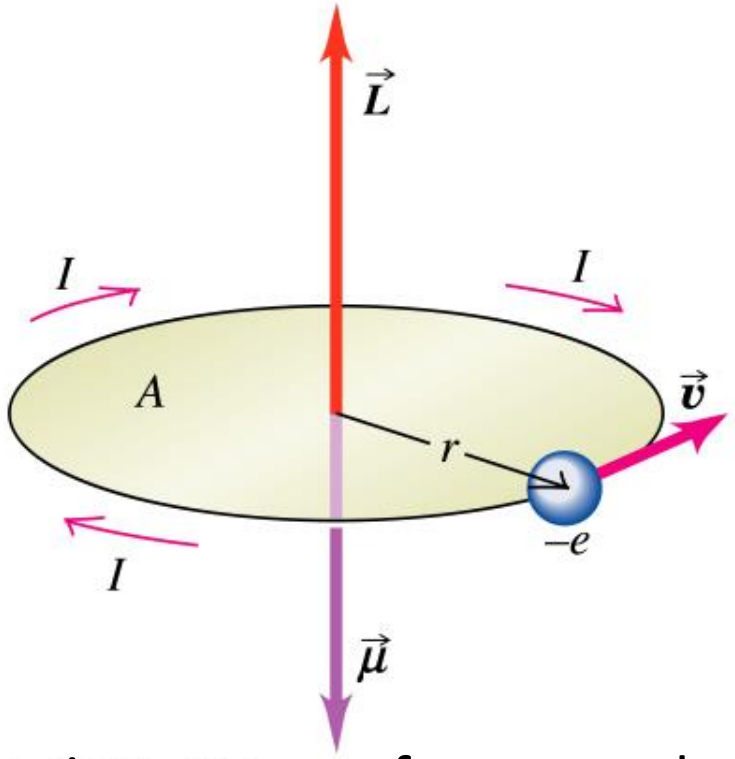
Borh magneton

Orbiting electrons form a current loop which give rise to a magnetic field.



$$i = -\frac{e}{T} = -\frac{e\,v}{2\pi r} \qquad A = \pi r^2$$

$$\mu = -\frac{e\,v}{2\pi}\pi r^2 = -\frac{e\,v\,r\,m_e}{2\,m_e} \qquad \hbar = v\,m_e\,r$$

For the electron: $\mu_b = \dfrac{e\hbar}{2m_e} = 9.27\,10^{-24}\,\dfrac{J}{T}$

Magnetic moment of a current loop:

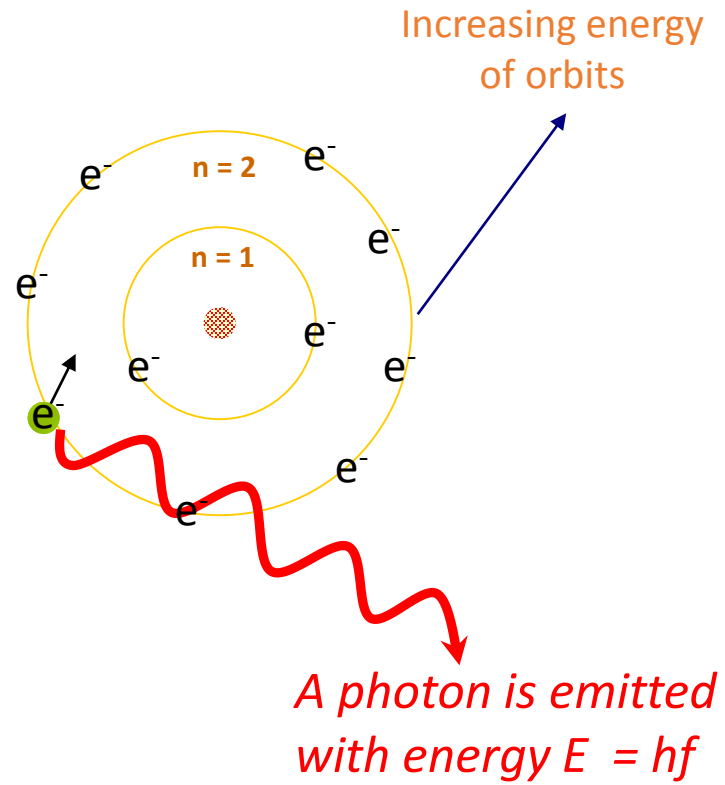
$|\mu| = iA$

current — area enclosed by current loop

For the electron, the Bohr magneton is the simplest model possible to the smallest possible current to the smallest possible area closed by the current loop

Rutherfod (1911) - Borh (1913) model of atom

1) Borh use the classical mechanics
2) The only permitted orbital are those for with $L_{orb} = n\hbar$
3) For these orbitals the electrons don't radiate electromagnetic waves
4) The energy of photon is : $E = h f$



$$\frac{e^2}{4\pi\epsilon_0 r^2} = \frac{m_e v^2}{r} \quad \Rightarrow \quad L = n\hbar \quad \Rightarrow \quad v = \frac{n\hbar}{m_e r}$$

Electrostatitc force — Centrifugal force

$$k = \frac{1}{4\pi e_0}$$

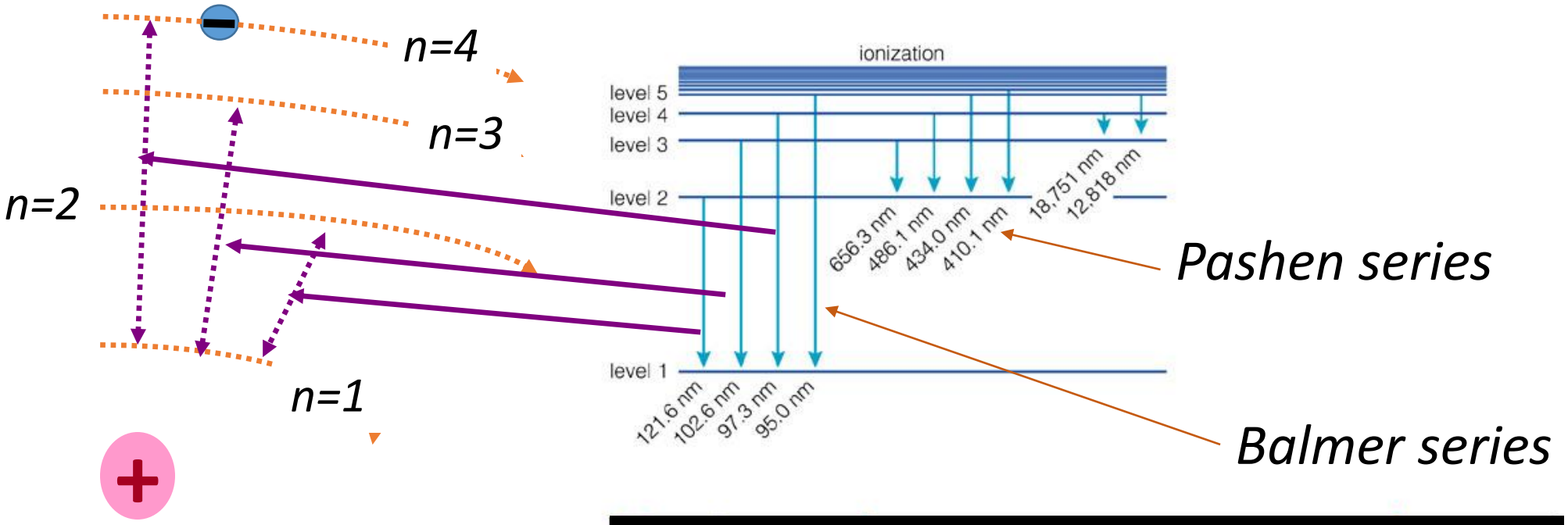
$$r_n = \frac{\hbar^2 n^2}{m_e k e^2}$$

$$r_n = a_0 n^2$$

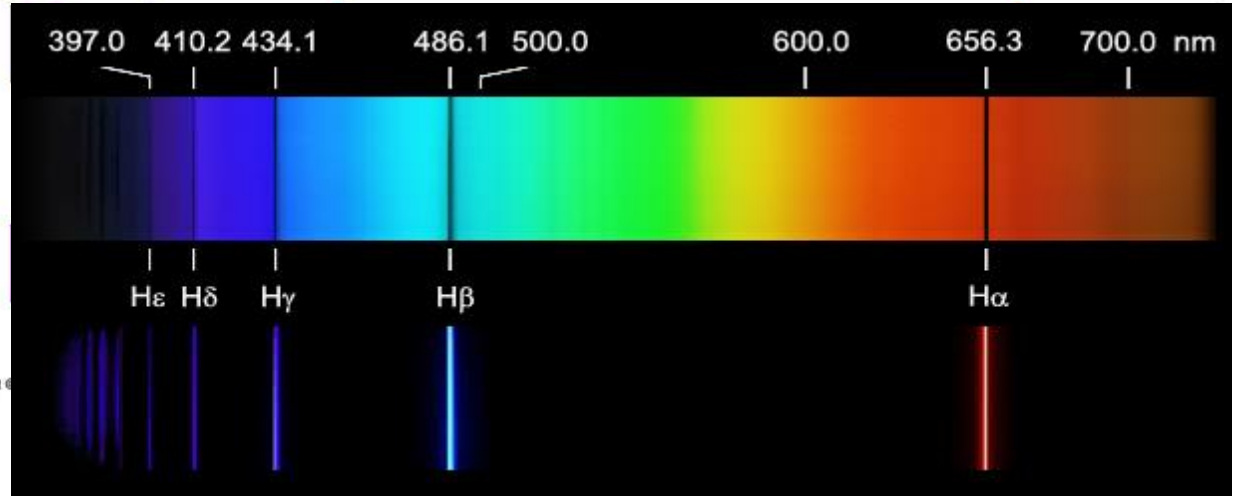
Borh radius

$$a_0 \equiv \frac{\hbar^2}{m_e k e^2} = 0.05297 \text{ nm}$$

Hydrogen energy levels (Borh- Rutherford Model)

