Magnetism to Spintronics

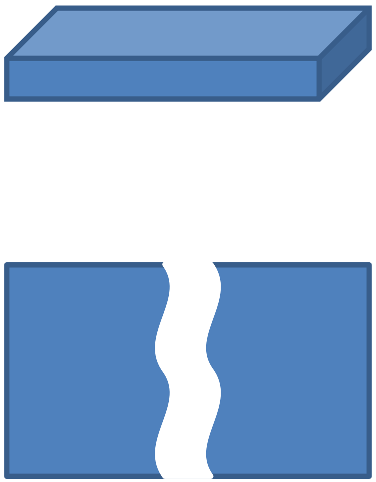
Introduction to Solid State Physics
Kittel 8th ed
Chap. 11-13

&

Condensed Matter Physics
Marder 2nd ed
Chap. 24-26

Magnetism -1

Why do most broken permanent magnets repel each other?



Cooperative phenomena

- Elementary excitations in solids describe the response of a solid to a perturbation
  - Quasiparticles

    usually fermions, resemble the particles that make the system, e.g. quasi-electrons
  - Collective excitations

    usually bosons, describe collective motions

    use second quantization with Fermi-Dirac or Bose-Einstein statistics

Magnetism

- the Bohr–van Leeuwen theorem

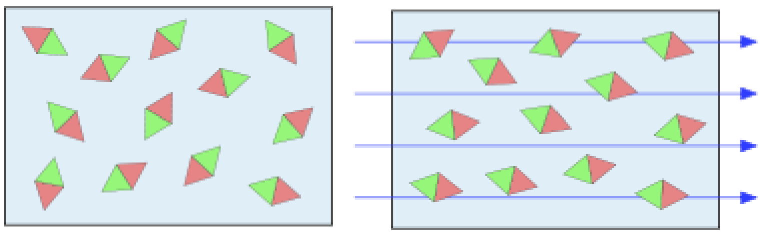
  when statistical mechanics and classical mechanics are applied consistently, the thermal average of the magnetization is always zero.
- Magnetism in solids is solely a quantum mechanical effect
- Origin of the magnetic moment:
  - Electron spin $\vec{S}$
  - Electron orbital momentum $\vec{L}$
- From (macroscopic) response to external magnetic field $\vec{H}$
  - Diamagnetism $\chi < 0$, $\chi \sim 1 \times 10^{-6}$, insensitive to temperature
  - Paramagnetism $\chi > 0$, $\chi = \frac{C}{T}$ Curie law

    $\chi = \frac{C}{T+\Delta}$ Curie-Weiss law
  - Ferromagnetism exchange interaction (quantum)

