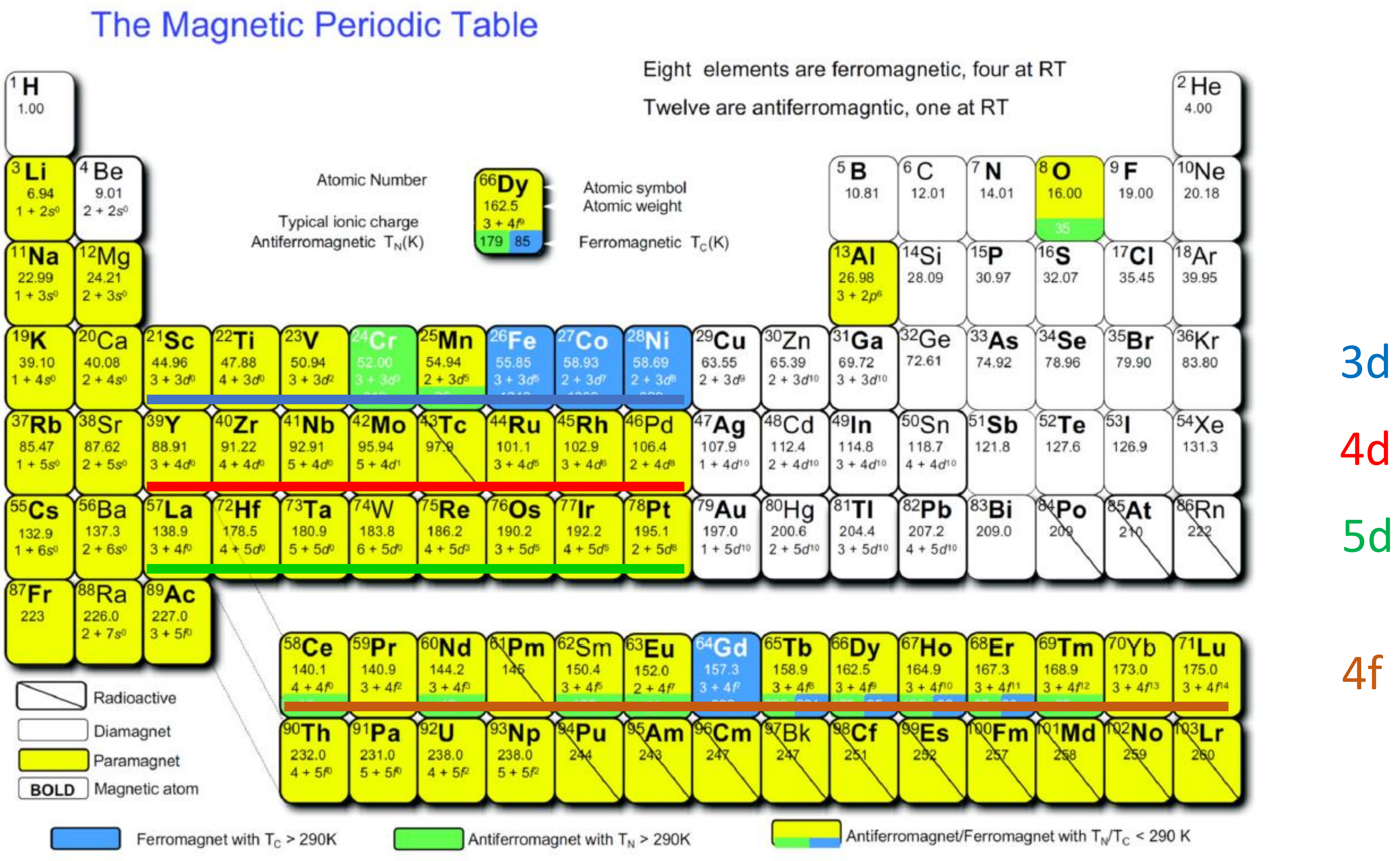
Orbital	n	l	$R_{n,l}$
1s	1	0	$2\left(\frac{Z}{a}\right)^{3/2}\mathrm{e}^{-\rho/2}$
2s	2	0	$\frac{1}{8^{1/2}}\left(\frac{Z}{a}\right)^{3/2}(2-\rho)\mathrm{e}^{-\rho/2}$
2p	2	1	$\frac{1}{24^{1/2}}\left(\frac{Z}{a}\right)^{3/2}\rho\mathrm{e}^{-\rho/2}$
3s	3	0	$\frac{1}{243^{1/2}}\left(\frac{Z}{a}\right)^{3/2}(6-6\rho+\rho^2)\mathrm{e}^{-\rho/2}$
3p	3	1	$\frac{1}{486^{1/2}}\left(\frac{Z}{a}\right)^{3/2}(4-\rho)\rho\mathrm{e}^{-\rho/2}$
3d	3	2	$\frac{1}{2430^{1/2}}\left(\frac{Z}{a}\right)^{3/2}\rho^2\mathrm{e}^{-\rho/2}$

$a = a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.0529\ nm$
is the Bohr radius

$\mu \approx m_e$

$$\rho = \frac{2Zr}{na_0}$$

- The polynomial term dominates close to the nucleus
- The exponential term describes the vanishing wave function at large distances

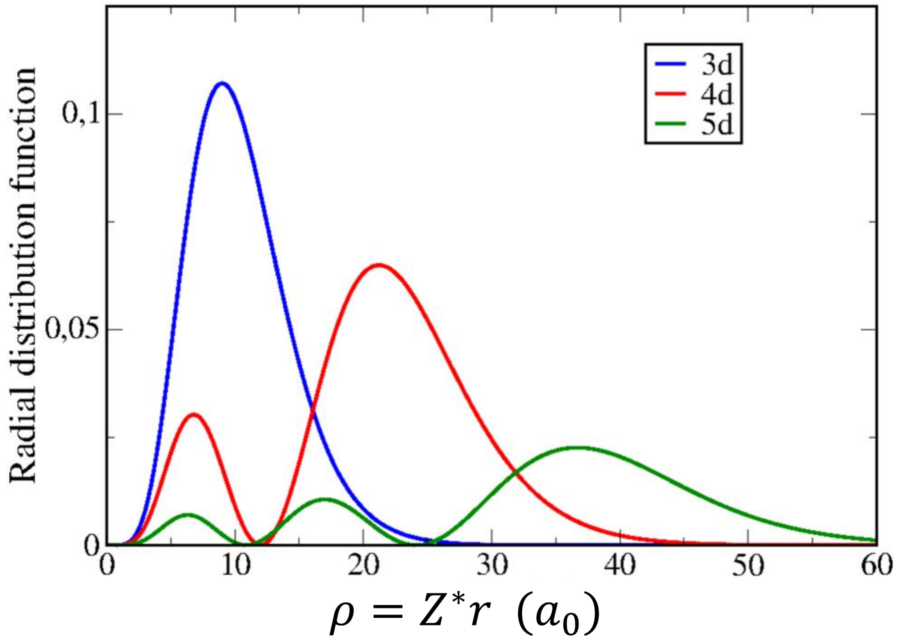


J.M.D. Coey, *Magnetism and magnetic materials* (Cambridge Univ. Press)