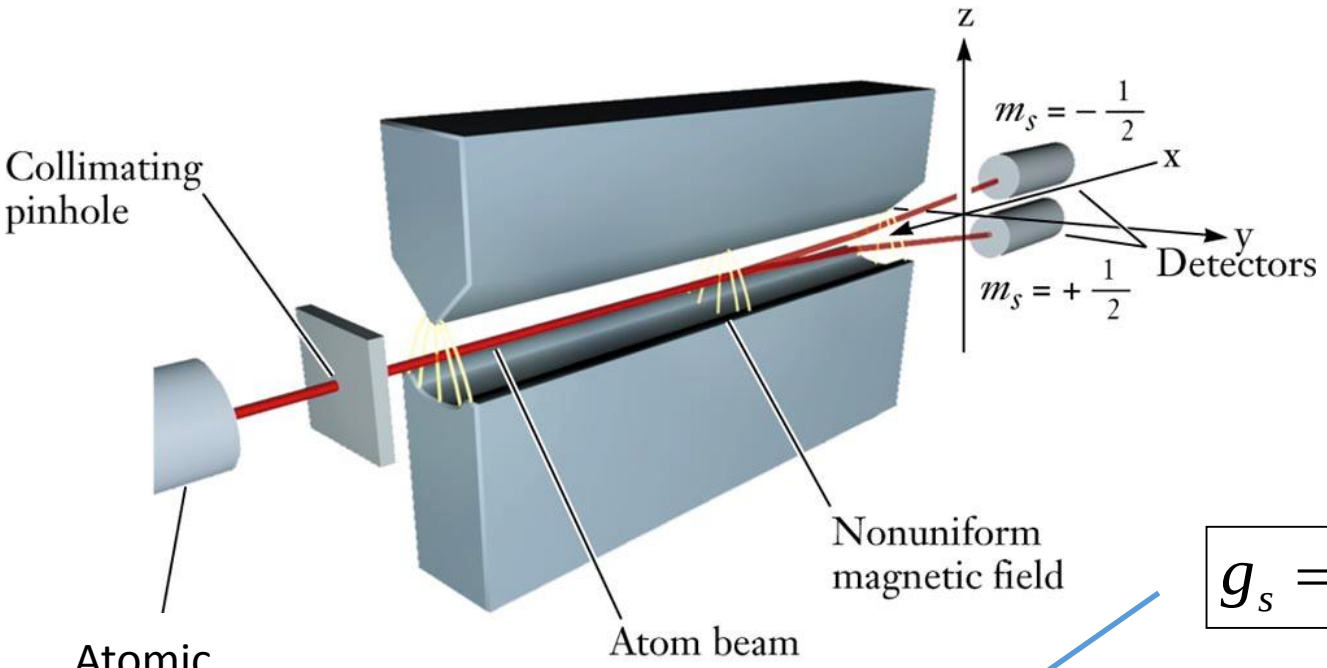


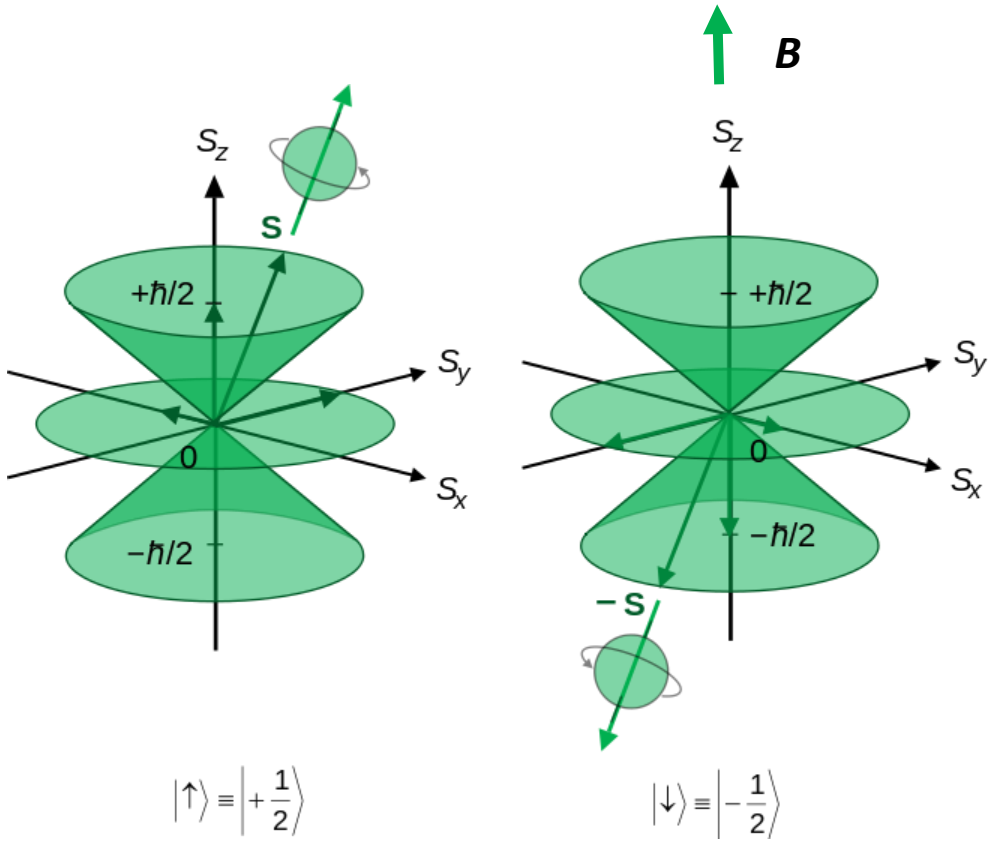
$$E_n = -\frac{m_e e^4}{(4\pi\varepsilon_0)^2 2\hbar^2 n^2} = -\frac{13.6\,\text{eV}}{n^2} \quad ,$$



Stern Gerlach experiment (1922)

A classic experiment that shows a difference between quantum and classical mechanics. Only two discrete deflections show up, corresponding to "spin up" and "spin down" for neutral particles.





$$g_s = 2.0023$$

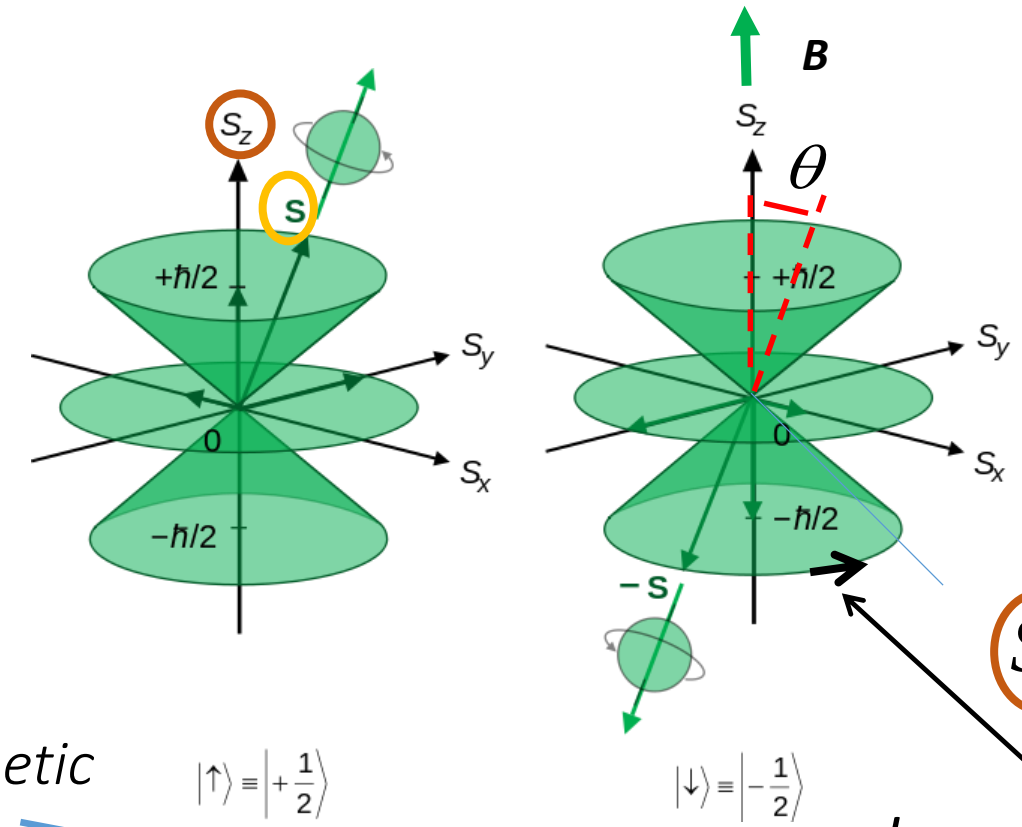
Spin magnetic moment →

$$\boldsymbol{\mu}_s = -g_s \frac{e}{2m_e}\mathbf{S}_z = -g_s \frac{e}{2m_e} m_s \hbar = -g_s \mu_b m_s$$

$m_s = +1/2$ (spin up)

$m_s = -1/2$ (spin down)

The spin orientation



Because of the uncertainty principle, it is impossible to orient the spin S parallel to B

$$\cos(\theta)S \geq \frac{\hbar}{2}$$

$$S_z = m_s\hbar$$

$$m_s = +1/2 \quad (\text{spin up})$$

$$m_s = -1/2 \quad (\text{spin down})$$

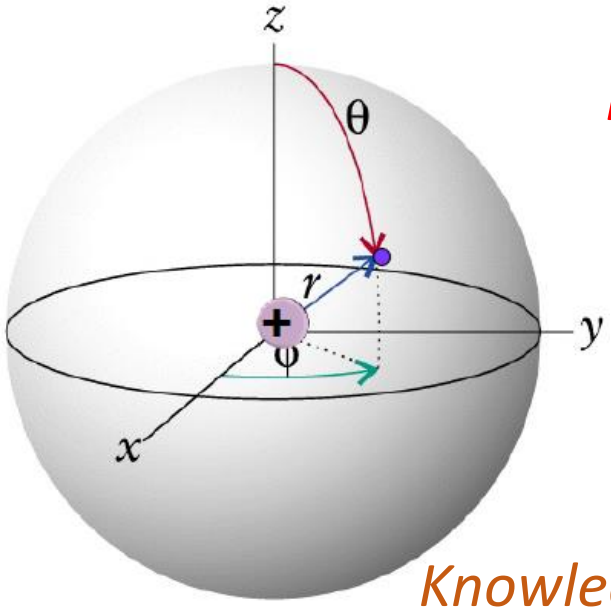
Gyromagnetic ratio

Larmor precession

Larmor frequency $\Rightarrow \omega = \frac{g_l \mu_B}{\hbar} B = 28GHz * B$

$$S = \sqrt{s(s+1)}\hbar = \sqrt{1/2(1/2+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

The Schrödinger equation (1922) to the hydrogen atom (without spin)



Kinetics energy

Potential energy

Total energy

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(x,y,z)+V\psi(x,y,z)=E\psi(x,y,z)$$

Wave function represent the probability amplitude.

It is a deterministic function (M. Born).

Knowledge of Ψ (r, t) then enables (in the Copenhagen interpretation) to know the dynamic of the wave function (its evolution in the space-time).

For the relativist case see Dirac equation.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{r^2sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}+\frac{2\mu}{\hbar}(\mathrm{E\text{-}V})\Psi=0$$

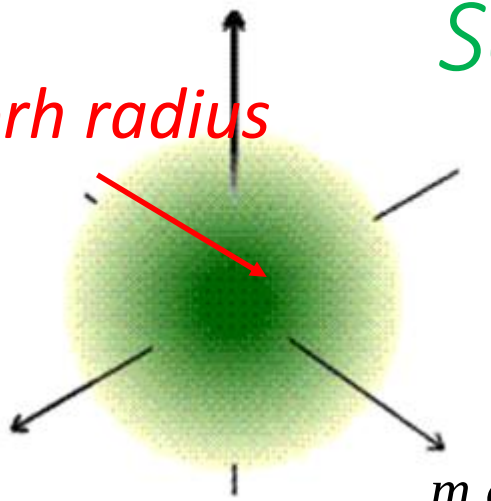
Kinetics energy

Total energy

Potential energy

The Schrödinger equation to the hydrogen atom
Solutions of radial equation 1S, 2S.

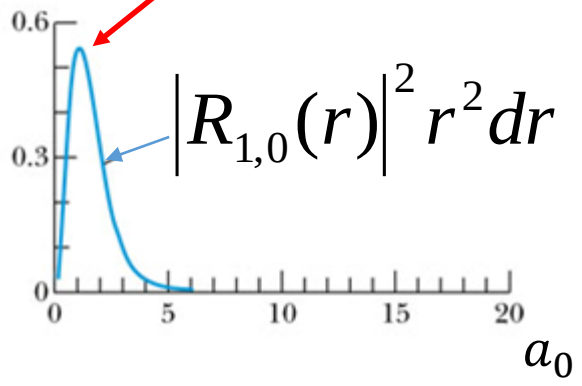
Borh radius



Orbital 1s (n=1, l=0), volume probability density for the ground state of the hydrogen atom

$$E_1 = -\frac{m_e e^4}{(4\pi\varepsilon_0)^2 2\hbar^2} = -13.6\,\text{eV}$$

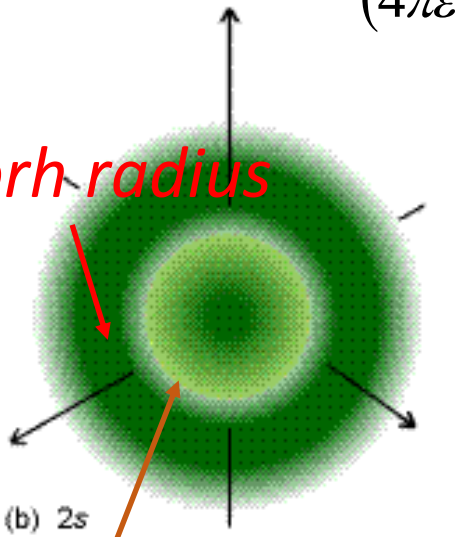
Borh radius



$$|R_{1,0}(r)|^2 r^2 dr$$

2 electrons maximum

Borh radius



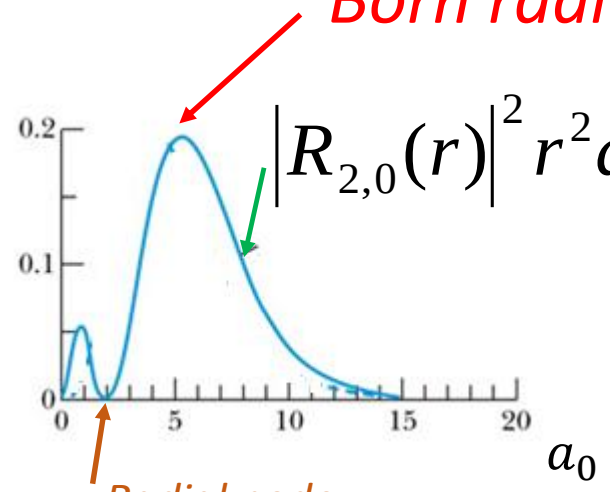
Radial node

Orbital 2s (n=2, l=0), volume probability density for the hydrogen atom in the quantum state, the gap in the dot density pattern marks a spherical surface over which the radial wave function is zero

$$E_2 = -\frac{m_e e^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\frac{1}{4} = -\frac{13.6\,\text{eV}}{4} = -3.4\,\text{eV}$$

$$a_0 = 5.29\times10^{-11}\,\text{m}$$

Borh radius



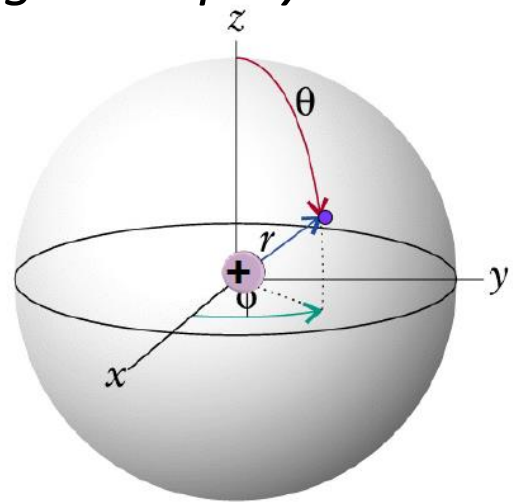
$$|R_{2,0}(r)|^2 r^2 dr$$

Radial node

The Schrödinger equation to the hydrogen atom
Solutions of harmonic equation

$$\frac{1}{\sin(\theta)}\frac{d}{d\theta}\left(\sin(\theta)\frac{d}{d\theta}P_l^{m_l}(\theta)\right)+\left[l(l+1)-\frac{m_l^2}{sin^2(\theta)}\right]P_l^{m_l}(\theta)=0$$