Magnetism

巨觀： 順磁性

Paramagnetism

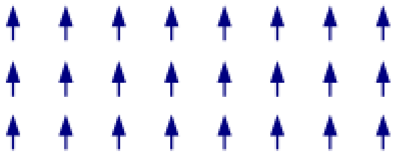


逆磁性

diamagnetism

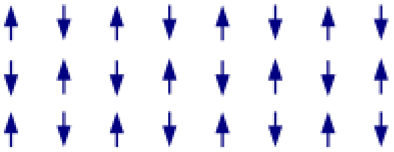
微觀： 鐵磁性

Ferromagnetism



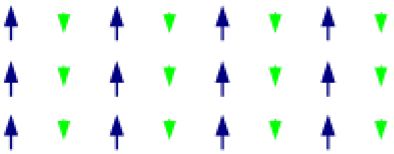
反鐵磁性

Antiferromagnetism

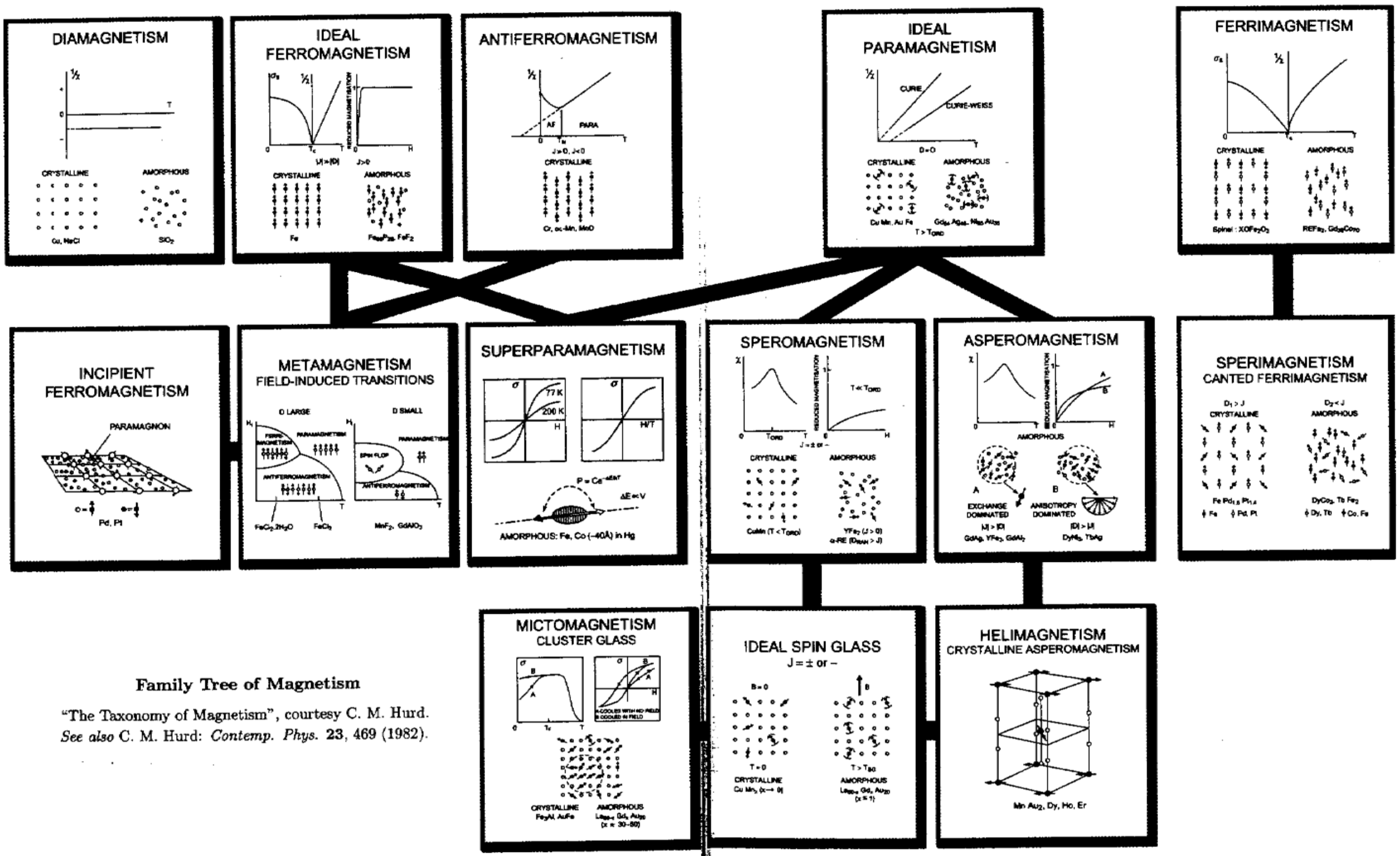


亞鐵磁性

Ferrimagnetism



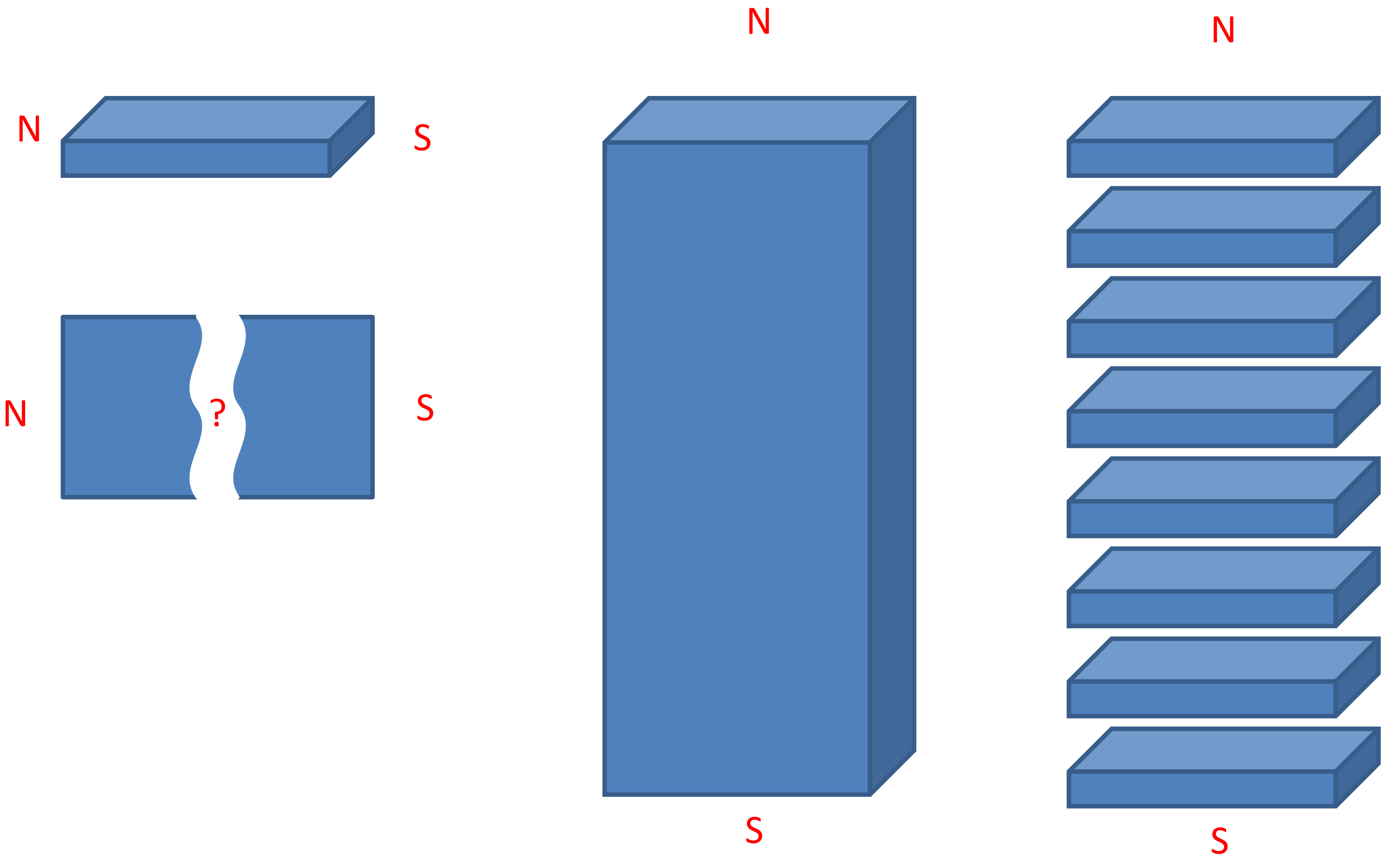
Family Tree of Magnetism



Family Tree of Magnetism

"The Taxonomy of Magnetism", courtesy C. M. Hurd. *See also* C. M. Hurd: *Contemp. Phys.* **23**, 469 (1982).

Why do most broken permanent magnets repel each other?



- Classical and quantum theory for diamagnetism
  - Calculate $\langle r^2 \rangle$
- Classical and quantum theory for paramagnetism
  - Superparamagnetism, Langevin function
  - Hund's rules
  - Magnetic state ${}^{2S+1}L_J$
  - Crystal field
  - Quenching of orbital angular momentum L_z
    - **Angular momentum operator**
    - **Spherical harmonics**
  - Jahn-Teller effect
  - Paramagnetic susceptibility of conduction electrons

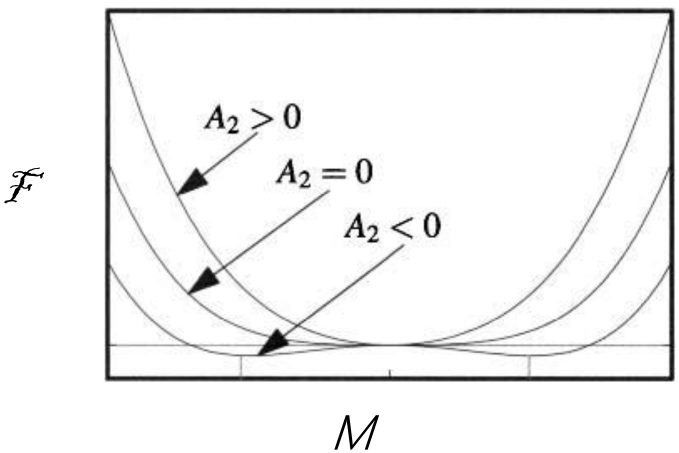
- *Ferromagnetism*
  - Microscopic – ferro, antiferro, ferri magnetism
  - Exchange interaction
  - Exchange splitting – source of magnetization

    two-electron system spin-independent Schrodinger equation
  - Type of exchange: direct exchange, super exchange, indirect exchange, itinerant exchange
  - Spin Hamiltonian and Heisenberg model
  - Molecular-field (mean-field) approximation

Critical phenomena

- Universality: Divergences near the critical point are identical in a variety of apparently different physical systems and also in a collection of simple models.
- **Scaling:** The key to understand the critical point lies in understanding the relationship between systems of different sizes. Formal development of this idea led to the *renormalization group* of Wilson (1975).

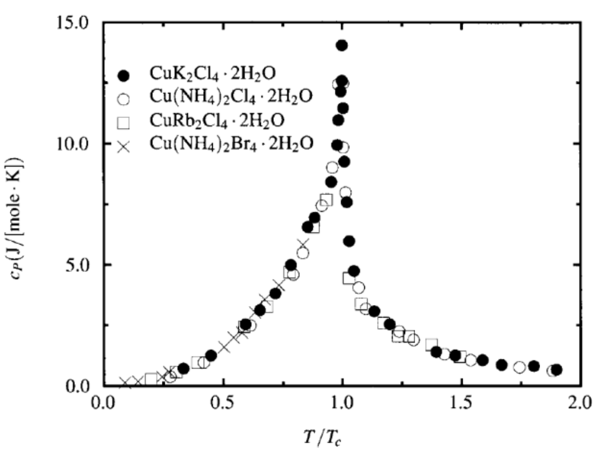
Landau Free Energy



$$F(M, T) = A_0(T) + A_2(T)M^2 + A_4(T)M^4 + HM$$

$$t \equiv \frac{T - T_C}{T_C}$$

$$F = a_2 t M^2 + a_4 M^4 + HM$$



Molar heat capacities of four ferromagnetic copper salts versus scaled temperature T/T_c. [Source Jongh and Miedema (1974).]

Correspondence between Liquids and Magnets

- ***Specific Heat*— α**
- ***Magnetization and Density*— β**
- ***Compressibility and** Susceptibility*— γ
- ***Critical Isotherm*— δ**
- ***Correlation Length* — ν**
- ***Power-Law Decay at Critical Point*— η**

Summary of critical exponents, showing correspondence between fluid-gas systems, magnetic systems, and the three-dimensional Ising model.

Exponent	Fluid	Magnet	Mean Field Theory	Experiment	3d Ising
α	$C_V \sim \|t\|^{-\alpha}$	$C_V \sim \|t\|^{-\alpha}$	discontinuity	0.11–0.12	0.110
β	$\Delta n \sim \|t\|^{\beta}$	$M \sim \|t\|^{\beta}$	$\frac{1}{2}$	0.35–0.37	0.325
γ	$K_T \sim \|t\|^{-\gamma}$	$\chi \sim \|t\|^{-\gamma}$	1	1.21–1.35	1.241
δ	$P \sim \|\Delta n\|^{\delta}$	$\|H\| \sim \|M\|^{\delta}$	3	4.0–4.6	4.82
ν	$\xi \sim \|t\|^{-\nu}$	$\xi \sim \|t\|^{-\nu}$		0.61–0.64	0.63
η	$g(r) \sim r^{-1-\eta}$	$g(r) \sim r^{-1-\eta}$		0.02–0.06	0.032

Source: Vicentini-Missoni (1972) p. 67, Cummins (1971), p. 417, and Goldenfeld (1992) p. 384.