Radial distribution probability in real atoms

Radial distribution probability: $r^2 R_{nl}^2(r)$ ⟺ Charge density

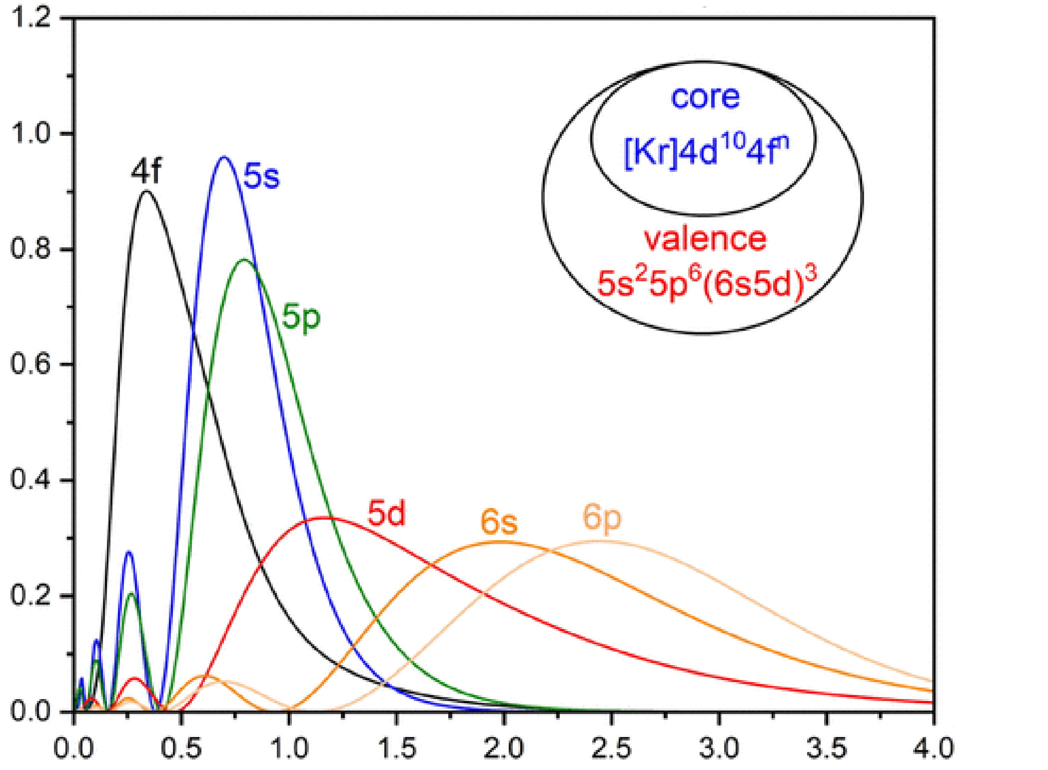
Transition metals



Radial distribution function as a function of the distance from the nucleus *r* expressed in atomic units. $Z^* = Z - \sigma$ is the effective nuclear charge with σ a screening constant. As the principal quantum number *n* increases, *Z** remains almost constant for *d* valence electrons and their radial distribution is thus more and more extended.

J. Phys.: Condens. Matter **29** 263001 (2017)

Lanthanides (or rare earths)

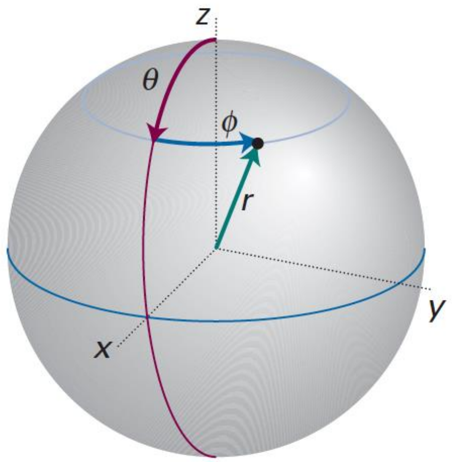


Radial distribution probability for 4f, 5s, 5p, 5d, 6s, and 6p orbitals of Nd atoms with the ($[Kr]4d^{10}5s^2 5p^6 6s^2 4f^4 5d^0 6p^0$) configuration.

J. Chem. Theory Comput. **19**, 82-96 (2023)

Hydrogenic angular wavefunctions: Spherical harmonics

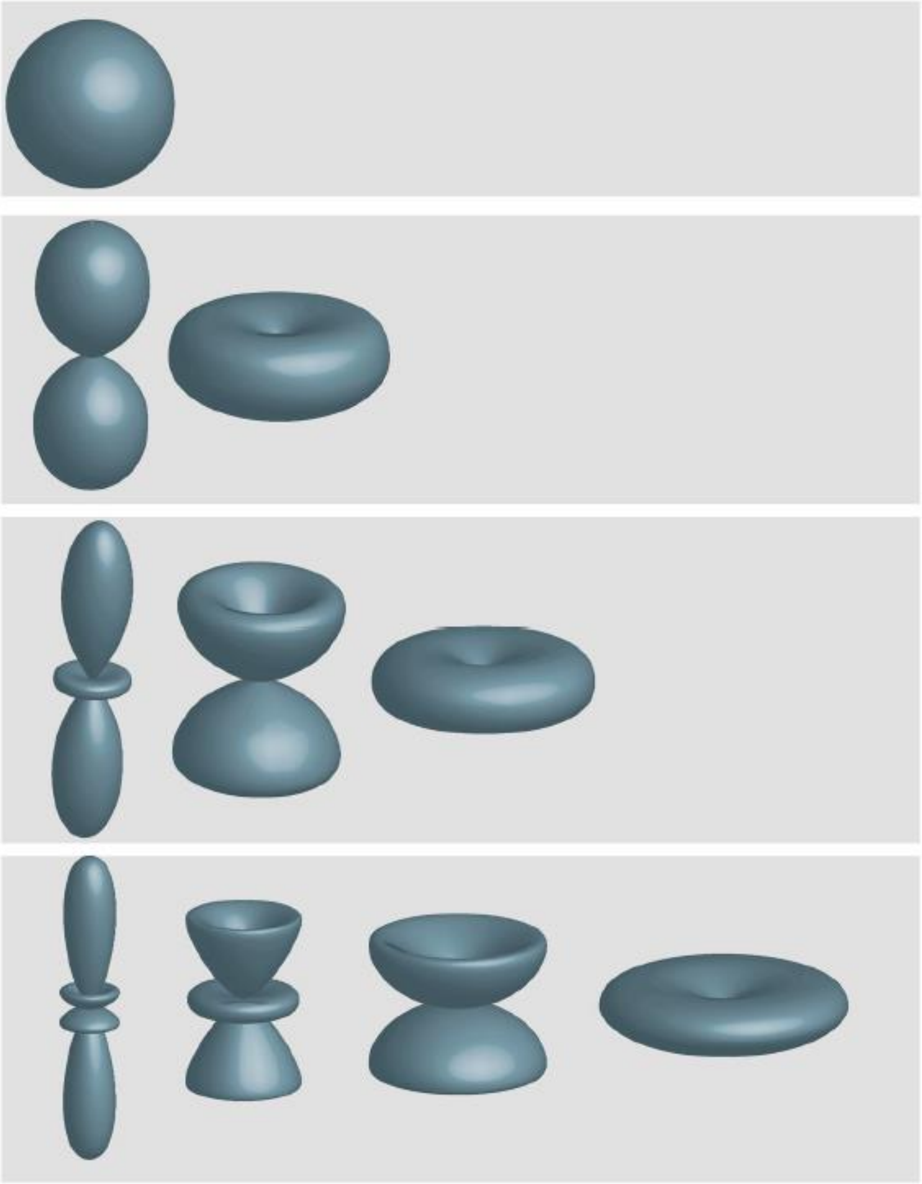
	l	m	$Y_{l,m}(\theta,\phi)$
s	0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
p	1	0	$\left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$
		±1	$\mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{\pm i\phi}$
d	2	0	$\left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$
		±1	$\mp\left(\frac{15}{8\pi}\right)^{1/2} \cos\theta \sin\theta\, e^{\pm i\phi}$
		±2	$\left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{\pm 2i\phi}$



f	3	0	$\left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$
		±1	$\mp\left(\frac{21}{64\pi}\right)^{1/2} (5\cos^2\theta - 1)\sin\theta\, e^{\pm i\phi}$
		±2	$\left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta \cos\theta\, e^{\pm 2i\phi}$
		±3	$\mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta\, e^{\pm 3i\phi}$