Legendre polynomials



$[P_l^{m_l}(\theta)]^2 \mathrm{d}\theta$

The probability density to find an electron in an angle θ with an apperture angle $d\theta$

Quantum number l called the orbital quantum number, is a measure of the magnitude of the angular momentum associated with the quantum state l = 0, 1, 2 ,3 ,…n-1

$[\Phi(\varphi)]^2 \mathrm{d}\varphi$

The probability density to find an electron in an angle φ with an apperture angle $d\varphi$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2} = -m_l^2\,\Phi(\varphi)$$

Quantum number m_l, called the orbital magnetic quantum number is related to the orientation in space of the angular momentum vector

$$-l \le m_l \le +l$$

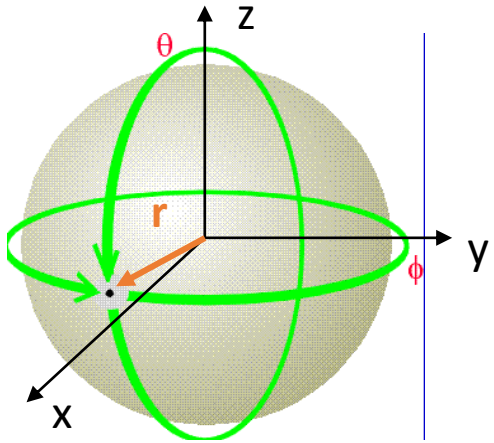
The Schrödinger equation to the hydrogen atom: orbital 2p (n=2, l=1)

$$p_0 = R_{2,1}(r)P_1^0(\theta)\Phi(\phi) = \frac{1}{4(2\pi)^{1/2}}\left(\frac{1}{a_0}\right)^{5/2} r\cos\theta\, e^{-\frac{r}{2a_0}} = r\cos\theta.f(r) = z.f(r) = p_z$$

$$p_{\pm1} = R_{2,1}(r)P_1^{\pm1}(\theta)\Phi(\phi) = \mp\frac{1}{8\pi^{1/2}}\left(\frac{1}{a_0}\right)^{5/2} r\, e^{-\frac{r}{2a_0}} \sin\theta\, e^{\pm i\phi}$$

$$= \mp\frac{1}{2^{1/2}} r\sin\theta\, e^{\pm i\phi} f(r)$$

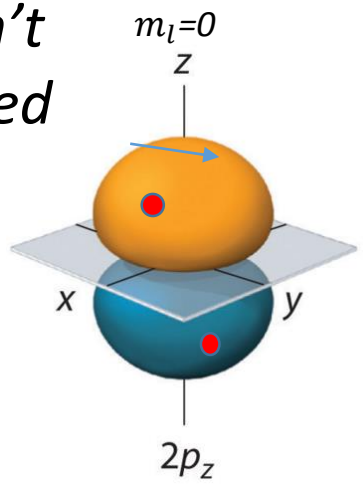
Different rotations: clockwise, counter-clockwise

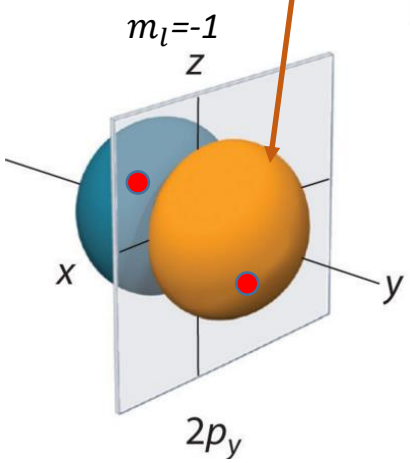


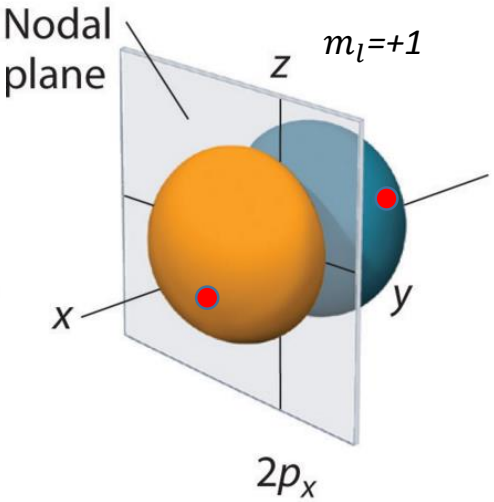
$$p_x = -\frac{1}{2^{1/2}}(p_{+1} - p_{-1}) = r\sin\theta\cos\phi\ f(r) = x\, f(r)$$

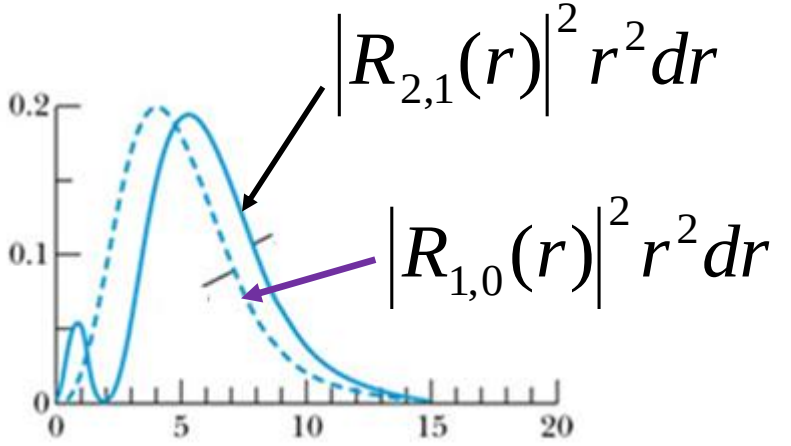
$$p_y = \frac{i}{2^{1/2}}(p_{+1} + p_{-1}) = r\sin\theta\sin\phi\ f(r) = y\, f(r)$$

We haven't represented f(r)







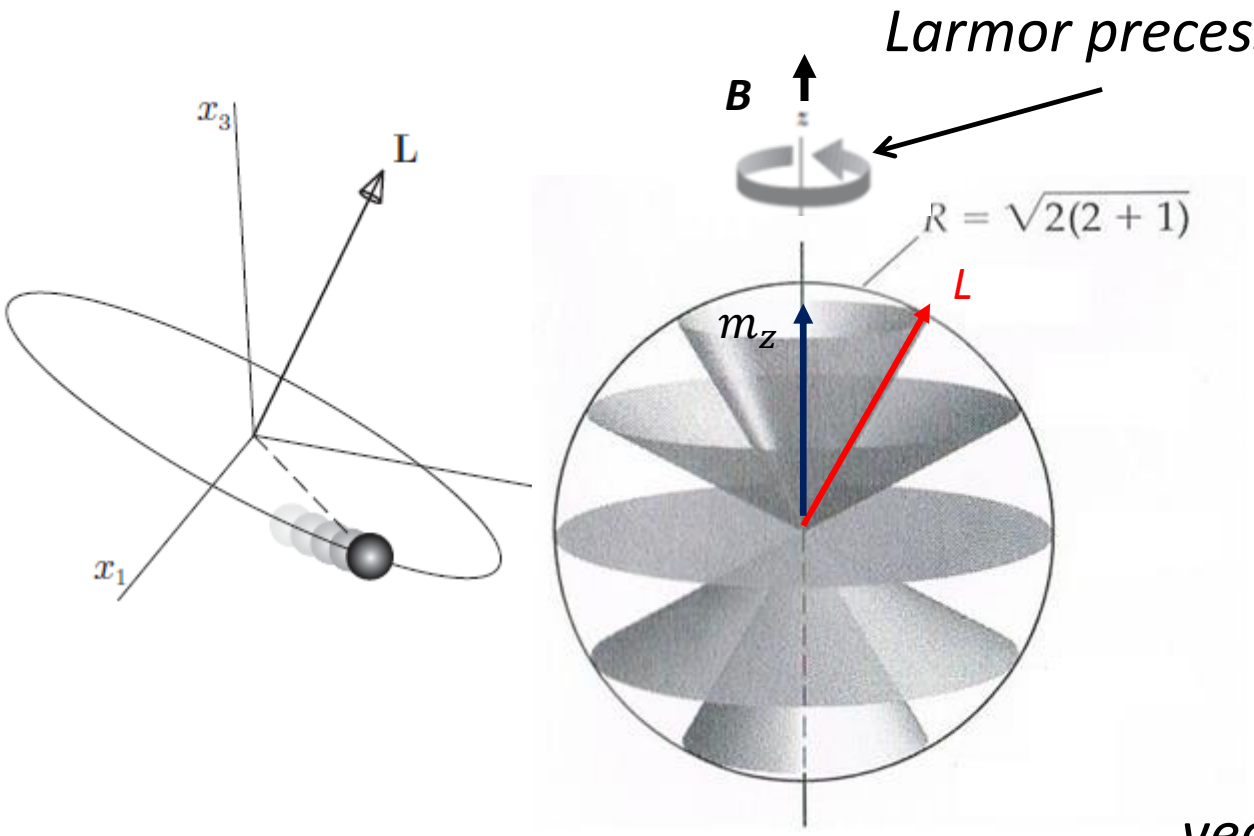


6 electrons maximum

The orbital angular momentum for l=2

$$-l \leq m_z \leq +l$$

Classical equation $\vec{L} = \vec{r} \times \vec{p}$



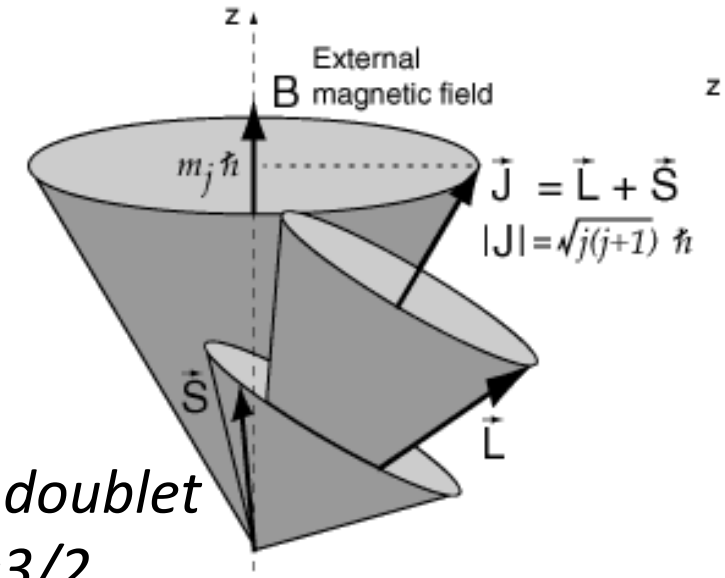
$$L_z = m_\ell \hbar \qquad L = \hbar\sqrt{\ell(\ell+1)} = \sqrt{6}\hbar$$

Because of the uncertainty principle, it is impossible to orient the orbital angular momentum l parallel to B

This figure shows the five quantized components l_z of the orbital angular momentum for an electron with l=2, as well as the associated orientations of the angular momentum vector (however, we should not take the figure literally as we cannot detect L this way)

Total angular momentum in a magnetic field

The total angular momentum can be visualized as processing about any externally applied magnetic field. We don't consider the spin-orbit interaction.