Relations Among Exponents

$$\alpha + 2\beta + \gamma = 2 \qquad (2-\eta)\nu = \gamma$$

$$\delta = 1 + \frac{\gamma}{\beta} \qquad 2 - \alpha = 3\nu$$

- # Stoner band ferromagnetism

Teodorescu, C. M.; Lungu, G. A. (November 2008). "Band ferromagnetism in systems of variable dimensionality", *Journal of Optoelectronics and Advanced Materials* **10** (11), 3058–3068.

$$\mathcal{E} = \int_0^{\mathcal{E}_F - \Delta} d\mathcal{E}' \, D(\mathcal{E}')\mathcal{E}' + \frac{1}{2} \int_{\mathcal{E}_F - \Delta}^{\mathcal{E}_F + \Delta} d\mathcal{E}' \, D(\mathcal{E}')\mathcal{E}' - \frac{1}{2} nJ \, \langle S \rangle^2$$

$$\langle S \rangle = \frac{1}{2n} \int_{\mathcal{E}_F - \Delta}^{\mathcal{E}_F + \Delta} d\mathcal{E}' \, \frac{1}{2} D(\mathcal{E}') = \frac{1}{2n} D(\mathcal{E}_F)\Delta$$

$$\left.\frac{\partial \mathcal{E}}{\partial \Delta}\right|_{\mathcal{E}_F} = \Delta D(\mathcal{E}_F) - \frac{J}{4n} D(\mathcal{E}_F)^2 \Delta$$

$$\left.\frac{\partial \mathcal{E}}{\partial \Delta}\right|_{\mathcal{E}_F} = 0 \Rightarrow \frac{J}{n} D(\mathcal{E}_F) = 4$$

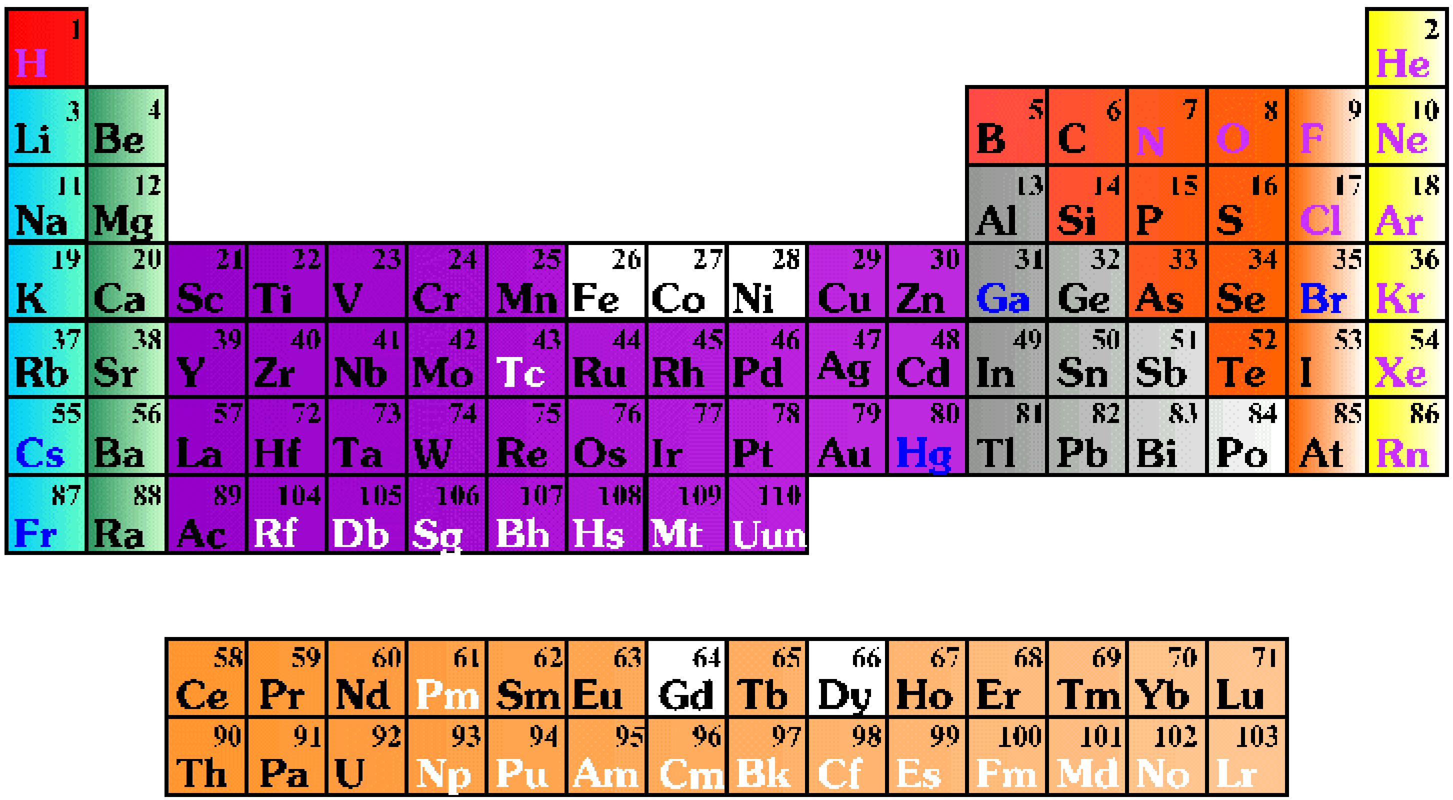
--Ferromagnetic elements: such as 鐵 Fe, 鈷 Co, 鎳 Ni,

釓 Gd, 鏑 Dy; 錳 Mn, 鈀 Pd ??

--Some elements with ferromagnetic properties

合金, alloys,

錳氧化物 MnOx, ……



Platonic solid

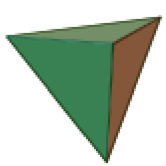
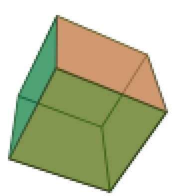
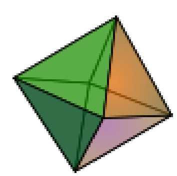
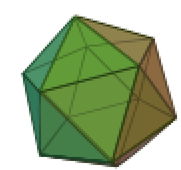
From Wikipedia

In geometry, a Platonic solid is a convex polyhedron that is regular, in the sense of a regular polygon. Specifically, the faces of a Platonic solid are congruent regular polygons, with the same number of faces meeting at each vertex; thus, all its edges are congruent, as are its vertices and angles.

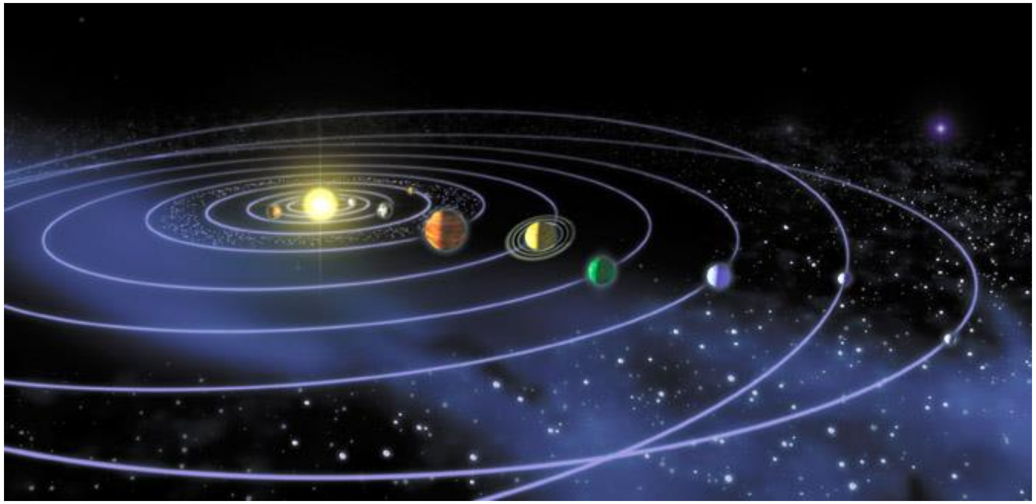
There are precisely five Platonic solids (shown below):

The name of each figure is derived from its number of faces: respectively 4, 6, 8, 12, and 20.

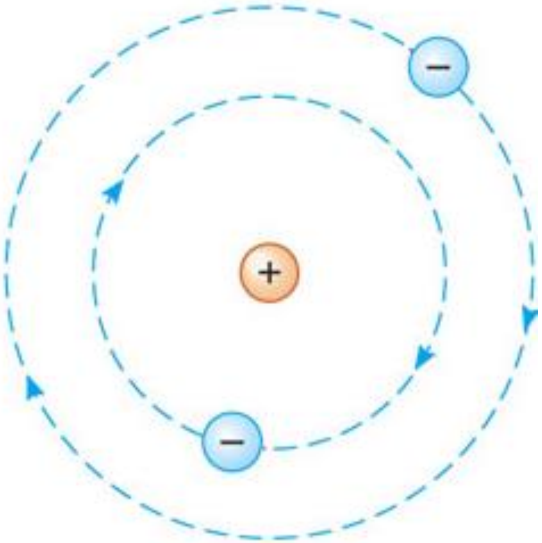
The aesthetic beauty and symmetry of the Platonic solids have made them a favorite subject of geometers for thousands of years. They are named for the ancient Greek philosopher Plato who theorized that the classical elements were constructed from the regular solids.