Angular momentum

electron density angular distribution



$l = 0$ — s

$l = 1$ — p

$l = 2$ — d

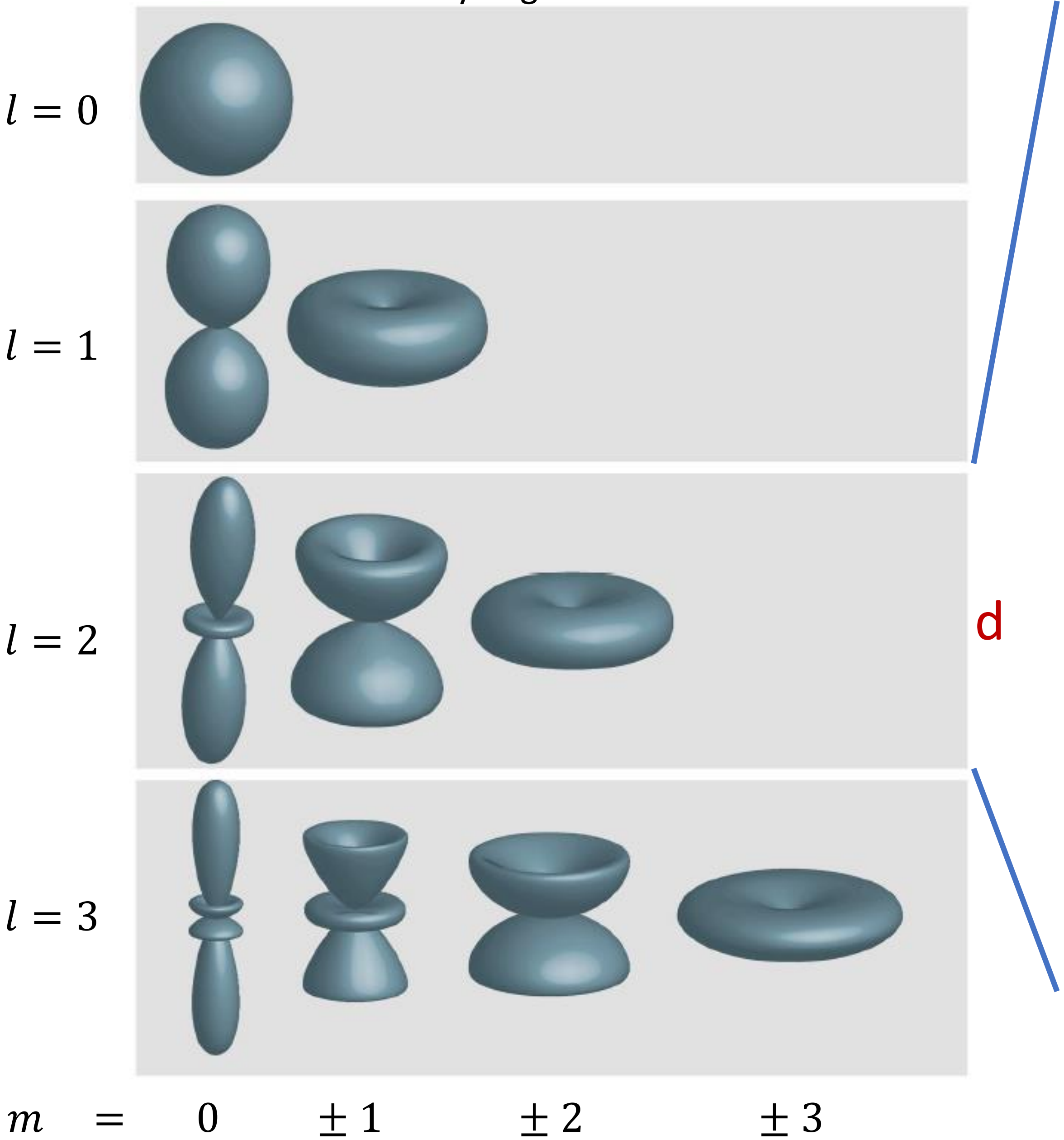
$l = 3$ — f

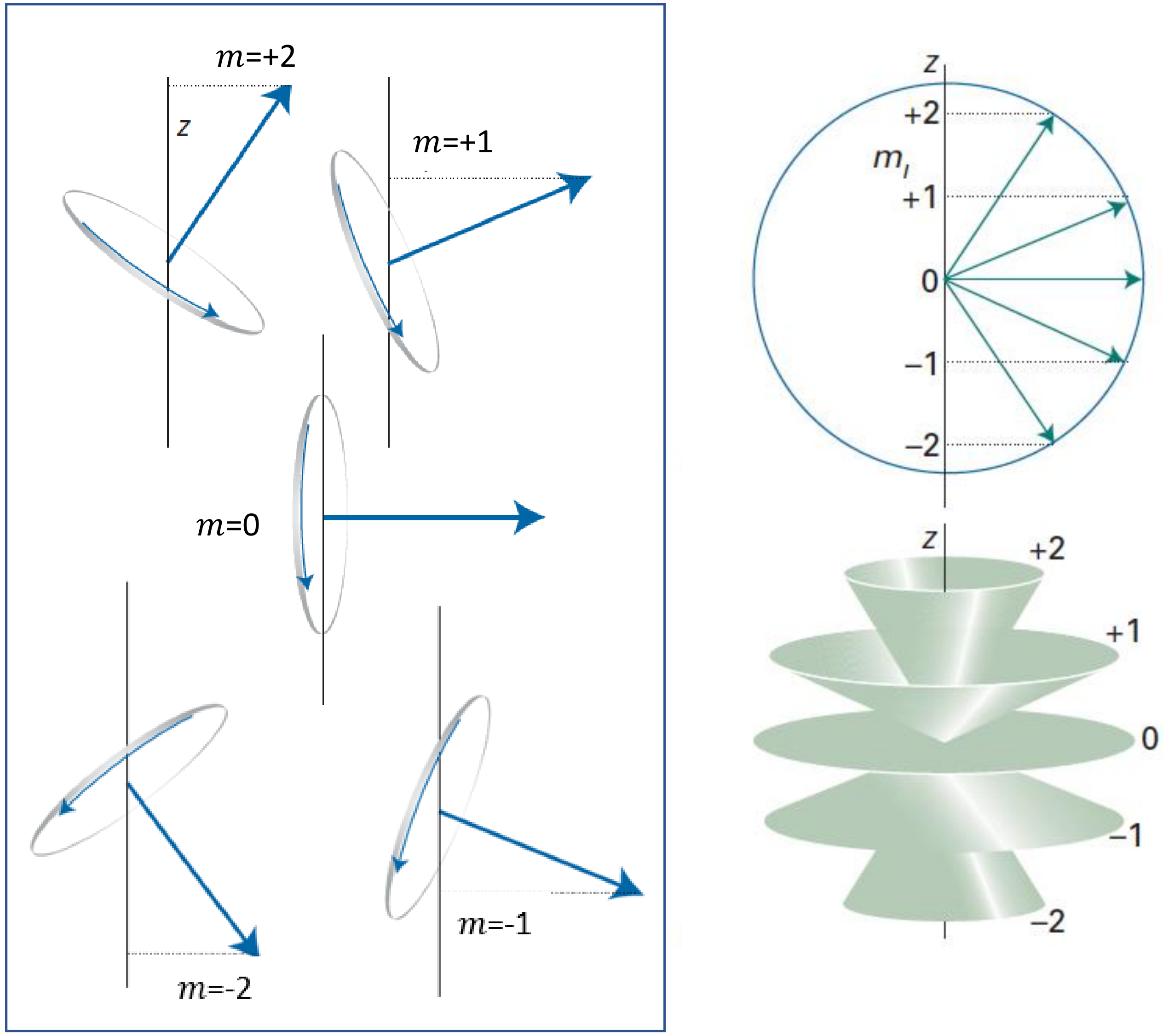
$m \;=\; 0 \quad \pm 1 \quad \pm 2 \quad \pm 3$

	l	m_l	$Y_{l,m}(\theta,\phi)$
s	0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
p	1	0	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
		±1	$\mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$
d	2	0	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$
		±1	$\mp\left(\frac{15}{8\pi}\right)^{1/2}\cos\theta\sin\theta\, e^{\pm i\phi}$
		±2	$\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$
f	3	0	$\left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta-3\cos\theta)$
		±1	$\mp\left(\frac{21}{64\pi}\right)^{1/2}(5\cos^2\theta-1)\sin\theta\, e^{\pm i\phi}$
		±2	$\left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
		±3	$\mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta\, e^{\pm 3i\phi}$