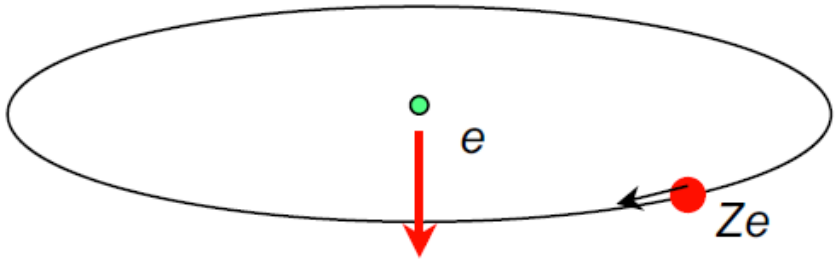


the sodium doublet with j=3/2

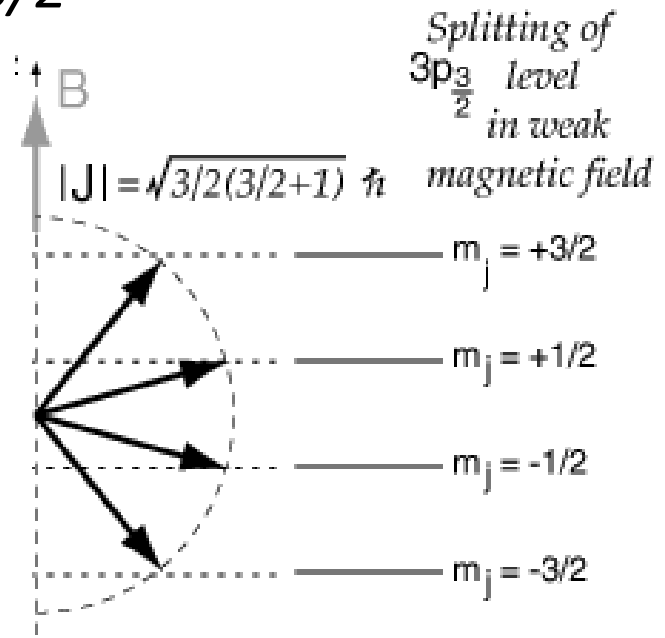
From the electron's point of view, the nucleus revolves round it. It is a current loop

It is a current loop $I = Ze\ v/2\pi r$ *Which produces a magnetic field* $\mu_0 I/2r$ *at the centre* $B_{so} = \mu_0 Zev/2\pi r^2$

$E_{so} = -\mu_b B_{so}$ *. Since* $r \approx a_0/Z$ *and* $m_e vr = \hbar$



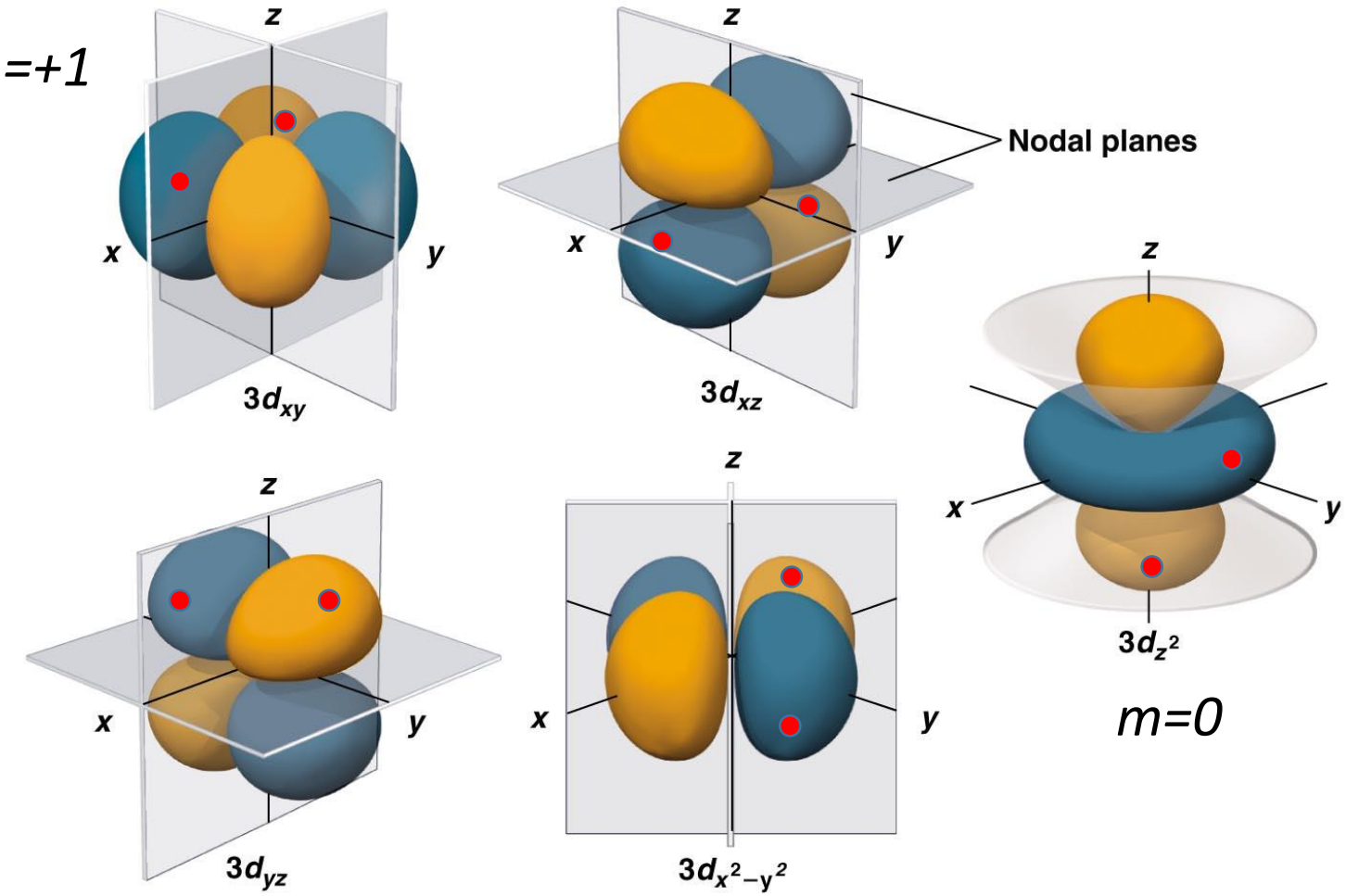
$$E_{so} \approx -\mu_0 \mu_B{}^2 Z^4 / 4\pi a_0{}^3$$



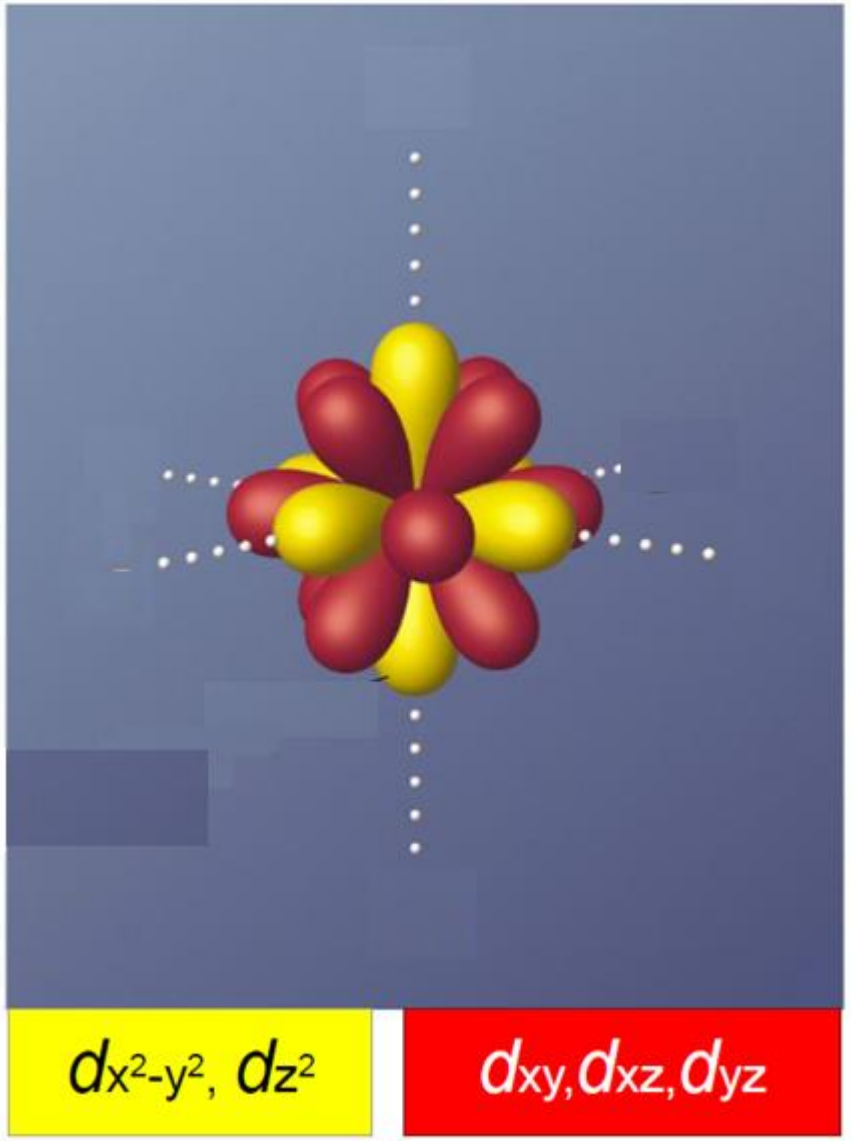
Note if we consider that the spin-orbit, the formula indicates that spin orbit-coupling interactions are significantly larger for atoms that are further down a particular column of the periodic table.

The Schrödinger equation to the hydrogen atom: orbital 3d (n=3, l=2)

m=+1

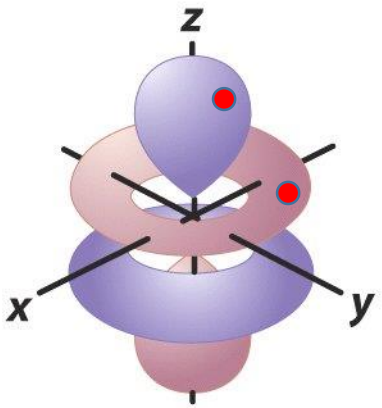


m=0

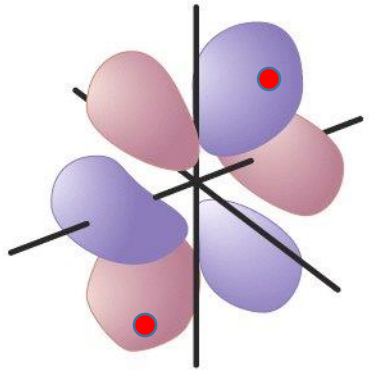


10 electrons maximum

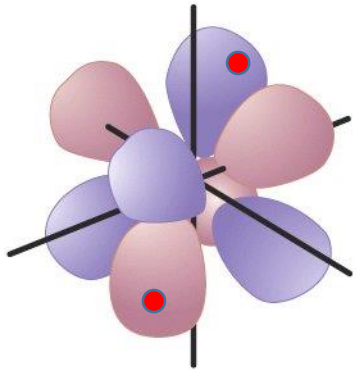
The Schrödinger equation to the hydrogen atom: orbital 4d (n=4, l=3)



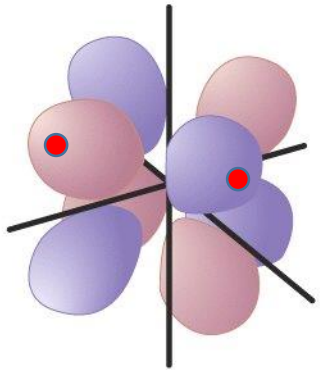
$5z^3 - 3zr^2$



$5xz^2 - xr^2$

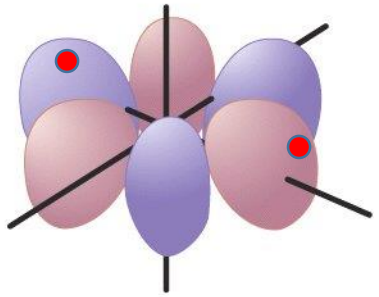


$zx^2 - zy^2$

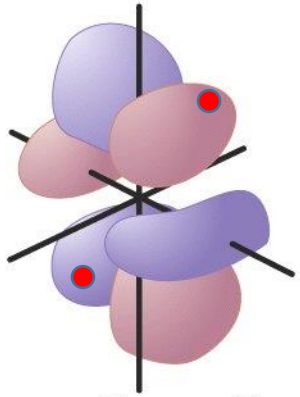


xyz

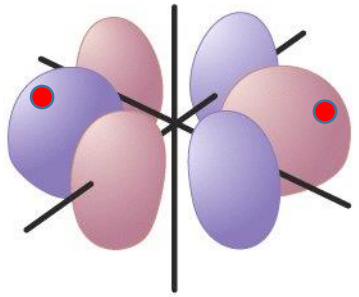
14 electrons maximum



$y^3 - 3yx^2$



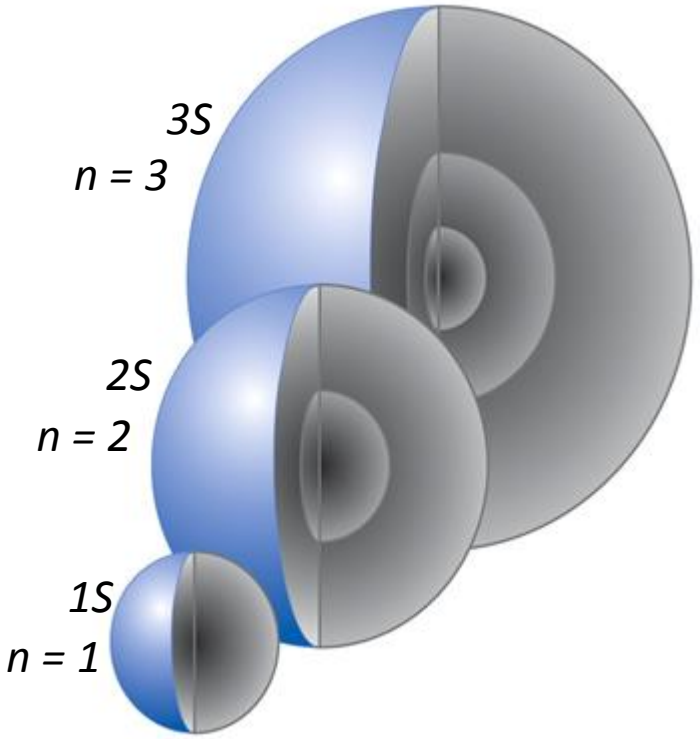
$5yz^2 - yr^2$



$x^3 - 3xy^2$

Quantum Numbers

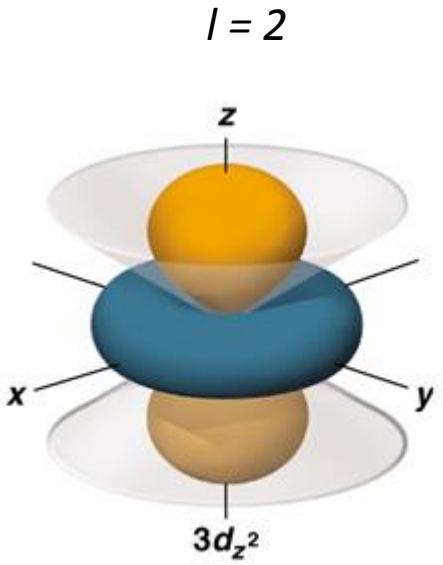
❖ **The *principal quantum number* (*n*) has possible values of:**