 Tetrahedron	 Cube hexahedron	 Octahedron	 Dodecahedron	 Icosahedron

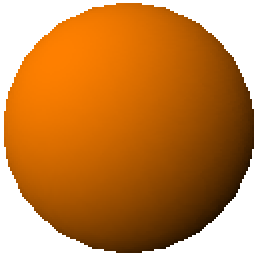
Solar system

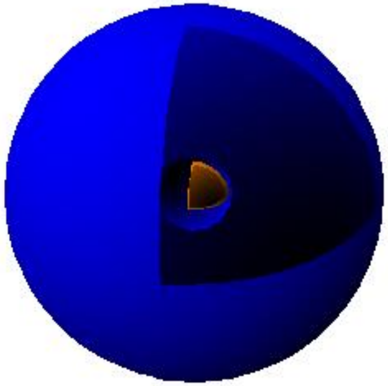


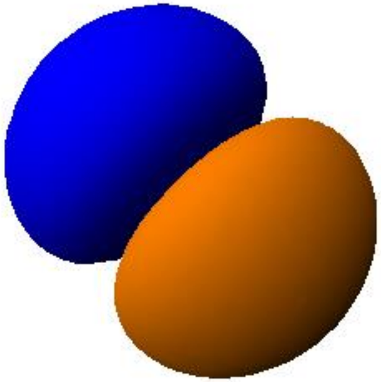
Electronic orbit



s, p electron orbits



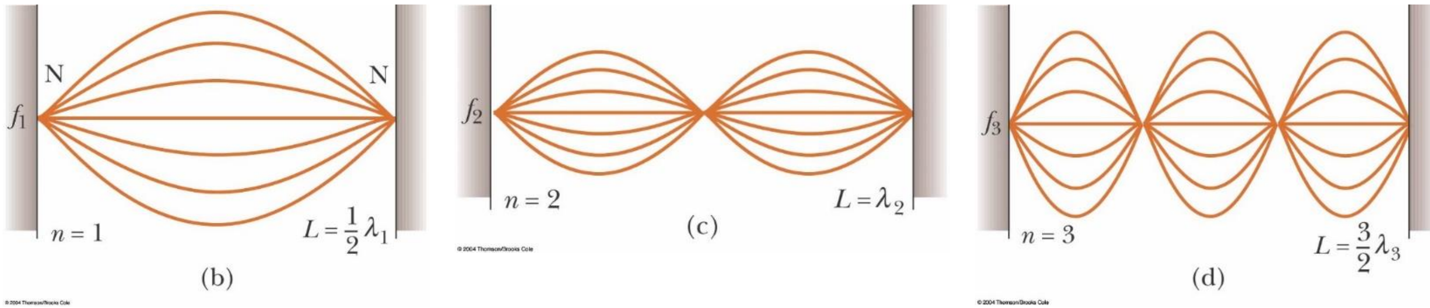




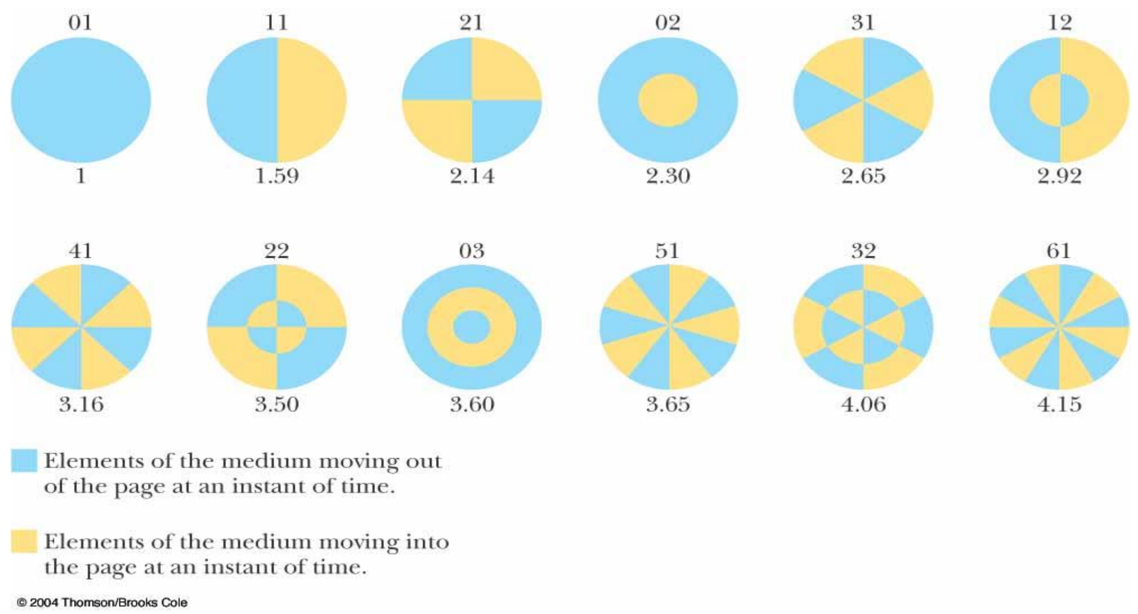
Orbital viewer

Resonance

One-dimensional



Two-dimensional



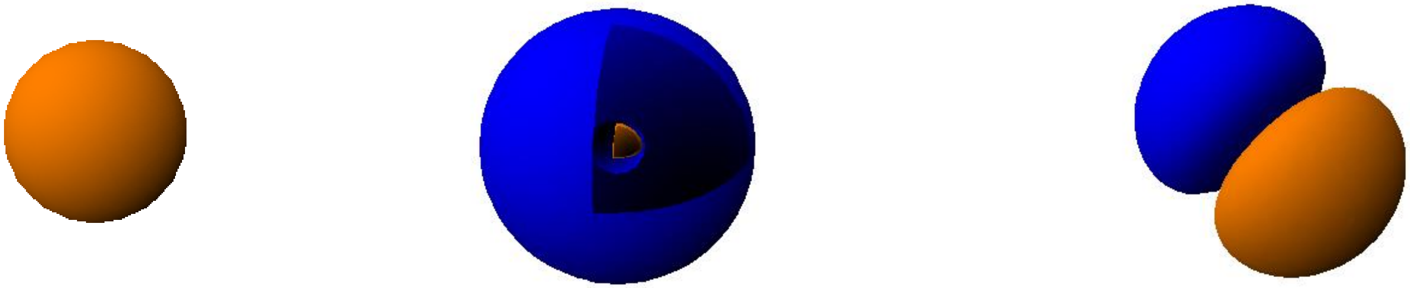
Three-dimensional

Hydrogen atom

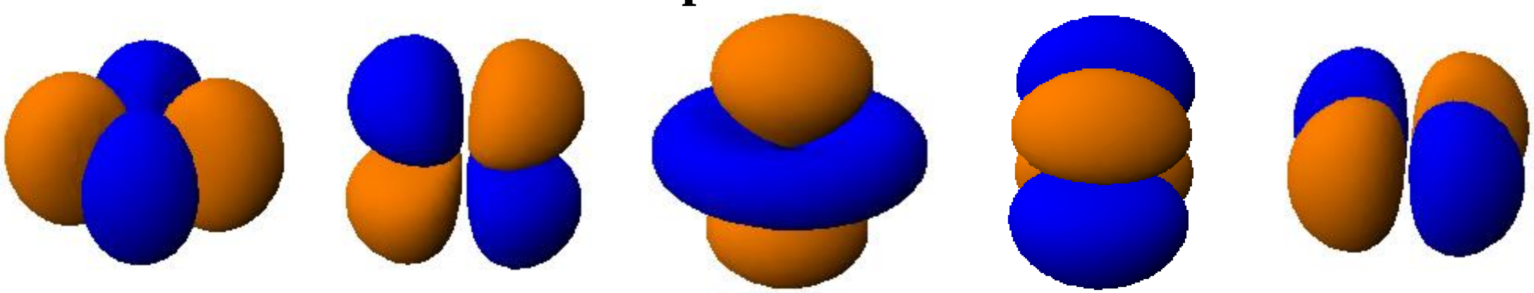
3d transition metals:

Mn atom has 5 d↑ electrons, Bulk Mn is NOT magnetic.