Angular momentum

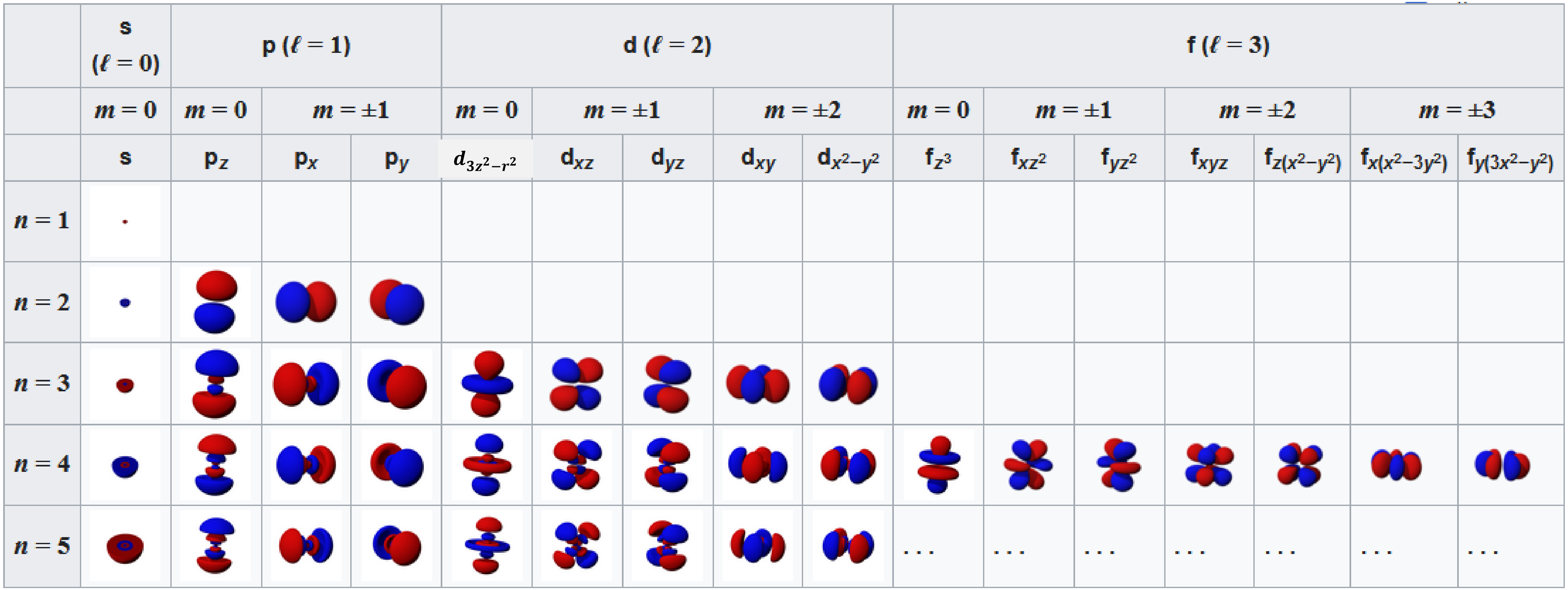
electron density angular distribution





The angular part of the wave function describes the angular distribution of the electron during its precessional motion

Orbitals (real wave functions): used in crystals and molecules



$$= \begin{cases} \frac{i}{\sqrt{2}}\left(\psi_{n,\ell,-|m|} - (-1)^m \psi_{n,\ell,|m|}\right) & \text{for } m < 0 \\ \psi_{n,\ell,|m|} & \text{for } m = 0 \\ \frac{1}{\sqrt{2}}\left(\psi_{n,\ell,-|m|} + (-1)^m \psi_{n,\ell,|m|}\right) & \text{for } m > 0 \end{cases}$$

$\Rightarrow$

$$s = \frac{1}{\sqrt{4\pi}} = Y_{0,0}$$

$$p_x = \sqrt{\frac{3}{4\pi}}\frac{x}{r} = \frac{1}{\sqrt{2}}(Y_{1,-1} - Y_{1,+1})$$

$$p_y = \sqrt{\frac{3}{4\pi}}\frac{y}{r} = \frac{i}{\sqrt{2}}(Y_{1,-1} + Y_{1,+1})$$

$$p_z = \sqrt{\frac{3}{4\pi}}\frac{z}{r} = Y_{1,0}$$

$$d_{xy} = \sqrt{\frac{15}{4\pi}}\frac{xy}{r^2} = \frac{i}{\sqrt{2}}(Y_{2,-2} - Y_{2,+2})$$

$$d_{xz} = \sqrt{\frac{15}{4\pi}}\frac{xz}{r^2} = \frac{1}{\sqrt{2}}(Y_{2,-1} - Y_{2,+1})$$

$$d_{yz} = \sqrt{\frac{15}{4\pi}}\frac{yz}{r^2} = \frac{i}{\sqrt{2}}(Y_{2,-1} + Y_{2,+1})$$

$$d_{x^2-y^2} = \sqrt{\frac{15}{16\pi}}\frac{(x^2-y^2)}{r^2} = \frac{1}{\sqrt{2}}(Y_{2,-2} + Y_{2,+2})$$

$$d_{3z^2-r^2} = \sqrt{\frac{5}{16\pi}}\frac{(3z^2-r^2)}{r^2} = Y_{2,0}$$

Electron spin

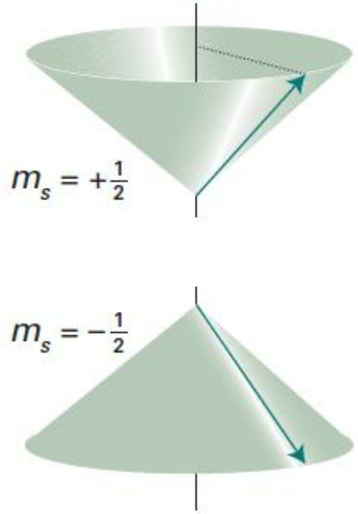
$$\Psi_{nlms} = R_{nl}(r) Y_l^m s$$

Intrinsic angular momentum of the electron

$s = {}^1/_2$ spin quantum number, magnitude : $|\boldsymbol{s}| = \sqrt{s(s+1)}\hbar = {}^{\sqrt{3}}/_2\,\hbar$

$m_s = \pm{}^1/_2$ spin magnetic quantum number, component along z ,
magnitude: $s_z = m_s\hbar = \pm{}^1/_2\,\hbar$

$m_s = +{}^1/_2 = \uparrow, \quad m_s = -{}^1/_2 = \downarrow$



Spin magnetic moment: $\boldsymbol{\mu}_s = -g_e \frac{\mu_B}{\hbar}\,\boldsymbol{s}$

Spin magnetic moment along quantization axis: $\mu_{s_z} = -g_e \frac{\mu_B}{\hbar} s_z$