$$n = 1, 2, 3, \ldots \infty$$

It describes the relative size of the orbital

Quantum Numbers

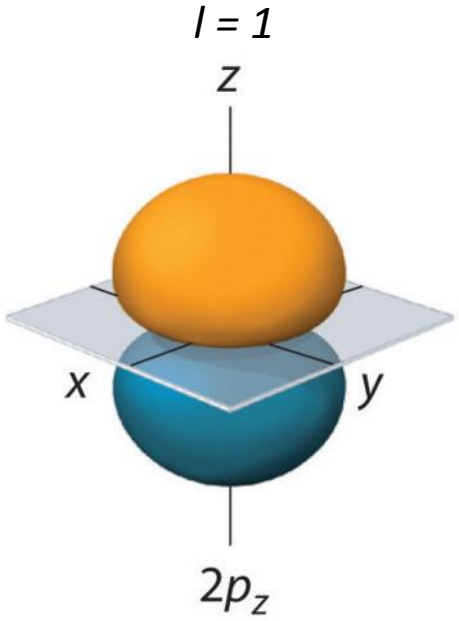


❖ **The *angular momentum quantum number* (*ℓ*)**

has possible values of:

$$\ell = 0, 1, 2, \ldots n-1$$

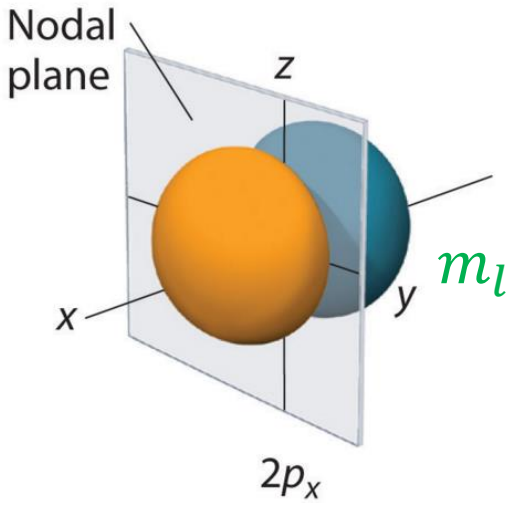
It describes the shape of the orbital.



☆ *The value of ℓ is often referred to by a letter equivalent;*

0 = s, 1 = p, 2 = d, 3 = f, ... (the rest are alphabetical)

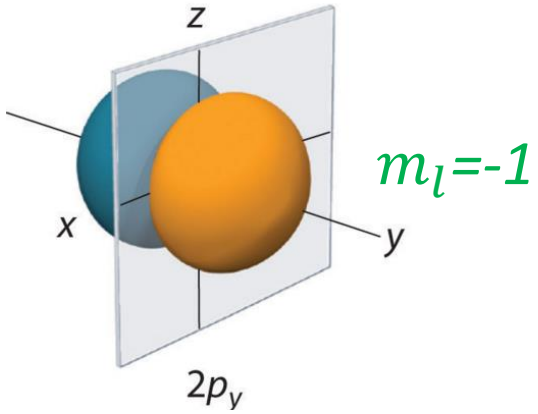
Quantum Numbers



m_l=+1

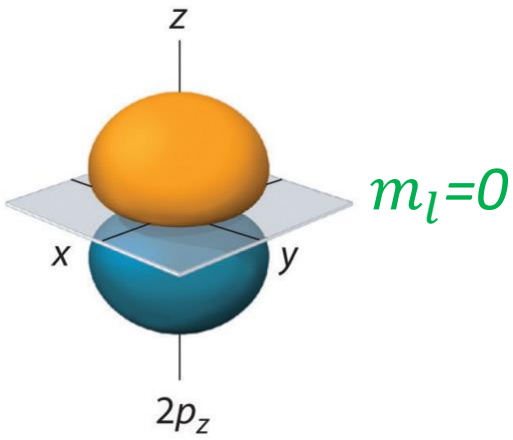
❖ ***The magnetic quantum number (m_ℓ) has values:***

$$m_\ell = -\ell, \ldots -1, 0, 1, \ldots \ell$$



m_l=-1

It describes the orientation of the orbital in space.



m_l=0

Quantum Numbers

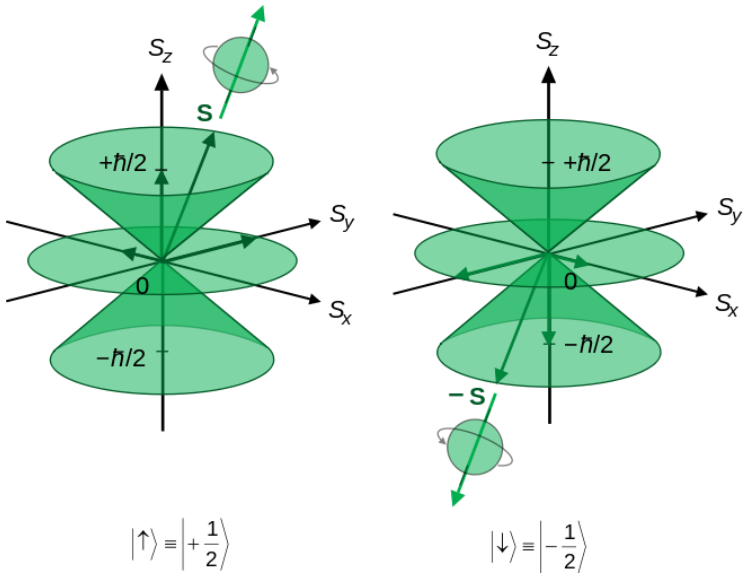
❖ ***The spin angular momentum number (m_s)***

has possible values of:

$$m_s = \pm\frac{1}{2}$$

It describes the orientation of the spin.

The vertical axis is used as reference.



Pauli exclusion principle (1925)

Wolfgang Pauli postulated the (Pauli) exclusion principle, which states that no two electrons in one atom can exist in the same quantum state.

"State" refers to the four quantum numbers n, ℓ, m_ℓ, m_s. Obviously, all electrons have the same s.

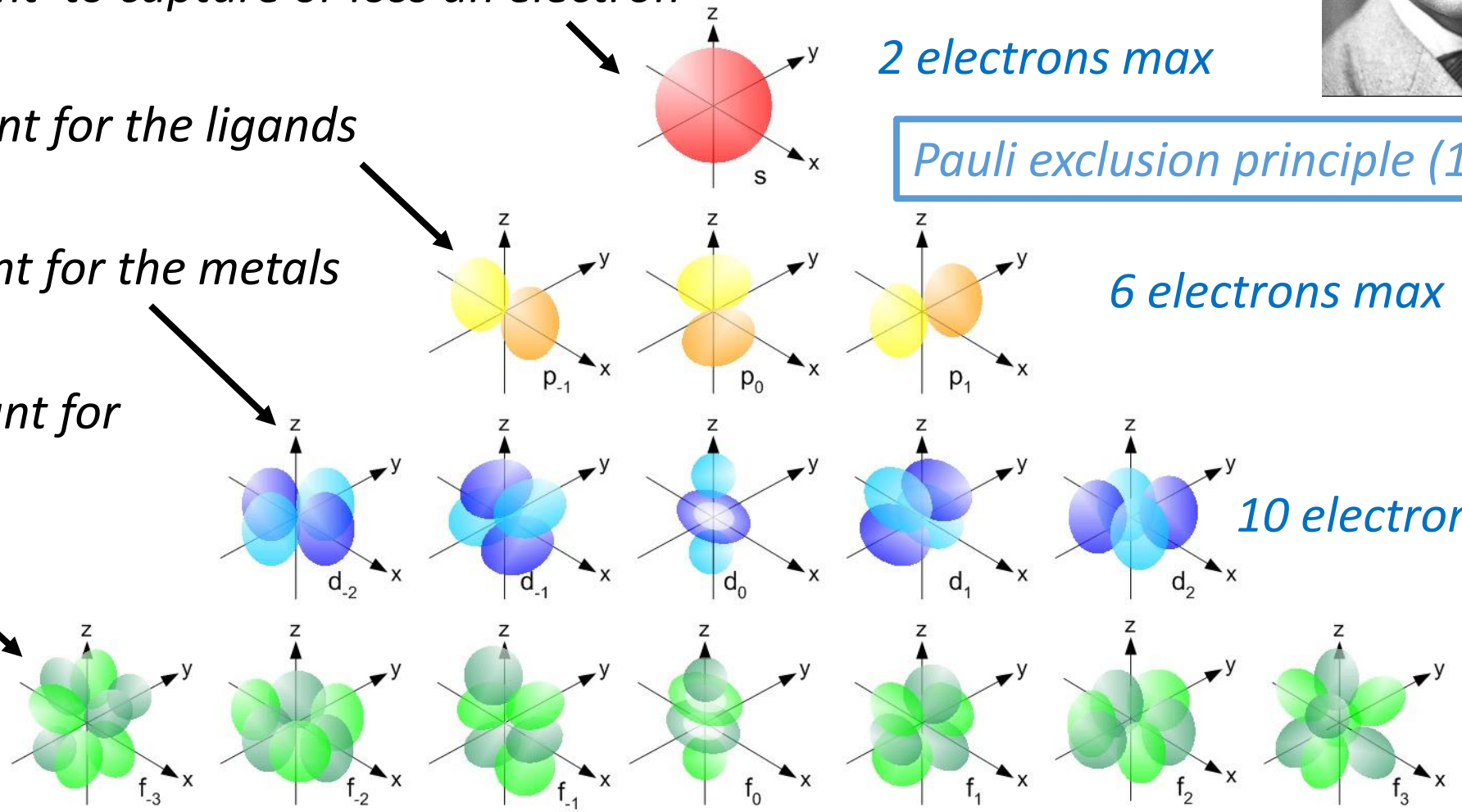
Subshells Schrödinger (1922)