s, p electron orbital

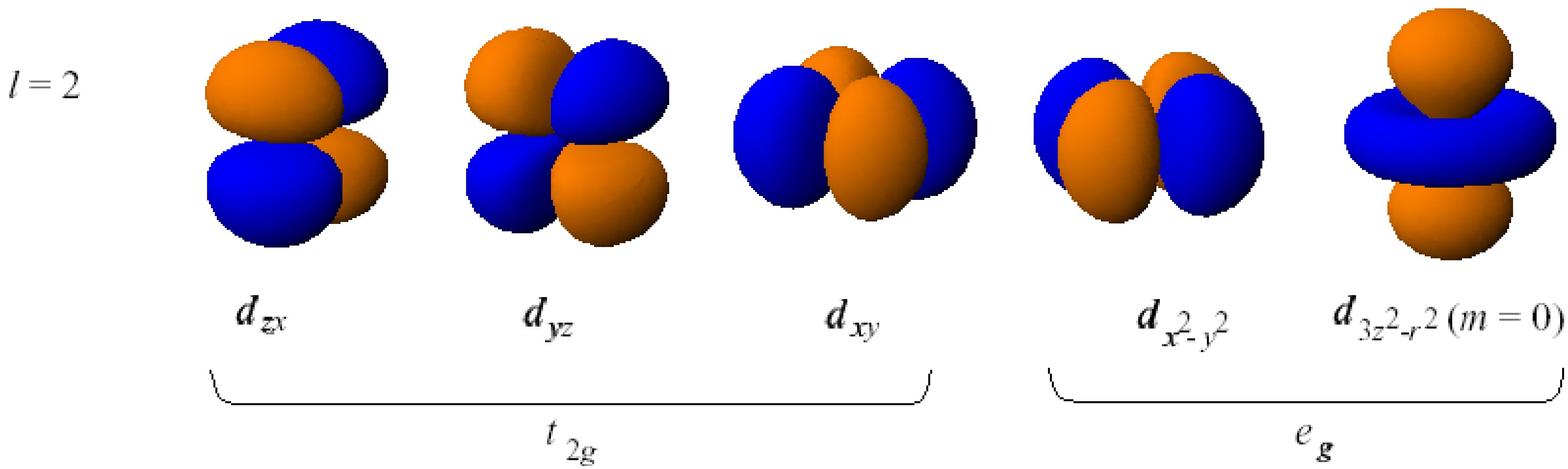


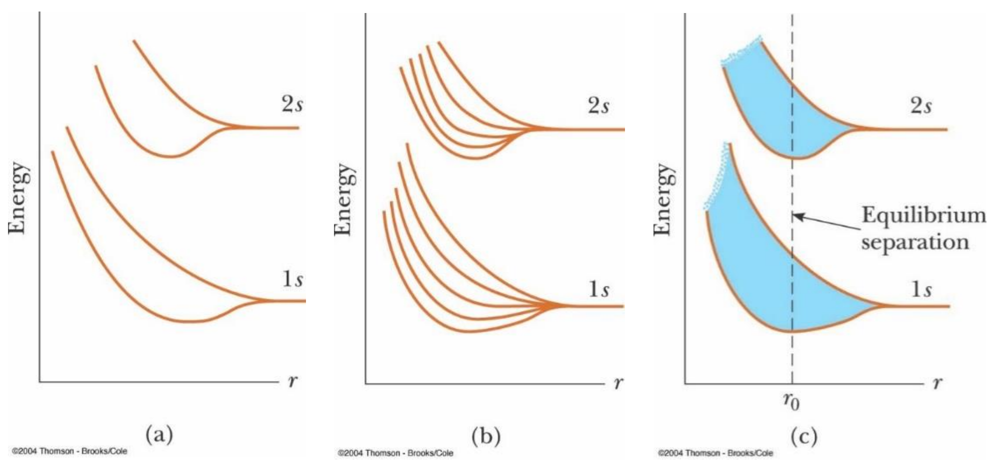
3d electron distribution in real space



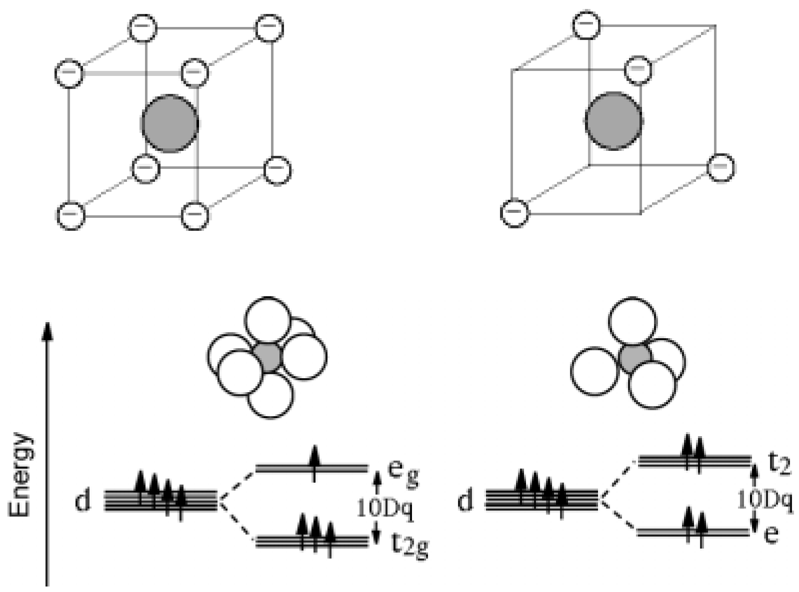
Co atom has 5d↑ electrons and 2d↓ electrons
Bulk Co is magnetic.