($\mu_B = \frac{e\hbar}{2m_e} = 0.058\ \mathrm{meV/T}$ is the Bohr magneton; $g_e = 2.0023$ is the electron g-factor)

Total magnetic moment of one electron: $\boldsymbol{m}_{tot} = \boldsymbol{\mu}_s + \boldsymbol{\mu}_l = -\frac{\mu_B}{\hbar}(2\boldsymbol{s} + \boldsymbol{l})$

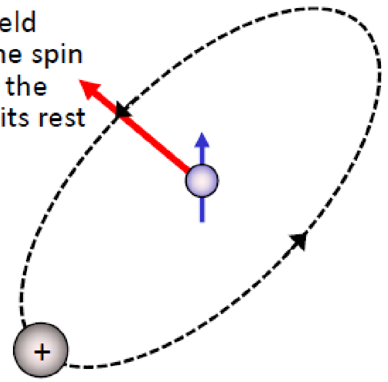
Total magnetic moment along *z:* $m_{tot_z} = \mu_{s_z} + \mu_{l_z} = -\frac{\mu_B}{\hbar}(2s_z + l_z)$

Spin-orbit interaction

The **spin–orbit interaction** (also called **spin–orbit coupling**) is a relativistic interaction of a particle's spin with its motion inside a potential.

Atomic potential: $V(r) = \dfrac{Ze}{4\pi\varepsilon_0 r}$ $\qquad \boldsymbol{\nabla} V = \dfrac{1}{r}\dfrac{dV(r)}{dr}\boldsymbol{r}$

magnetic field acting on the spin moment of the electron in its rest frame



Reference frame of the electron:

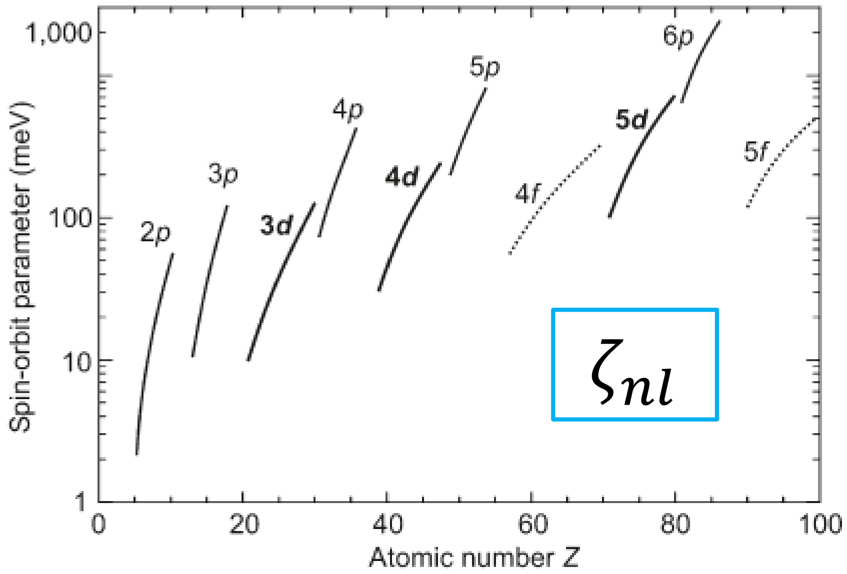
the electron's spin "sees" a positively charged nucleus orbiting around it, giving rise to an electric current and consequently a magnetic field produced by this current

$$H_{SO} = \frac{e\hbar}{2m_e^2c^2}\boldsymbol{s}\cdot(\boldsymbol{p}\wedge\boldsymbol{\nabla}V) = \frac{e\hbar}{2m_e^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\boldsymbol{s}\cdot(\boldsymbol{p}\wedge\boldsymbol{r}) =$$

$$= -\frac{e\hbar^2}{2m_e^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\boldsymbol{s}\cdot\boldsymbol{l} = \xi_{nl}(r)\boldsymbol{s}\cdot\boldsymbol{l}$$

$$\zeta_{nl} = \int_0^\infty R_{nl}(r)\xi_{nl}(r)R_{nl}^*(r)r^2dr$$

Z increases $\Rightarrow V(r)$ increases $\Rightarrow \zeta_{nl}$ increases



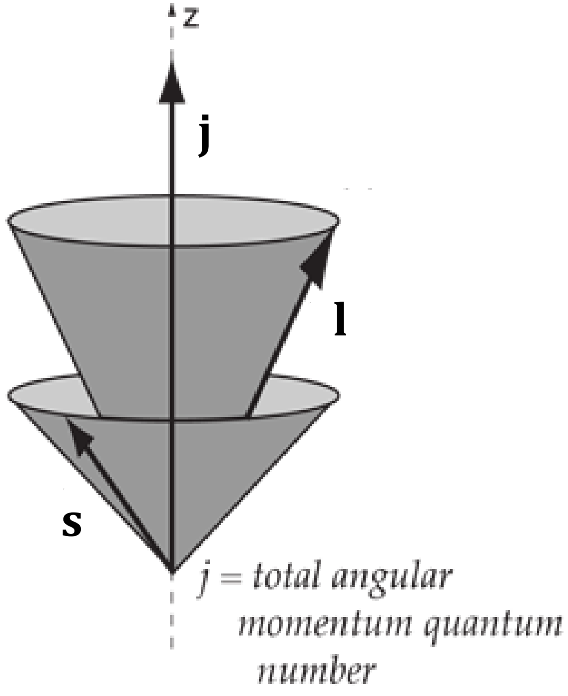
Still only one electron but ***l*** and ***s*** are coupled

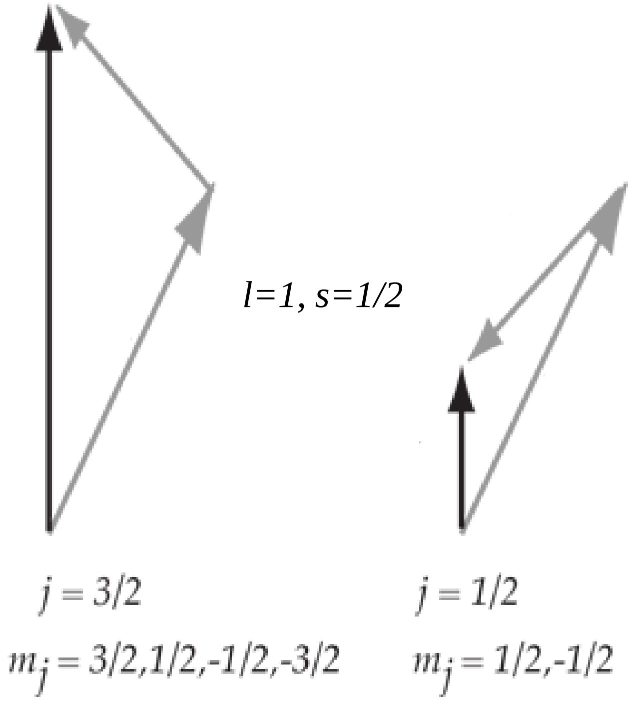
$|l, s, l_z, s_z> \Rightarrow |l, s, j, j_z>$

Total angular moment: $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$

$|\boldsymbol{j}| = \sqrt{j(j+1)}\hbar, \qquad j_z = m_j\hbar$

$j = |l-s|, \ldots, l+s; \quad m_j = j, \ldots -j$





Total angular magnetic moment: $\boldsymbol{\mu}_j = -g_j \frac{\mu_B}{\hbar}\boldsymbol{j}$

Total angular magnetic moment along *z* : $\mu_{j_z} = -g_j \frac{\mu_B}{\hbar} j_z$