Subshell very important to capture or loss an electron

Subshell very important for the ligands

Subshell very important for the metals

Subshell very important for rare earths



2 electrons max

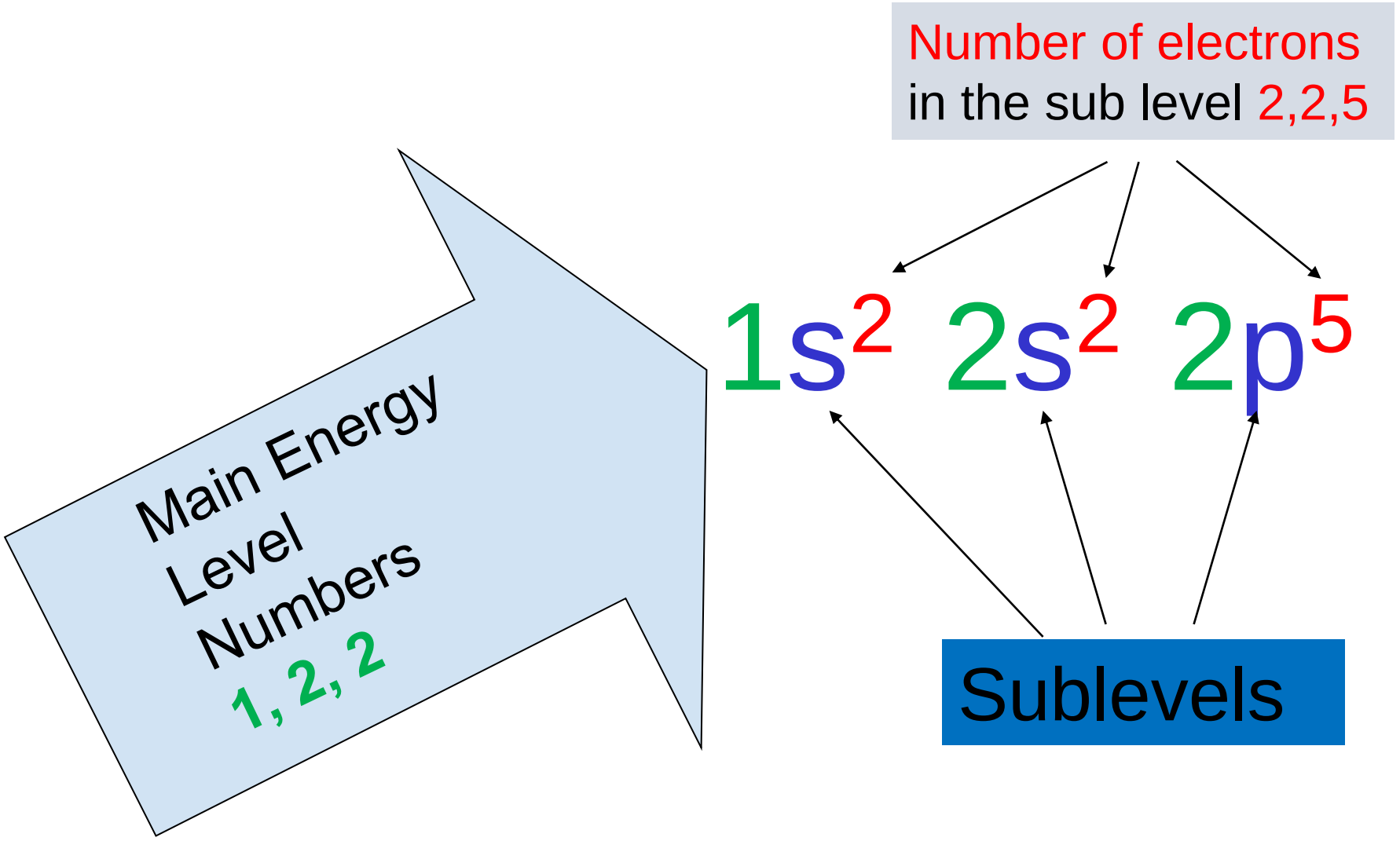
Pauli exclusion principle (1925)

6 electrons max

10 electrons max

14 electrons max

Standard Notation of Fluorine

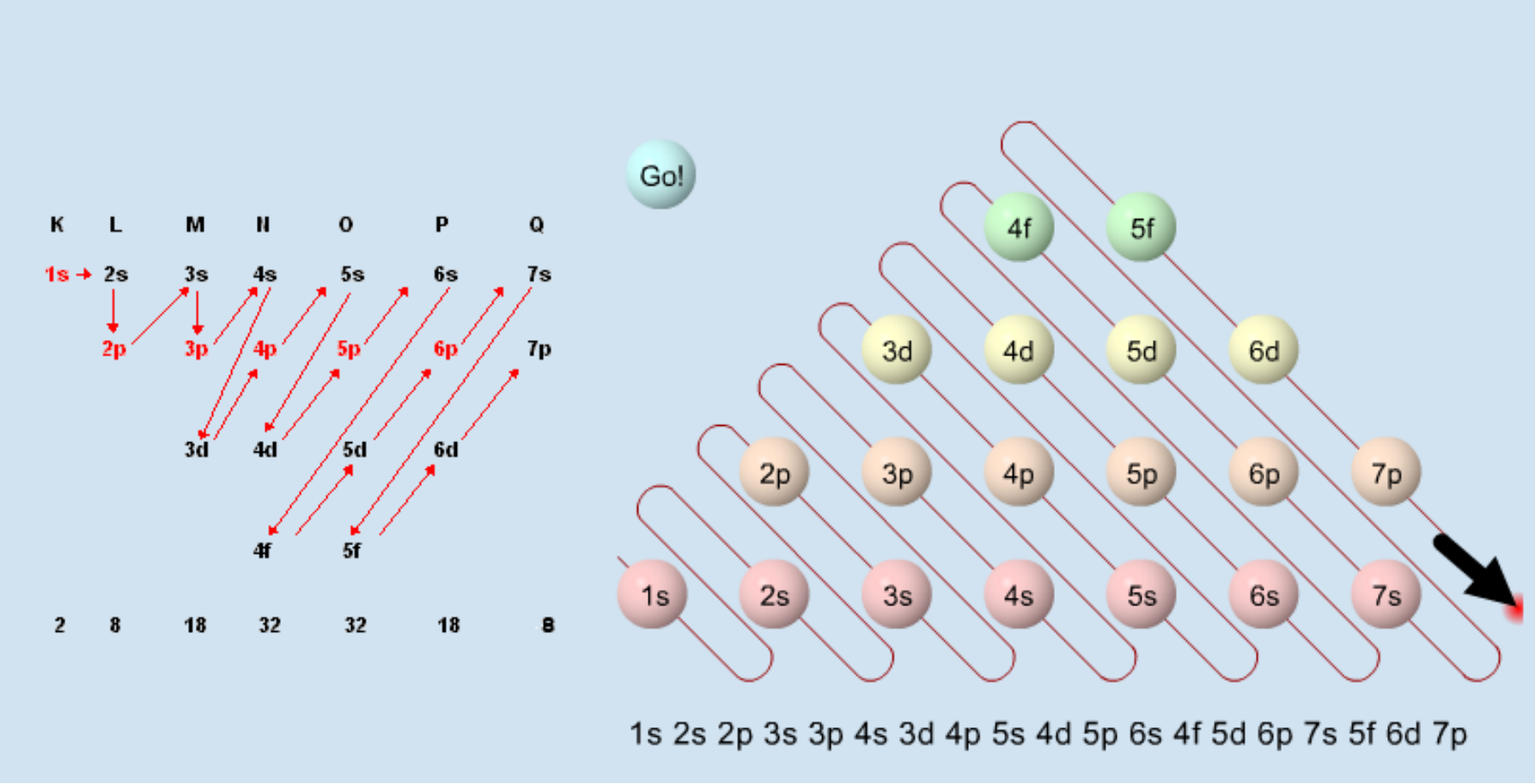


Hund's rule

Orbital Filling Order (Diagonal Rule).

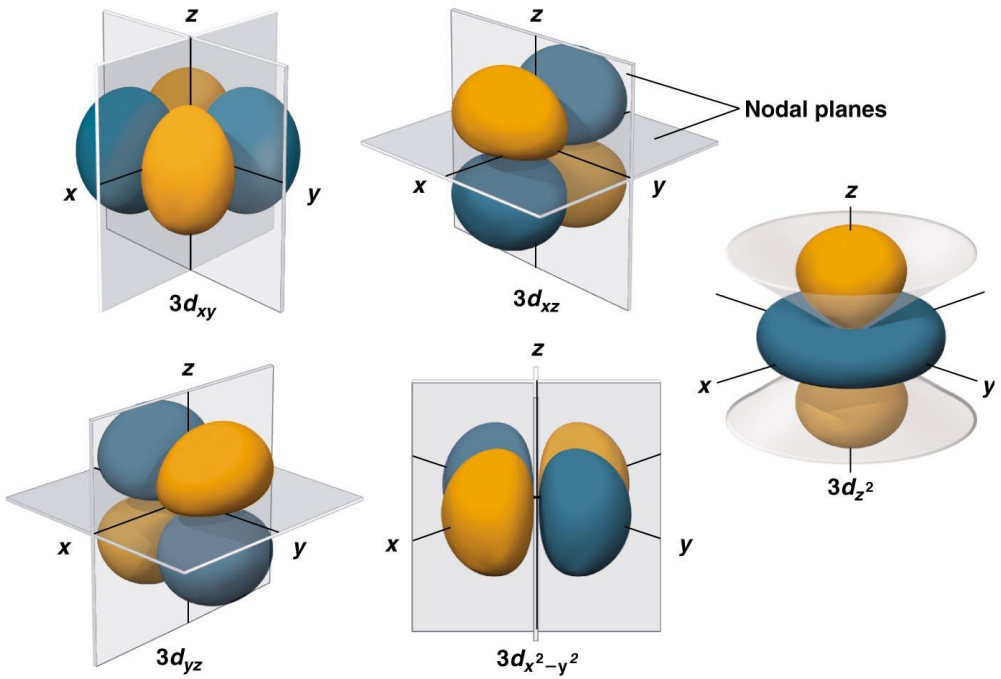
It is a semi-empirical law with exceptions case

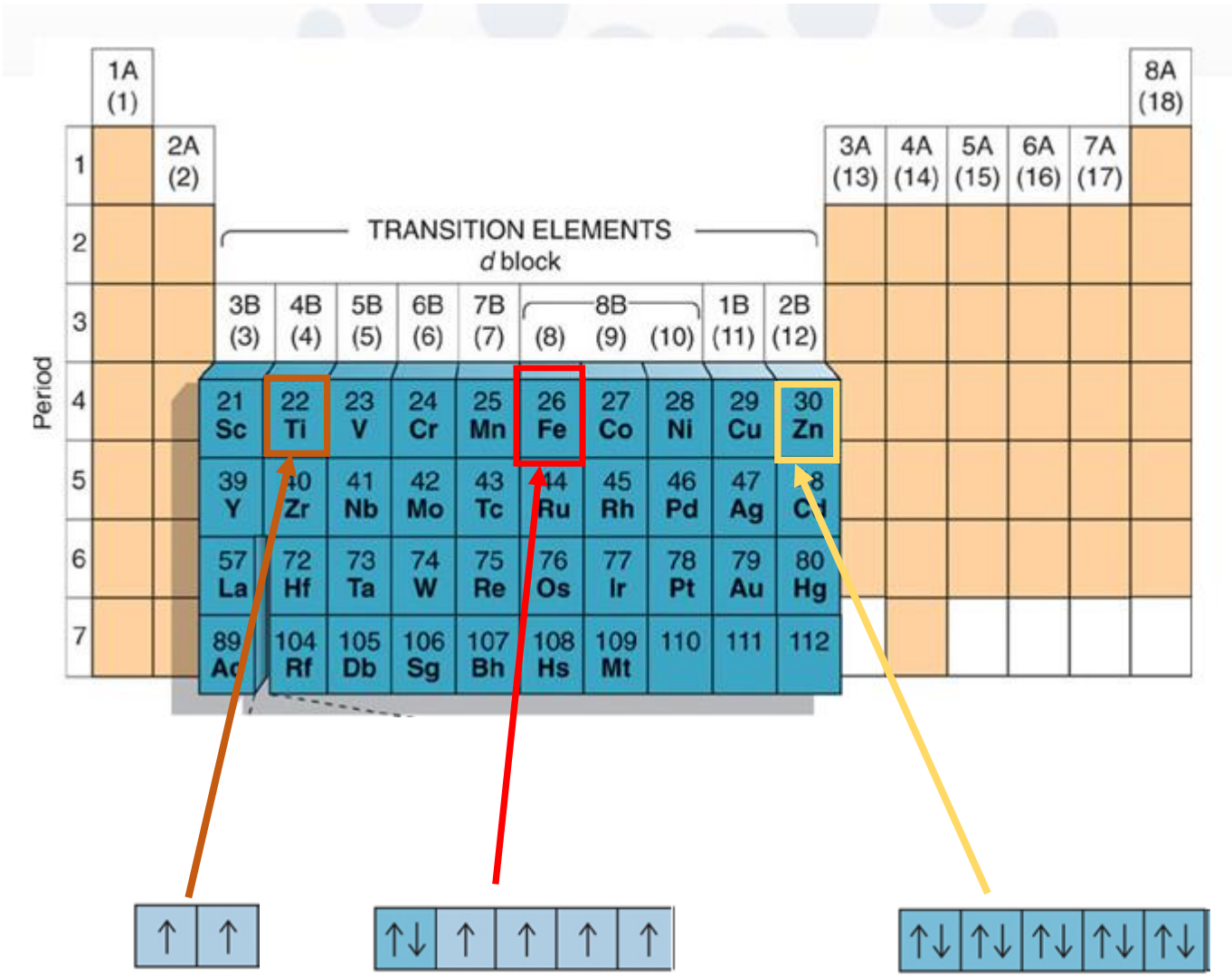
Minimize the coulomb interaction + Pauli exclusion principle.