d orbitals

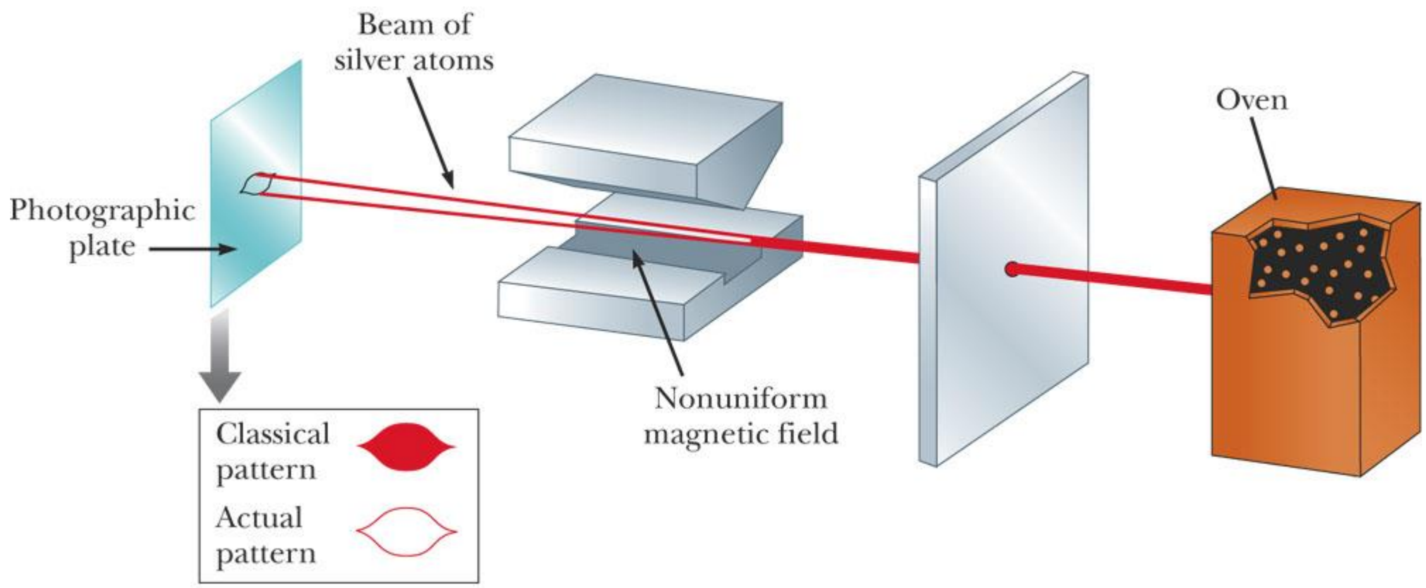


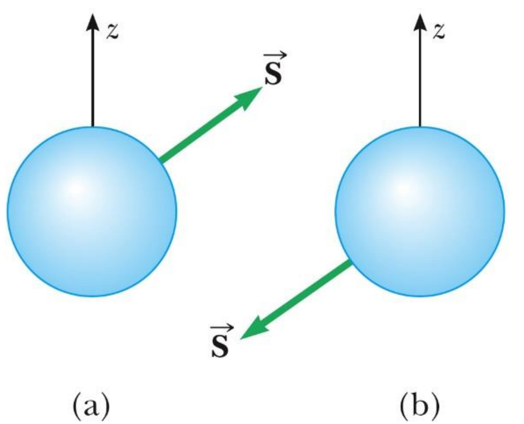


Crystal-field splitting



Stern-Gerlach Experiment

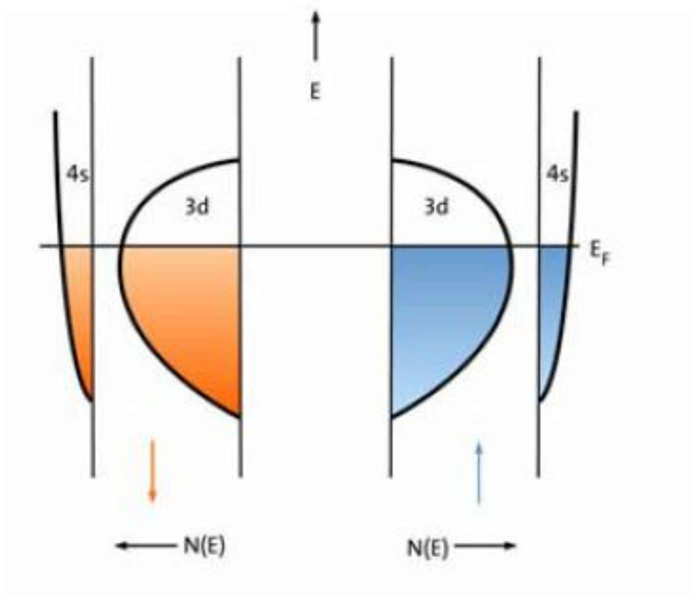




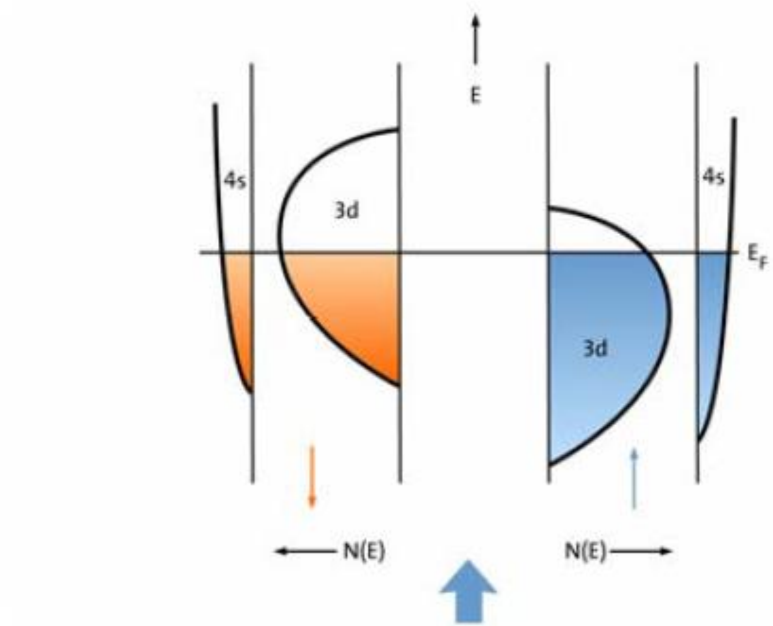
There are two kinds of electrons:
spin-up and spin-down.

Stoner criterion for ferromagnetism

I $N(E_F) > 1$, I is the **Stoner exchange parameter** and $N(E_F)$ is the density of states at the Fermi energy.



For the non-magnetic state there are identical density of states for the two spins.



For a ferromagnetic state, N↑ > N↓. The polarization is indicated by the thick blue arrow.

Schematic plot for the energy band structure of 3d transition metals.

Teodorescu and Lungu, "Band ferromagnetism in systems of variable dimensionality". *J Optoelectronics and Adv. Mat.* **10,** 3058–3068 (2008).

Exchange interaction

https://en.wikipedia.org/wiki/Exchange_interaction

Exchange interaction - Wi...

Русский
Українська
Tiếng Việt
Edit links

Exchange Interactions between localized electron magnetic moments [edit]

Quantum mechanical particles are classified as bosons or fermions. The spin–statistics theorem of quantum field theory demands that all particles with half-integer spin behave as fermions and all particles with integer spin behave as bosons. Multiple bosons may occupy the same quantum state; by the Pauli exclusion principle, however, no two fermions can occupy the same state. Since electrons have spin 1/2, they are fermions. This means that the overall wave function of a system must be antisymmetric when two electrons are exchanged, i.e. interchanged with respect to both spatial and spin coordinates. First, however, exchange will be explained with the neglect of spin.

Exchange of spatial coordinates [edit]

Taking a hydrogen molecule-like system (i.e. one with two electrons), we may attempt to model the state of each electron by first assuming the electrons behave independently, and taking wave functions in position space of $\Phi_a(r_1)$ for the first electron and $\Phi_b(r_2)$ for the second electron. We assume that Φ_a and Φ_b are orthogonal, and that each corresponds to an energy eigenstate of its electron. Now, we may construct a wave function for the overall system in position space by using an antisymmetric combination of the product wave functions in position space:

$$\Psi_A(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}[\Phi_a(\vec{r}_1)\Phi_b(\vec{r}_2) - \Phi_b(\vec{r}_1)\Phi_a(\vec{r}_2)] \qquad (1)$$

Alternatively, we may also construct the overall position–space wave function by using a symmetric combination of the product wave functions in position space:

$$\Psi_S(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}[\Phi_a(\vec{r}_1)\Phi_b(\vec{r}_2) + \Phi_b(\vec{r}_1)\Phi_a(\vec{r}_2)] \qquad (2)$$

Treating the exchange interaction in the hydrogen molecule by the perturbation method, the overall Hamiltonian is:

$\mathcal{H} = \mathcal{H}^{(0)} + \mathcal{H}^{(1)}$

where $\mathcal{H}^{(0)} = -\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{e^2}{r_1} - \frac{e^2}{r_2}$ and $\mathcal{H}^{(1)} = \left(\frac{e^2}{R_{ab}} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{b2}}\right)$

Two eigenvalues for the system energy are found:

$$E_{+/-} = E_{(0)} + \frac{C \pm J_{ex}}{1 \pm B^2} \qquad (3)$$

where the E_+ is the spatially symmetric solution and E_- is the spatially antisymmetric solution. A variational calculation yields similar results. $\mathcal{H}$ can be diagonalized by using the position–space functions given by Eqs. (1) and (2). In Eq. (3), C is the **Coulomb integral**, B is the **overlap integral**, and J_{ex} is the **exchange integral**. These integrals are given by:

$$C = \int \Phi_a(\vec{r}_1)^2 \left(\frac{1}{R_{ab}} + \frac{1}{r_{12}} - \frac{1}{r_{a1}} - \frac{1}{r_{b2}}\right) \Phi_b(\vec{r}_2)^2 \, d^3r_1 \, d^3r_2 \qquad (4)$$

$$B = \int \Phi_b(\vec{r}_2)\Phi_a(\vec{r}_2) \, d^3r_2 \qquad (5)$$

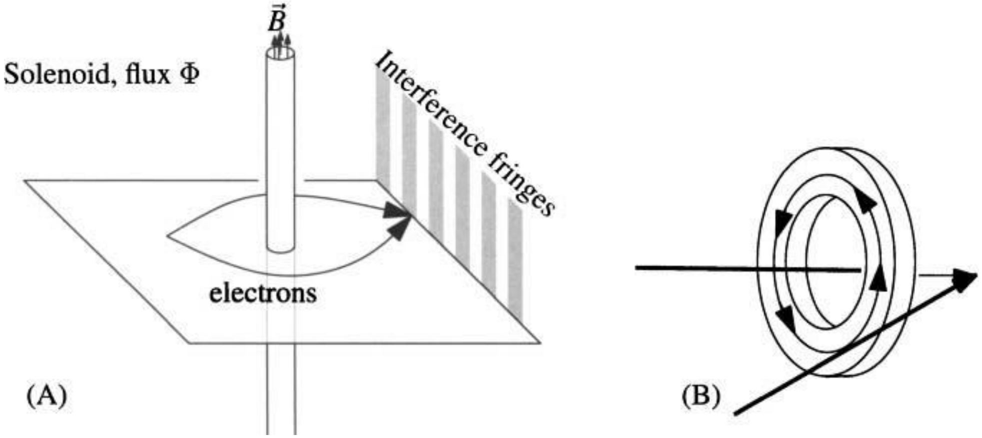
$$J_{ex} = \int \Phi_a(\vec{r}_1)\Phi_b(\vec{r}_2) \left(\frac{1}{R_{ab}} + \frac{1}{r_{12}} - \frac{1}{r_{a1}} - \frac{1}{r_{b2}}\right) \Phi_b(\vec{r}_1)\Phi_a(\vec{r}_2) \, d^3r_1 \, d^3r_2 \qquad (6)$$