N.B.: the total angular magnetic moment is also $\boldsymbol{\mu}_j = -g_j \frac{\mu_B}{\hbar}\boldsymbol{j} \Leftrightarrow \boldsymbol{m}_{tot} = -\frac{\mu_B}{\hbar}(2\boldsymbol{s} + \boldsymbol{l})$

N.B.: g_j describes the fact that ***l*** and ***s*** are not parallel

Landé g-factor $\quad g_j = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$

Many-electron atoms

All the electrons interact with one another, analytical solution not possible
orbital approximation → electron configuration (n, l)
Pauli exclusion principle → max two electrons per orbital

$$H_{atom} = \sum_{i=1}^{Z} \left(\frac{p_i^2}{2me} + V(r_i)\right) + \sum_{i<j}^{Z} \frac{e^2}{|r_i - r_j|} + \sum_{i=1}^{Z} (\boldsymbol{l}_i \cdot \boldsymbol{s}_i)\, \xi_{nl}(r_i) + \mu_B(\boldsymbol{L} + 2\boldsymbol{S}) \cdot \boldsymbol{B} = H_C + V_{ee} + V_{so} + V_{Zeeman}$$

L and ***S*** coupled by SOC

$$H_{SO} = V_{SO} = \sum_i \xi_{nl}(r_i)\boldsymbol{l}_i \cdot \boldsymbol{s}_i = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

$$\lambda = \pm \frac{\zeta_{nl}}{2S}$$

$$\boldsymbol{S} = \sum_{i=1}^{Z} \boldsymbol{s}_i$$

$$\boldsymbol{L} = \sum_{i=1}^{Z} \boldsymbol{l}_i$$

Magnetic moment of one atom

$$\boldsymbol{m}_{at} = \boldsymbol{\mu}_S + \boldsymbol{\mu}_L = -\frac{\mu_B}{\hbar}(2\boldsymbol{S} + \boldsymbol{L}) = -g_J \frac{\mu_B}{\hbar}\boldsymbol{J}$$

$$m_{at_z} = -\frac{\mu_B}{\hbar}(2S_z + L_z) = -g_J \frac{\mu_B}{\hbar} J_z$$

Orbital magnetic moment: $\mu_{L_z} = -L_z \frac{\mu_B}{\hbar}$

Spin Magnetic moment: $\mu_{S_z} = -2\, S_z \frac{\mu_B}{\hbar}$

Atomic magnetic moment: $m_{at_z} = -\, g_J J_z \frac{\mu_B}{\hbar}$

Filling of open subshells in atoms

See exercise: 1.1

For the **ground state** it follows the **Hund's rules**

Hund's rules:

1) Total spin $\boldsymbol{S} = \sum_i \boldsymbol{s}_i$ maximized ($\Rightarrow S = M_S = S_z/\hbar$)

2) Total orbital momentum $\boldsymbol{L} = \sum_i \boldsymbol{l}_i$ maximized ($\Rightarrow L = M_L = L_z/\hbar$)

(1 and 2) ⟺ Coulomb repulsion V_{ee}

3) ***L*** and ***S*** couple parallel ($J=|L+S|$) if band more than half filled
L and ***S*** couple antiparallel ($J=|L-S|$) if band less than half filled

⟺ Spin-orbit interaction V_{SO}

$$H_{SO} = V_{SO} = \sum_i \xi_{nl}(r_i)\boldsymbol{s}_i \cdot \boldsymbol{l}_i = \lambda \boldsymbol{L} \cdot \boldsymbol{S} \qquad \lambda = \pm \frac{\zeta_{nl}}{2S}$$

Ground state of Ti ([Ar] $4s^2\,3d^2$)

Y_l^m

	+2	+1	0	-1	-2
3d (l = 2)	↓	↓			
4s (l = 0)			↑↓		

$L = 3,\ S = 1,\ J = 2$

$\mu_L = -L\ \mu_B = -3\ \mu_B$,

$\mu_S = -2\,S\ \mu_B = -2\ \mu_B$,

$m_{at} = -g_J\,J\ \mu_B = -4/3\ \mu_B$

Magnetic moments in the ground state (!! forgetting $\hbar$!!)

Ground state of Fe ([Ar] $4s^2\,3d^6$)

	+2	+1	0	-1	-2
3d	↑↓	↑	↑	↑	↑
4s			↑↓		

$L = 2,\ S = 2,\ J = 4$

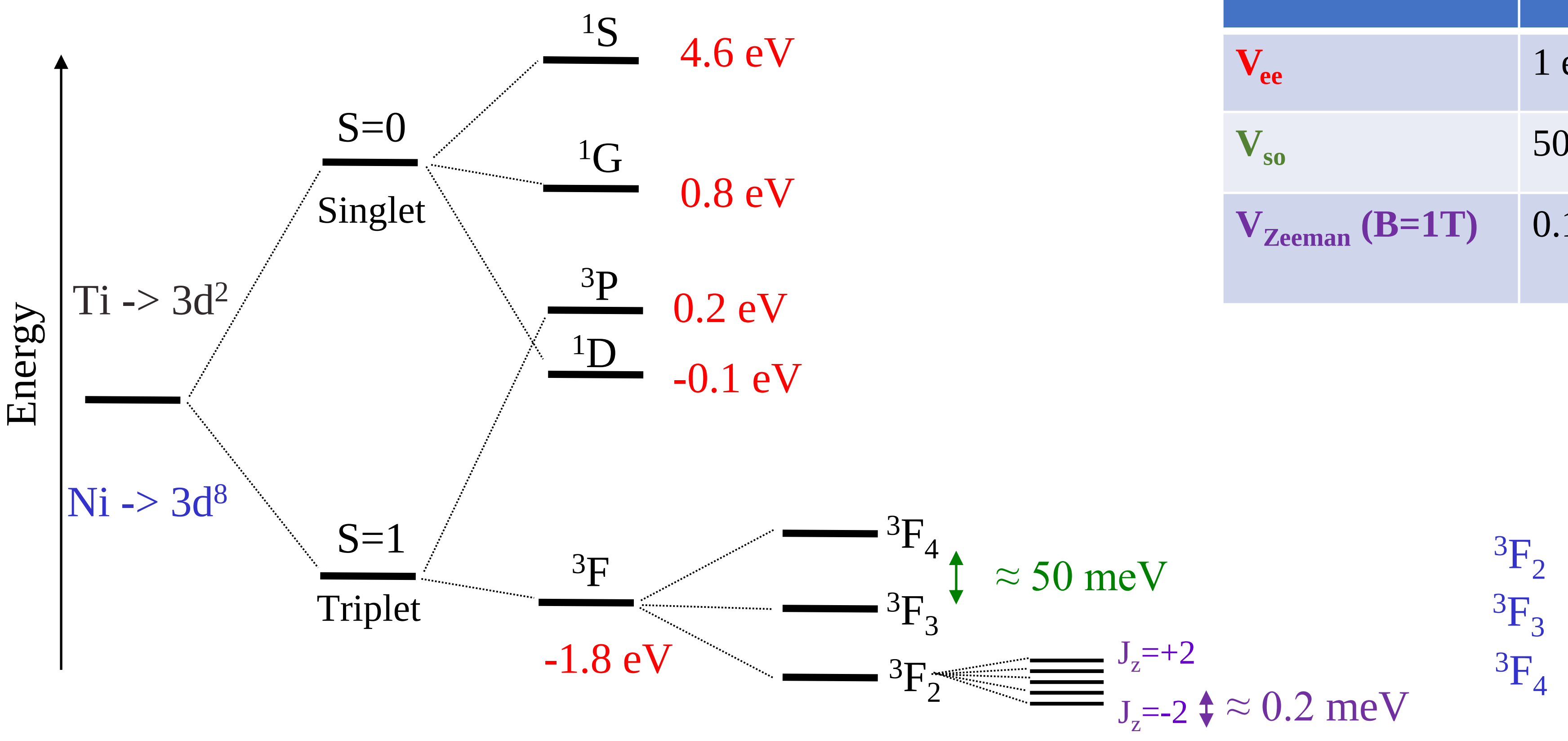
$\mu_L = -L\ \mu_B = -2\ \mu_B$,

$\mu_S = -2\,S\ \mu_B = -4\ \mu_B$,

$m_{at} = -g_J\,J\ \mu_B = -6\ \mu_B$

Energy spectrum of an isolated 3d atom

See exercises: 1.2 & 1.4



interaction term	3d transition metals	4f rare earths
V_{ee}	1 eV	1eV
V_{so}	50-100 meV	300-500 meV
V_{Zeeman} (B=1T)	0.1 -0.2 meV	0.1 -0.6 meV