The transition elements (d block)

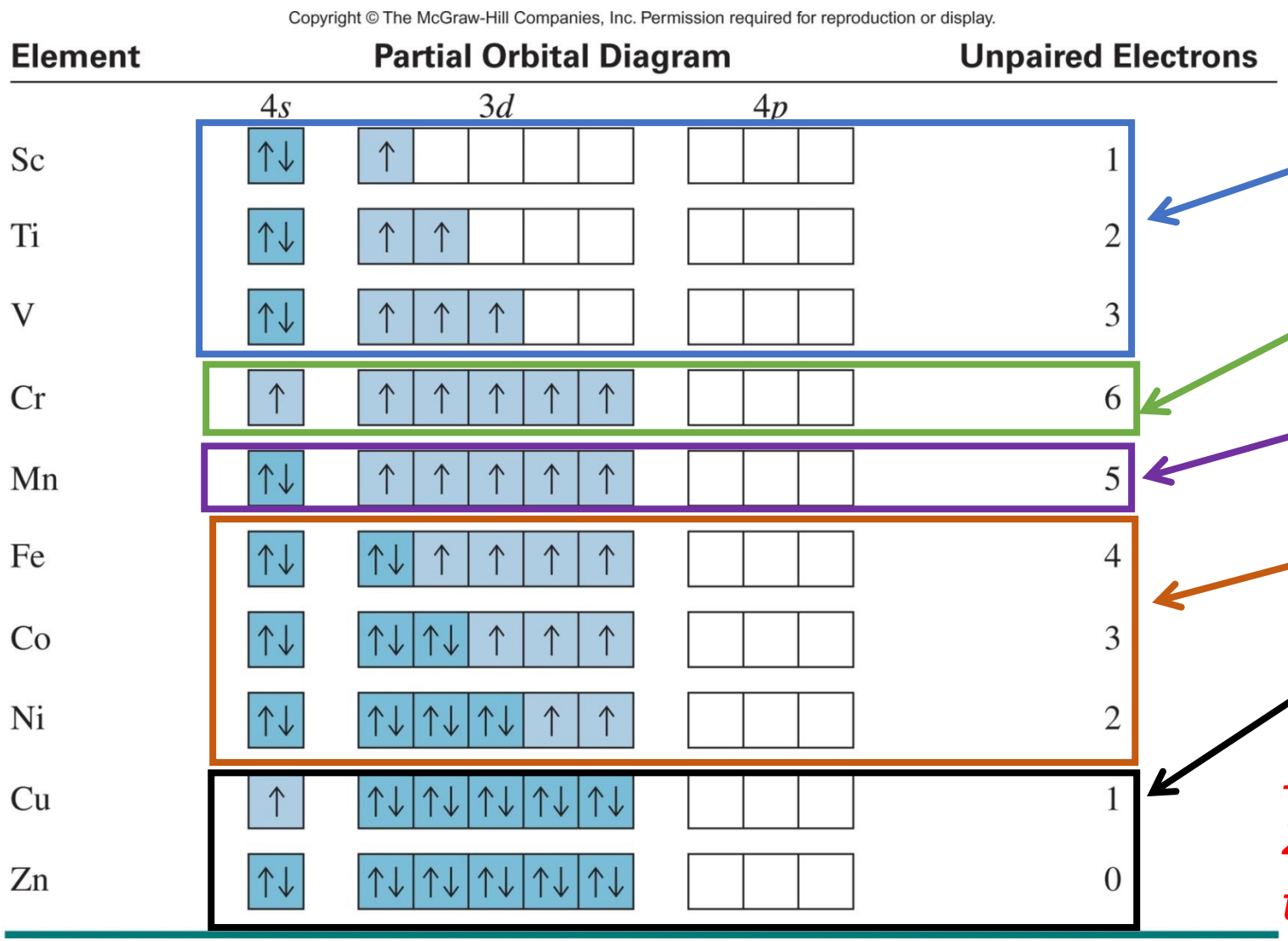
orbital 3d (n=3, l=2)





10 electrons maximum

Orbital occupancy for the transition metals



Paramagnetic

Antiferromagnetic !!!!
Néel temperature

Antiferromagnetic
or paramagnetic !!!!
Néel temperature

Ferromagnetic

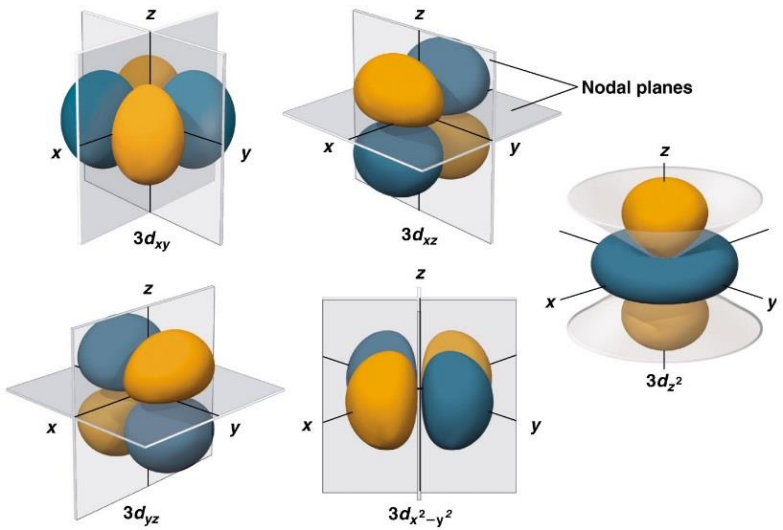
Diamagnetic

3d ferromagnetism

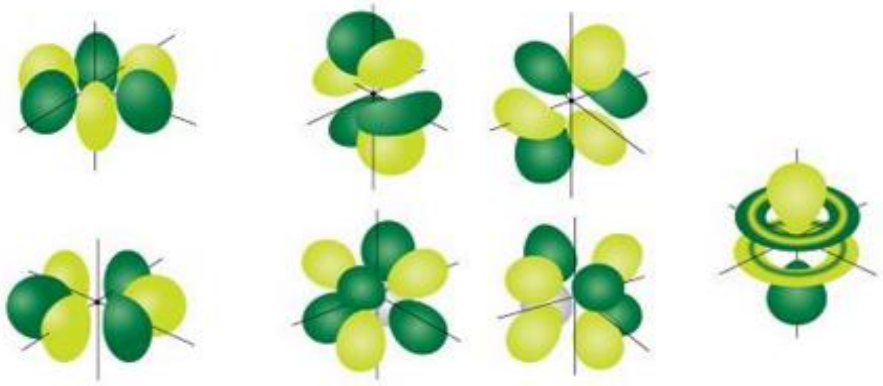
1) When the sub schell is not full.
2) Depend of the distance between the atoms and the radius shell 3d.
3) Exchange energy (Heisenberg 1927)

It is preferable to use the exchange model

3d subshell



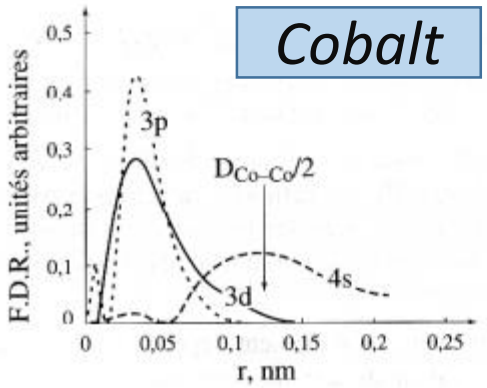
4f subshell



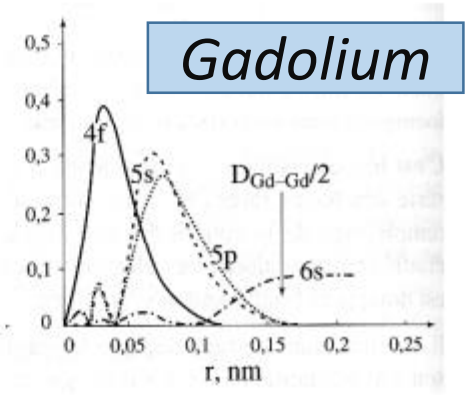
H																	He dia
Li para	Be dia											B dia	C dia	N dia	O AF	F dia	Ne dia
Na para	Mg para											Al para	Si dia	P dia	S dia	Cl dia	Ar dia
K para	Ca para	Sc para	Ti para	V para	Cr AF	Mn AF	Fe Ferro	Co Ferro	Ni Ferro	Cu dia	Zn dia	Ga dia	Ge dia	As dia	Se dia	Br dia	Kr dia
Rb para	Sr para	Y para	Zr para	Nb para	Mo para	*Tc*	Ru para	Rh para	Pd para	Ag dia	Cd dia	In dia	Sn *	Sb dia	Te dia	I dia	Xe dia
Cs para	Ba	La	Hf	Ta para	W para	Re para	Os para	Ir para	Pt para	Au dia	Hg dia	Tl dia	Pb dia	Bi dia	*Po*	*At*	Rn dia
Fr	*Ra*	*Ac*															
			Ce *	Pr para	Nd AF	*Pm*	Sm AF	Eu Ferri	Gd Ferro	Tb Ferro	Dy Ferro	Ho Ferri	Er Ferri	Tm Ferri	Yb para	Lu para	
			Th para	*Pa*	U para	*Np*	*Pu*	*Am*	*Cm*	*Bk*	*Cf*	*Es*	*Fm*	*Md*	*No*	*Lw*	

3d

4f



Cobalt



Gadolium

$Co : 3d^7 4s^2 \rightarrow Co^{2+} : 3d^7$

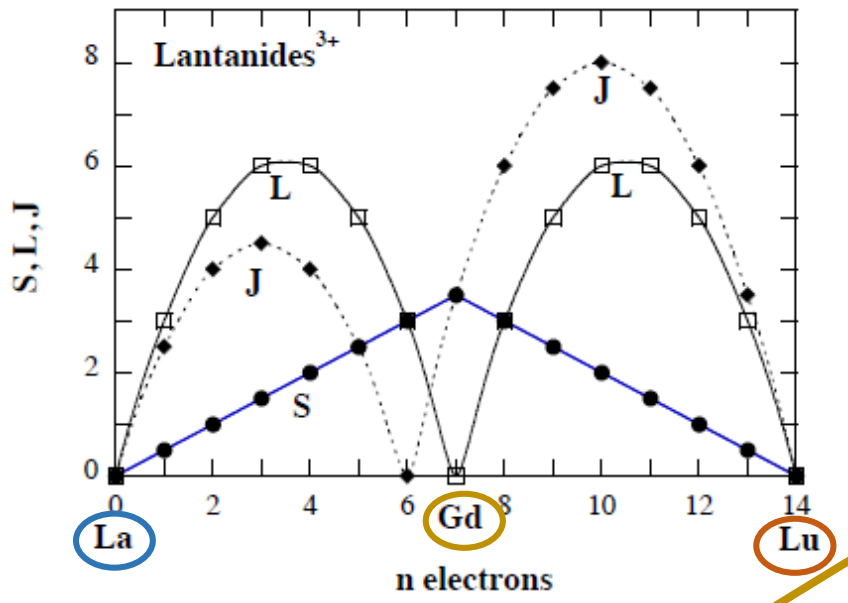
$Gd : 4f^7 5d^1 6s^2 \rightarrow Gd^{3+} : 4f^7$

3d magnetism created by itinerant electrons

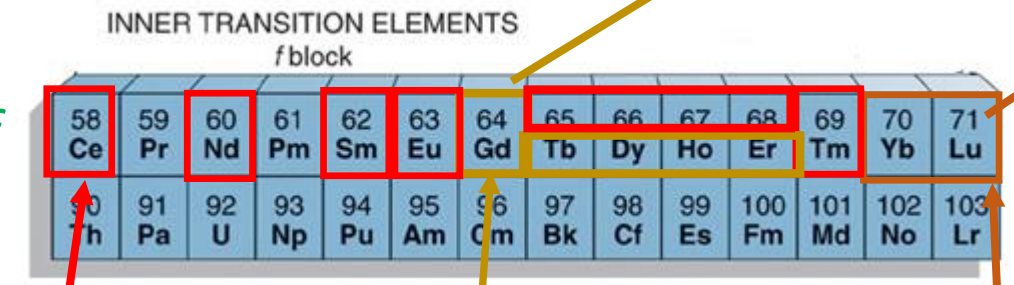
4f local magnetism created by the atoms

Lanthanides (4f block)

Paramagnetic properties depend temperature !



ion	shell	m_l +3	+2	+1	0	-1	-2	-3	S	L	J	term
Ce^{3+}	$4f^1$	↓							$\frac{1}{2}$	3	$\frac{5}{2}$	$^2F_{5/2}$
Pr^{3+}	$4f^2$	↓	↓						1	5	4	$^3H_4$
Nd^{3+}	$4f^3$	↓	↓	↓					$\frac{3}{2}$	6	$\frac{9}{2}$	$^4I_{9/2}$
Pm^{3+}	$4f^4$	↓	↓	↓	↓				2	6	4	$^5I_4$
Sm^{3+}	$4f^5$	↓	↓	↓	↓	↓			$\frac{5}{2}$	5	$\frac{5}{2}$	$^6I_{5/2}$
Eu^{3+}	$4f^6$	↓	↓	↓	↓	↓	↓		3	3	0	$^7F_0$
Gd^{3+}	$4f^7$	↓	↓	↓	↓	↓	↓	↓	$\frac{7}{2}$	0	$\frac{7}{2}$	$^8S_{7/2}$
Tb^{3+}	$4f^8$	↓↑	↑	↑	↑	↑	↑	↑	3	3	6	$^7F_6$
Dy^{3+}	$4f^9$	↓↑	↓↑	↑	↑	↑	↑	↑	$\frac{5}{2}$	5	$\frac{15}{2}$	$^6H_{15/2}$
Ho^{3+}	$4f^{10}$	↓↑	↓↑	↓↑	↑	↑	↑	↑	2	6	8	$^5I_8$
Er^{3+}	$4f^{11}$	↓↑	↓↑	↓↑	↓↑	↑	↑	↑	$\frac{3}{2}$	6	$\frac{15}{2}$	$^4I_{15/2}$
Tm^{3+}	$4f^{12}$	↓↑	↓↑	↓↑	↓↑	↓↑	↑	↑	1	5	6	$^3H_6$
Yb^{3+}	$4f^{13}$	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑	↑	$\frac{1}{2}$	3	$\frac{7}{2}$	$^2F_{7/2}$
Lu^{3+}	$4f^{14}$	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑	0	0	0	$^1S_0$