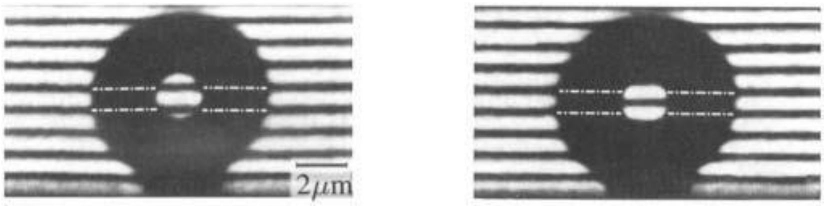
The terms in parentheses in Eqs. (4) and (6) correspond to: proton–proton repulsion (R_{ab}), electron–electron repulsion (r_{12}), and electron–proton attraction ($r_{a1/a2/b1/b2}$).All quantities are assumed to be real.

Although in the hydrogen molecule the exchange integral, Eq. (6), is negative, Heisenberg first suggested that it changes sign at some critical ratio of internuclear distance to

Berry Phase

Aharonov-Bohm Effect



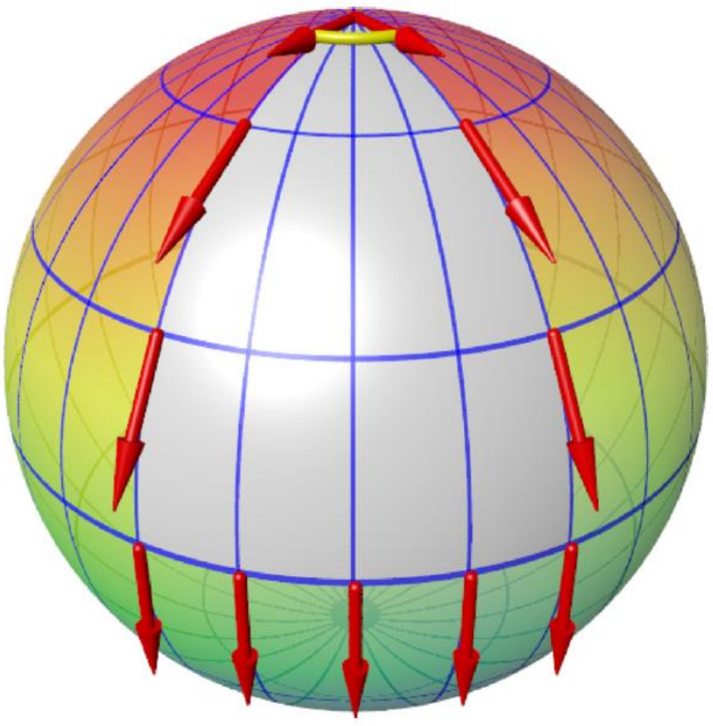


Electrons traveling around a flux tube suffer a phase change and can interfere with themselves even if they only travel through regions where B = 0.
(B) An open flux tube is not experimentally realizable, but a small toroidal magnet with no flux leakage can be constructed instead.

$$\Phi = \int d^2r\, B_z = \oint d\vec{r} \cdot \vec{A}$$

$$A_\phi = \frac{\Phi}{2\pi r}$$

Electron hologram showing interference fringes of electrons passing through small toroidal magnet. The magnetic flux passing through the torus is quantized so as to produce an integer multiple of π phase change in the electron wave functions. The electron is completely screened from the magnetic induction in the magnet. In (A) the phase change is 0, while in (B) the phase change is π. [Source: Tonomura (1993), p. 67.]



Parallel transport of a vector along a closed path on the sphere S2 leads to a geometric phase between initial and final state.

Real-space Berry phases: Skyrmion soccer (invited)
Karin Everschor-Sitte and Matthias Sitte
Journal of Applied Physics **115**, 172602 (2014); doi: 10.1063/1.4870695

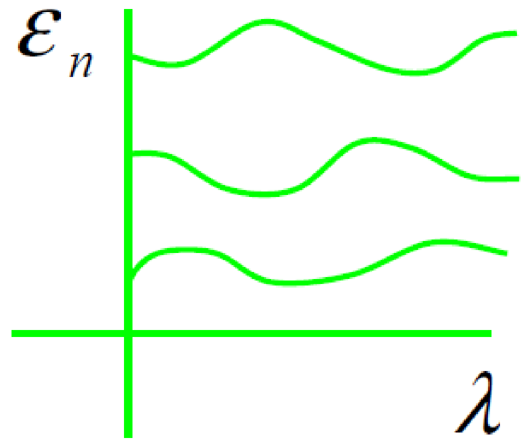
Berry phase formalism for intrinsic Hall effects

Berry phase
[Berry, Proc. Roy. Soc. London A 392, 451 (1984)]

From Prof. Guo Guang-Yu

Parameter dependent system:

$$\{ \varepsilon_n(\lambda), \psi_n(\lambda) \}$$

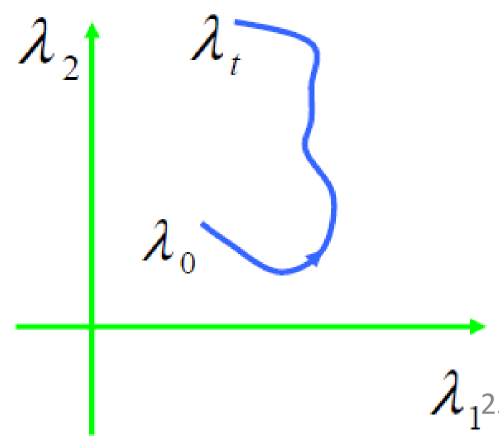


Adiabatic theorem:

$$\Psi(t) = \psi_n(\lambda(t))\; e^{-i\int_0^t dt\,\varepsilon_n/\hbar}\; e^{-i\gamma_n(t)}$$

Geometric phase:

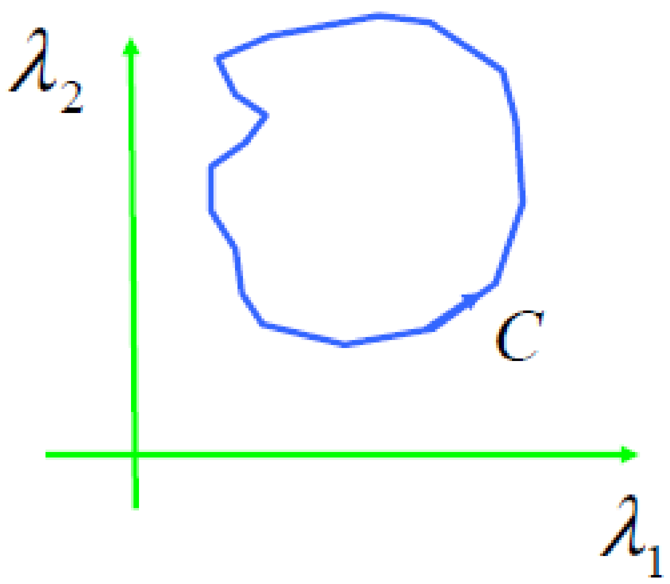
$$\gamma_n = \int_{\lambda_0}^{\lambda_t} d\lambda \left\langle \psi_n \middle| i\frac{\partial}{\partial\lambda} \middle| \psi_n \right\rangle$$



Well defined for a closed path

From Prof. Guo Guang-Yu

$$\gamma_n = \oint_C d\lambda \left\langle \psi_n \middle| i \frac{\partial}{\partial \lambda} \middle| \psi_n \right\rangle$$



Stokes theorem

$$\gamma_n = \iint d\lambda_1 d\lambda_2 \, \Omega$$

Berry Curvature

$$\Omega = i \frac{\partial}{\partial \lambda_1} \left\langle \psi \middle| \frac{\partial}{\partial \lambda_2} \middle| \psi \right\rangle - i \frac{\partial}{\partial \lambda_2} \left\langle \psi \middle| \frac{\partial}{\partial \lambda_1} \middle| \psi \right\rangle$$