$$V_{ee} = \sum_{i<j}^{Z} \frac{e^2}{|r_i - r_j|}$$

$$V_{SO} = \sum_{i=1}^{Z} (\boldsymbol{l}_i \cdot \boldsymbol{s}_i)\xi(r_i)$$

$$V_{Zee} = \mu_B(\boldsymbol{L} + 2\boldsymbol{S}) \cdot \boldsymbol{B}$$

Hund's rules ➡ max. S — max. L — min. J (band less than half filled) — max. J (band more than half filled)

Spectroscopic notation of multiplets terms: $^{2S+1}X_J$ with X= S, P, D, F, G, H, I, … for L = 0, 1, 2, 3, 4, 5, 6, …

See exercise: 1.3

$$H_{SO} = -\frac{e\hbar^2}{2m_e^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\boldsymbol{s}\cdot\boldsymbol{l} = \xi_{nl}(r)\boldsymbol{s}\cdot\boldsymbol{l}$$

$$\Psi_{nlm\sigma} = R_{nl}(r)Y_l^m\sigma$$

To calculate H_{SO} we need to move from vectors $(\boldsymbol{s}, \boldsymbol{l})$ to operators $(\hat{\boldsymbol{s}}, \hat{\boldsymbol{l}})$

$$\Delta E_{SO} = \sum_i^{occ}\langle\Psi_{nlm\sigma}|H_{SO}|\Psi_{nlm\sigma}\rangle = \sum_i^{occ}\langle R_{nl}|\xi_{nl}(r)|R_{nl}\rangle\langle Y_l^{m_i}\sigma_i|\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{s}}|Y_l^{m_i}\sigma_i\rangle = \zeta_{nl}\sum_i^{occ}\left\langle Y_l^{m_i}\sigma_i\middle|l_z s_z + \frac{1}{2}(l_+s_- + l_-s_+)\middle|Y_l^{m_i}\sigma_i\right\rangle$$

for simplicity we will use the same symbol for vectors and operators

Empirical formula: $\Delta E_{SO} = \lambda\boldsymbol{L}\cdot\boldsymbol{S} = \frac{\lambda}{2}[J(J+1) - L(L+1) - S(S+1)]$

$\lambda = \pm\frac{\zeta_{nl}}{2S}$ + (-) for shell less (more) than half filled

Ladder operator:

$$\hat{l}_\pm|Y_l^m\rangle = \hat{l}_\pm|l,m\rangle = $$
$$= l_\pm|Y_l^m\rangle = \sqrt{l(l+1) - m(m\pm1)}\,|l,m\pm1\rangle$$

Atom magnetic moment in real conditions

Atom described by quantum numbers $|LSJJ_z\rangle$, with J_z assuming $2J+1$ values between $-J$ and $+J$

At B = 0 T these $2J+1$ values are degenerate in energy
At $B \neq 0$ T the $2J+1$ states are split -> Zeeman split

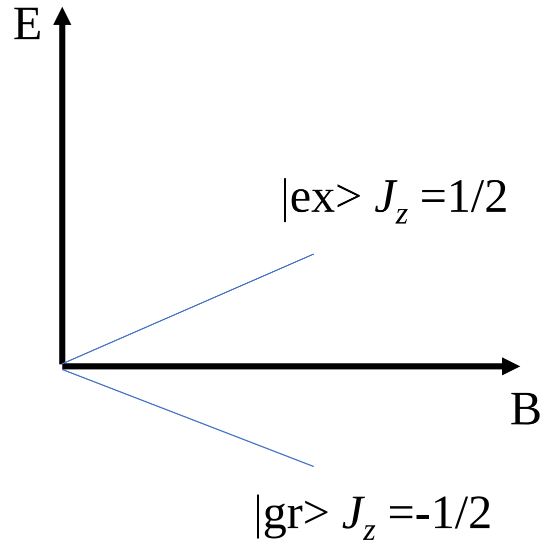
State occupation depends on B and T (Boltzmann statistic)

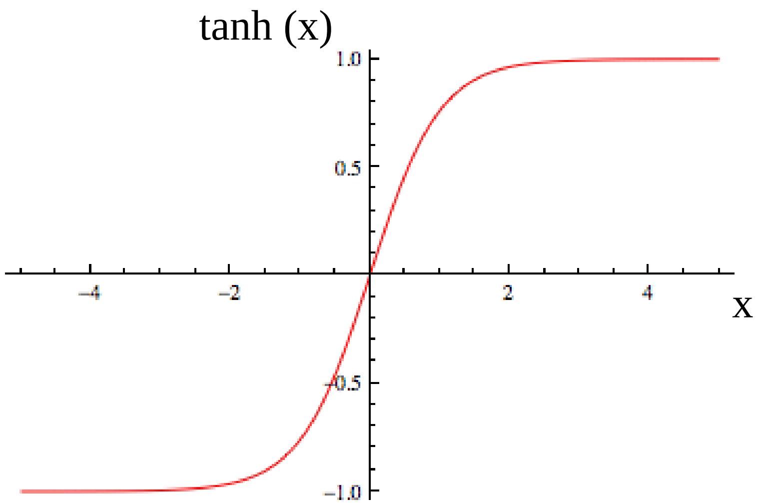
Example: atom with J = 1/2

two energy levels: $\pm J_z\, g_J\, m_B B$
occupation probability: $exp(\pm J_z\, g_J\, m_B B/k_B T)$

$$m_{at}(B,T) = m^{\uparrow} - m_{\downarrow} = J_z g_J \mu_B \left(\frac{e^x}{e^x + e^{-x}} - \frac{e^{-x}}{e^x + e^{-x}}\right) = J_z g_J \mu_B\, tanh(x) \qquad x = \frac{J_z g_J \mu_B B}{k_B T}$$

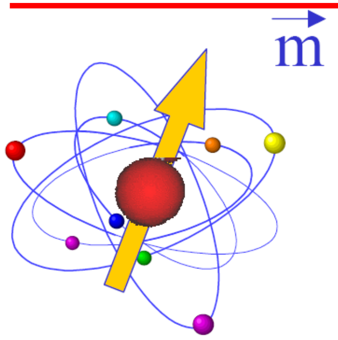
$$m_{at}(B,T) = \mu_B \tanh\left(\frac{\mu_B B}{k_B T}\right) \qquad with\ J_z = \frac{1}{2} \quad and \quad g_J = g = 2$$



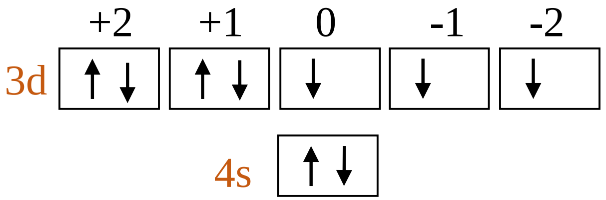


	tanh(x)	Occupation gr	Occupation ex
T = 0 or B = ∞	1	100%	0%
B = 0 or T = ∞	0	50%	50%
$B = 0.55\ k_B T/\mu_B$	0.5	75%	25%