Analogies

From Prof. Guo Guang-Yu

Berry curvature

$$\Omega(\vec{\lambda})$$

Magnetic field

$$B(\vec{r})$$

Berry connection

$$\langle \psi | i \frac{\partial}{\partial \lambda} | \psi \rangle$$

Vector potential

$$A(\vec{r})$$

Geometric phase

$$\oint d\lambda \, \langle \psi | i \frac{\partial}{\partial \lambda} | \psi \rangle = \iint d^2\lambda \;\; \Omega(\vec{\lambda})$$

Aharonov-Bohm phase

$$\oint dr \; A(\vec{r}) = \iint d^2 r \; B(\vec{r})$$

Chern number

$$\oiint d^2\lambda \;\; \Omega(\vec{\lambda}) = \text{integer}$$

Dirac monopole

$$\oiint d^2 r \;\; B(\vec{r}) = \text{integer } h/e$$

❑ Semiclassical dynamics of Bloch electrons

Old version [e.g., Aschroft, Mermin, 1976]

From Prof. Guo Guang-Yu

$$\dot{\mathbf{x}}_c = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}},$$

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\mathbf{E} - \frac{e}{\hbar}\dot{\mathbf{x}}_c \times \mathbf{B} = \frac{e}{\hbar}\frac{\partial \varphi(\mathbf{r})}{\partial \mathbf{r}} - \frac{e}{\hbar}\dot{\mathbf{x}}_c \times \mathbf{B}$$

❑ New version [Marder, 2000]

Berry phase correction [Chang & Niu, PRL (1995), PRB (1996)]

$$\dot{\mathbf{x}}_c = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}_n(\mathbf{k}),$$

$$\dot{\mathbf{k}} = \frac{e}{\hbar}\frac{\partial \varphi(\mathbf{r})}{\partial \mathbf{r}} - \frac{e}{\hbar}\dot{\mathbf{x}}_c \times \mathbf{B},$$

$$\mathbf{\Omega}_n(\mathbf{k}) = -\mathrm{Im}\left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right| \times \left| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle$$

(Berry curvature)

Demagnetization factor D

can be solved analytically in some cases, numerically in others

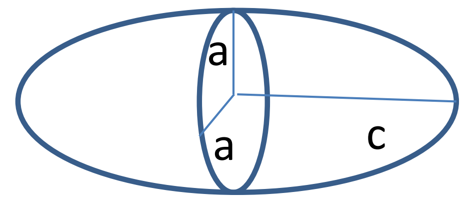
For an ellipsoid $D_x + D_y + D_z = 1$ (SI units) $D_x + D_y + D_z = 4\pi$ (cgs units)

Solution for Spheroid $a = b \neq c$

1. Prolate spheroid (football shape) $c/a = r > 1$; $a = b$, in cgs units

$$D_c = \frac{4\pi}{r^2-1}\left[\frac{r}{\sqrt{r^2-1}}\ln\left(r+\sqrt{r^2-1}\right)-1\right]$$

$$D_a = D_b = \frac{4\pi - D_c}{2}$$



Limiting case r >> 1 (long rod)

$$D_c = \frac{4\pi}{r^2}\left[\ln(2r)-1\right] \ll 1$$

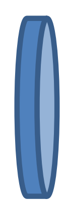
$$D_a = D_b = 2\pi$$

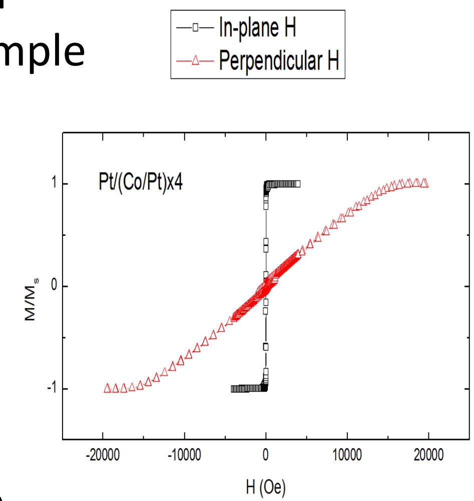
Note: you measure $2\pi M$ *without* knowing the sample

2. Oblate Spheroid (pancake shape) $c/a = r < 1$; $a = b$

$$D_c = \frac{4\pi}{1-r^2}\left[1-\frac{r}{\sqrt{1-r^2}}\cos^{-1} r\right]$$

$$D_a = D_b = \frac{4\pi - D_c}{2}$$





Limiting case r >> 1 (flat disk)

$$D_c = 4\pi$$

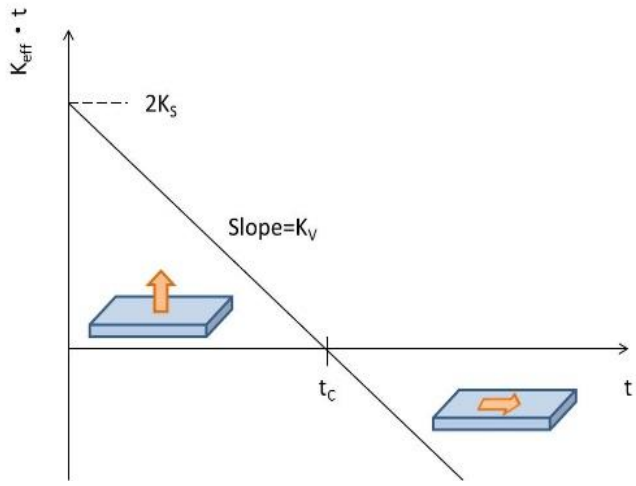
$$D_a = D_b = \pi^2 r \ll 1$$

Note: you measure $4\pi M$ *without* knowing the sample

Surface anisotropy

$$E = E_{exchange} + E_{Zeeman} + E_{mag} + E_{anisotropy} + \cdots$$

- E_{ex}: $\sum 2J\overrightarrow{S_i} \cdot \overrightarrow{S_j}$
- E_{Zeeman}: $\overrightarrow{M} \cdot \vec{H}$
- E_{mag}: $\frac{1}{8\pi}\int B^2 dV$
- $E_{anisotropy}$



For hcp Co$= K_1' \sin^2\theta + K_2{}' \sin^4\theta$

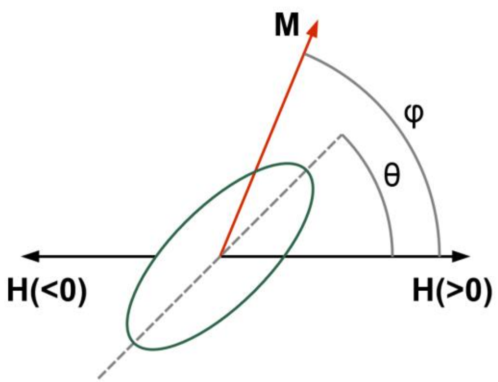
For bcc Fe $= K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + K_2(\alpha_1^2\alpha_2^2\alpha_3^2)$

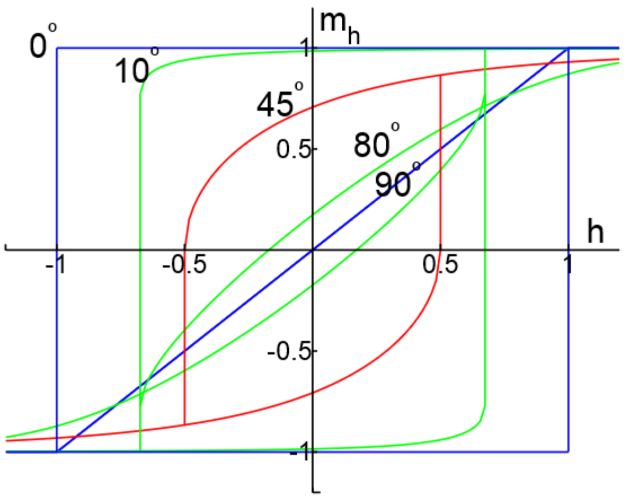
α_i: directional cosines

Surface anisotropy $K_{\text{eff}} = \frac{2K_S}{t} + K_V$ ➔ $K_{\text{eff}} \cdot t = 2K_S + K_V \cdot t$

Stoner–Wohlfarth model

A widely used model for the magnetization of single-domain ferromagnets. It is a simple example of magnetic hysteresis, and is useful for modeling small magnetic particles





$$E = K_u V \sin^2(\phi - \theta) - \mu_0 M_s V H \cos\phi,$$

where K_u is the uniaxial anisotropy parameter, V is the volume of the magnet, $\boldsymbol{M}_s$ is the saturation magnetization.