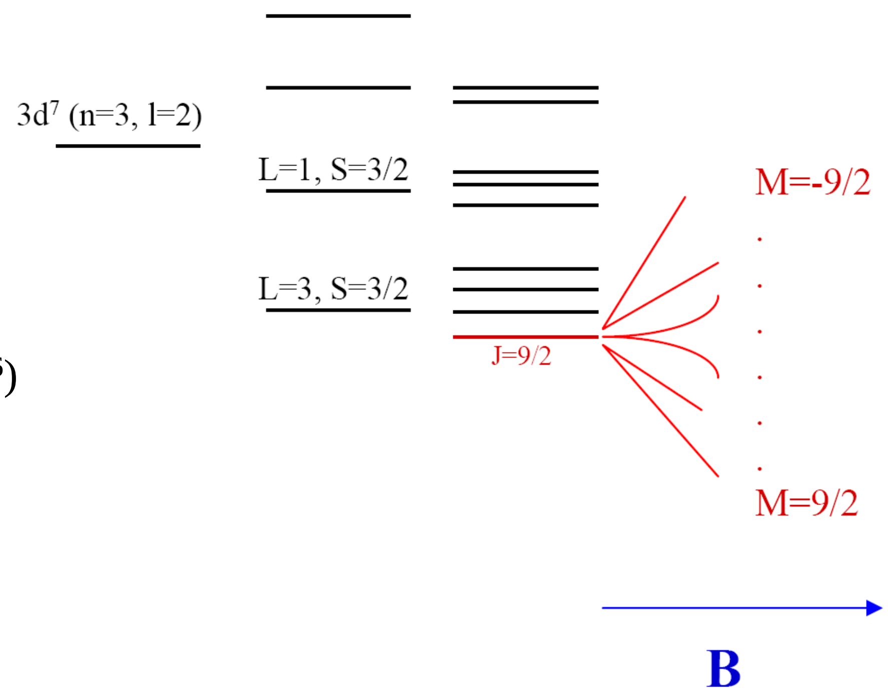
$m_{at}(B,T)$: Brillouin function



Ground state of Co ([Ar] $4s^2$ $3d^6$)



$L = 3, S = 3/2, J = 9/2$



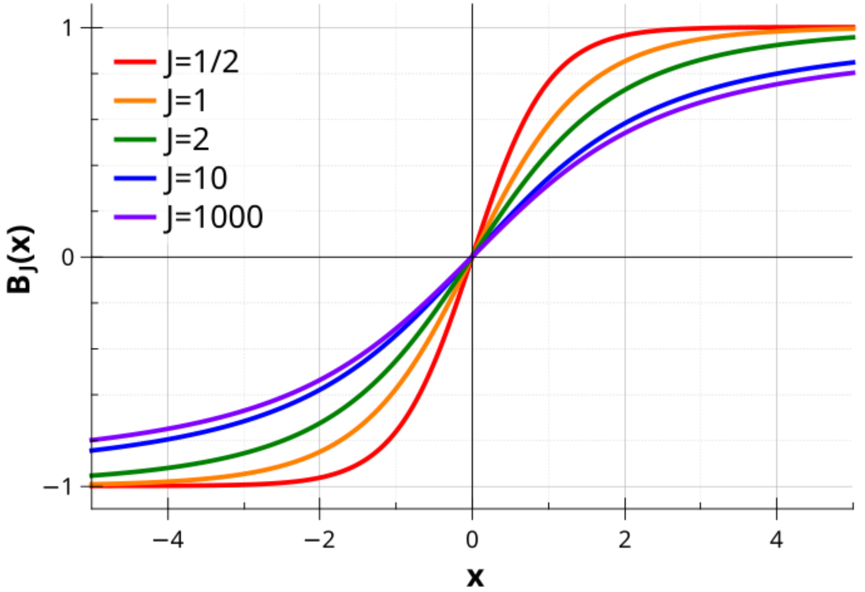
$$E = -\boldsymbol{m}_{at} \cdot \boldsymbol{B} = \frac{\mu_B}{\hbar} g_J J_z B = \mu_B g_J M B$$

$$m_{at} = \frac{1}{Z} \sum_{M=-J}^{J} \mu_B g_J M \, e^{\frac{-\mu_B g_J M B}{k_B T}} = \mu_B g_J J B(x) \qquad x = J\frac{\mu_B g_J B}{k_B T}$$

$$Z = \sum_{M=-J}^{J} e^{\frac{-\mu_B g_J M B}{k_B T}}$$

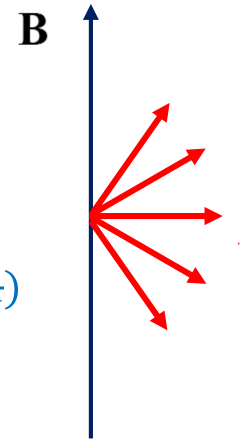
$$B(x) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J} x\right) - \frac{1}{2J} \coth\left(\frac{x}{2J}\right)$$

Brillouin function



Magnetic moment: quantum *vs.* classic description

quantum



$$m_{at}(B,T) = \mu_B g_J J B(x) \quad x = J\frac{\mu_B g_J B}{k_B T}$$

$$B(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{x}{2J}\right)$$

Brillouin function

$$E = -\boldsymbol{m}_{at}\cdot\boldsymbol{B} = \mu_B g_J J_z B$$

classic

$$m_{at}(B,T) = \mu\frac{\int_0^{2\pi} d\vartheta \int_0^{\pi} d\phi \sin\phi\cos\vartheta \;\, e^{-\frac{E}{k_B T}}}{\int_0^{2\pi} d\vartheta \int_0^{\pi} d\phi \sin\phi \;\, e^{-\frac{E}{k_B T}}}$$

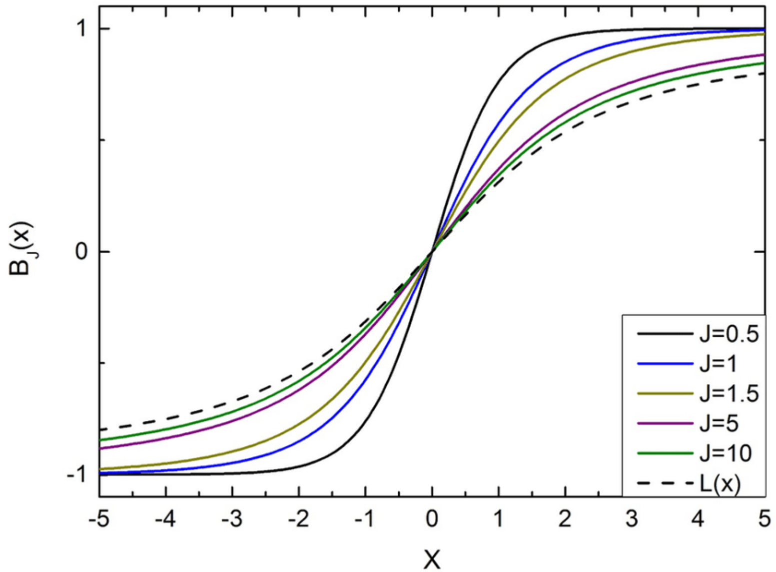
$$= \mu L\left(\frac{mB}{k_B T}\right)$$

$$L(x) = \coth x - \frac{1}{x}$$

Langevin function

$$E = -\boldsymbol{\mu}\cdot\boldsymbol{B} = \mu B\cos\theta$$

$$\chi = \frac{\partial m_{at}}{\partial B} = \frac{\left(\mu_B g_J\sqrt{J(J+1)}\,\right)^2}{3k_B T}$$



$$\chi = \frac{\partial m_{at}}{\partial B} = \frac{\mu^2}{3k_B T}$$