4f

5f

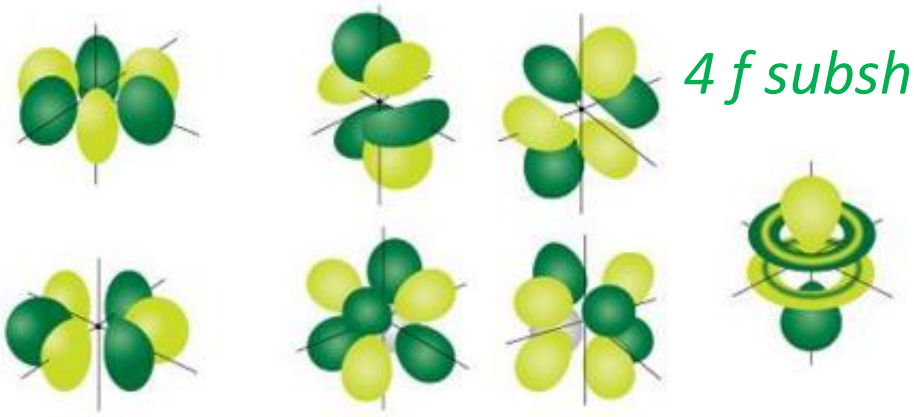
Lanthanides

Actinides

Antiferromagnetic

Ferromagnetic

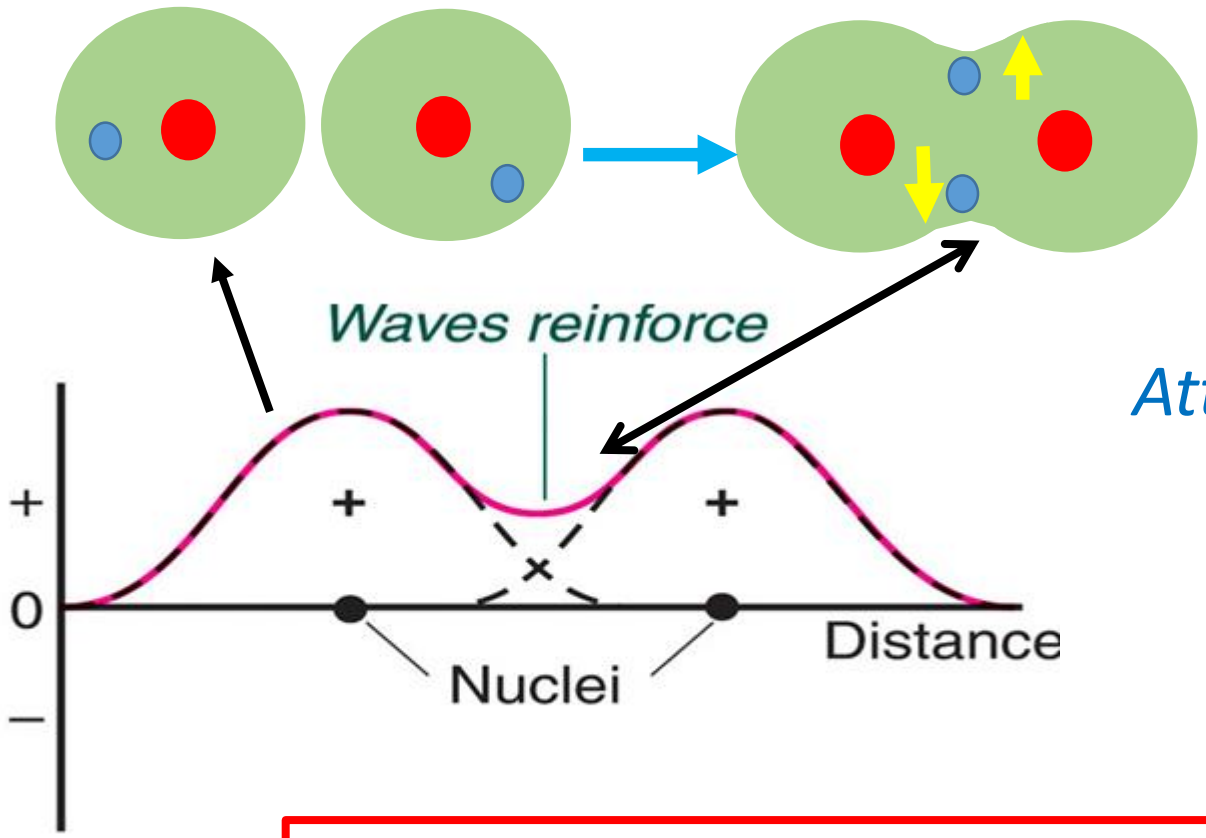
diamagnetic



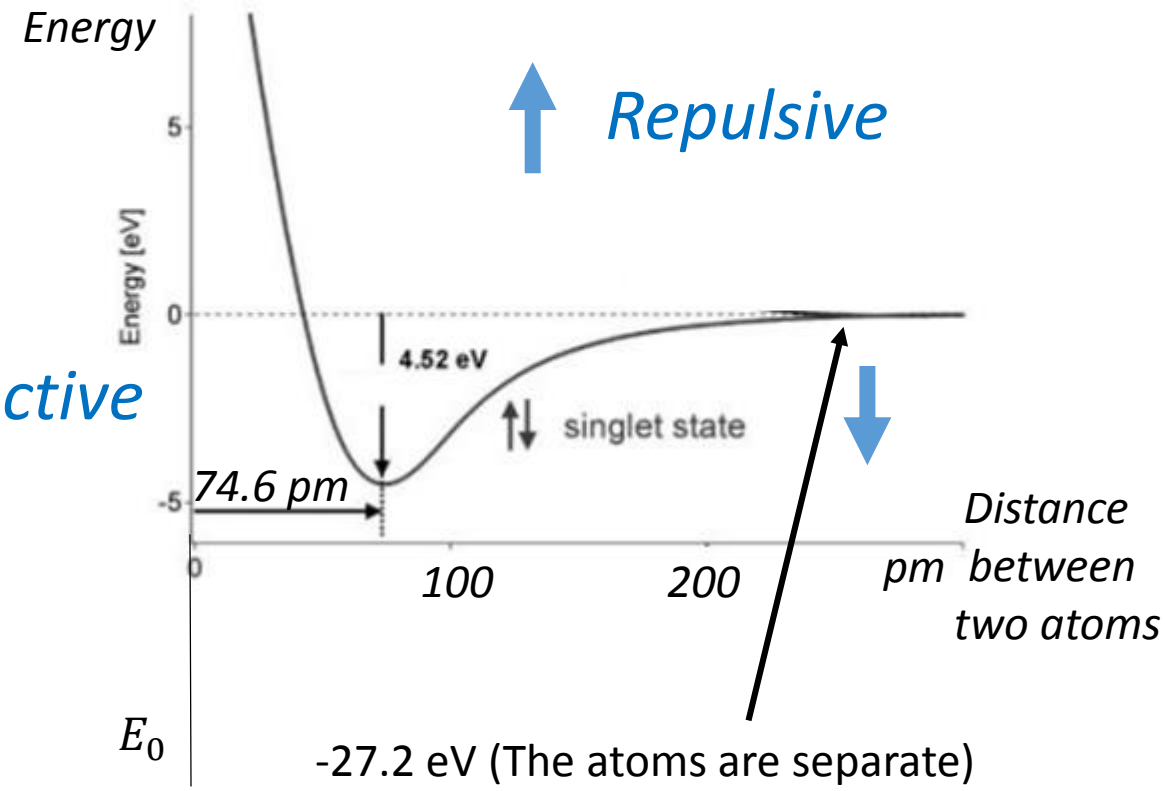
4 f subshell

Orbital model for H_2

Bonding



Attractive

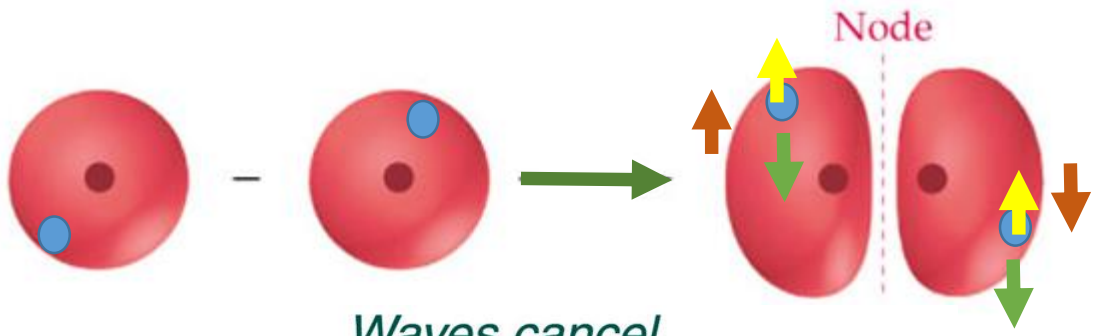


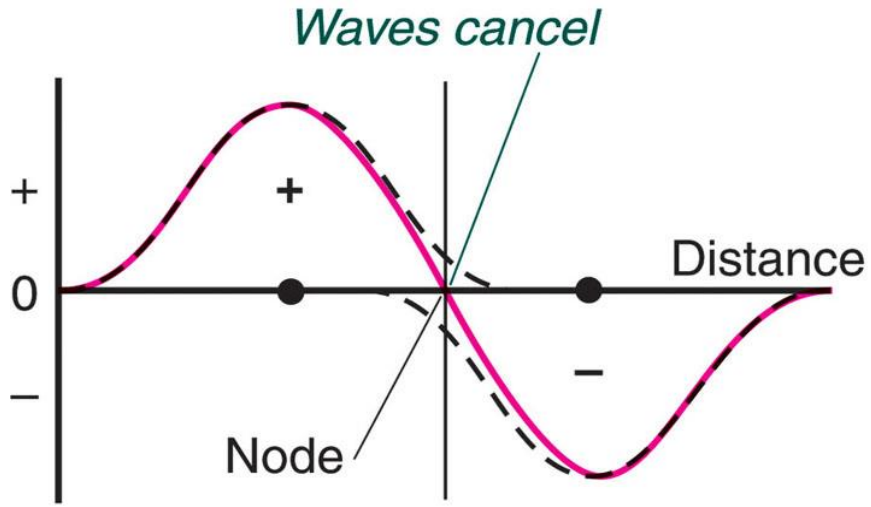
Pauli exclusion principle forbid the same spin orientation.

symmetric for the waves, antisymmetric for the spin

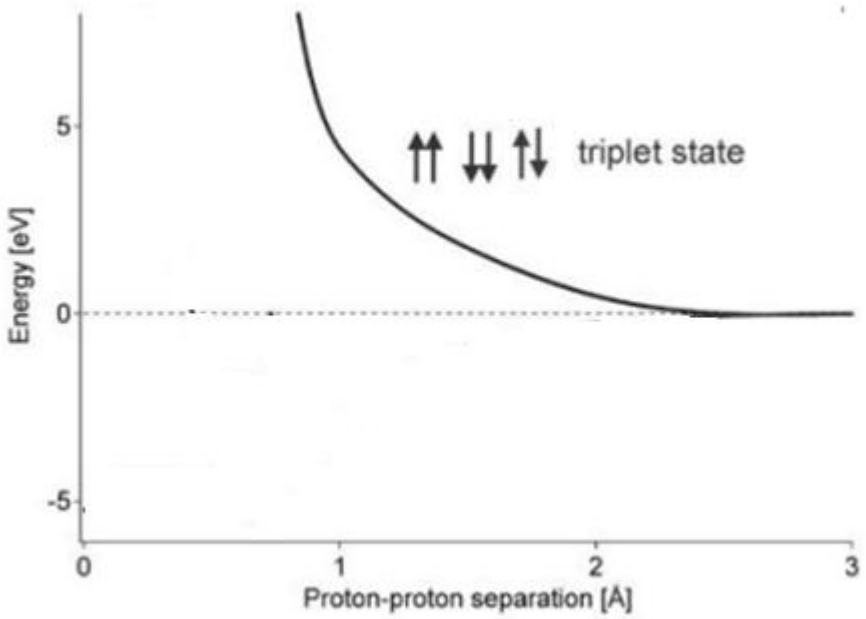
Orbital model for H_2

Antibonding





Antibonding
Not stable (Coulomb repulsion between protons)



Two different orbits 1S allow the same spin orientation.

symmetric for the spin, antisymmetric for the waves

Band theory (Solid state physics)

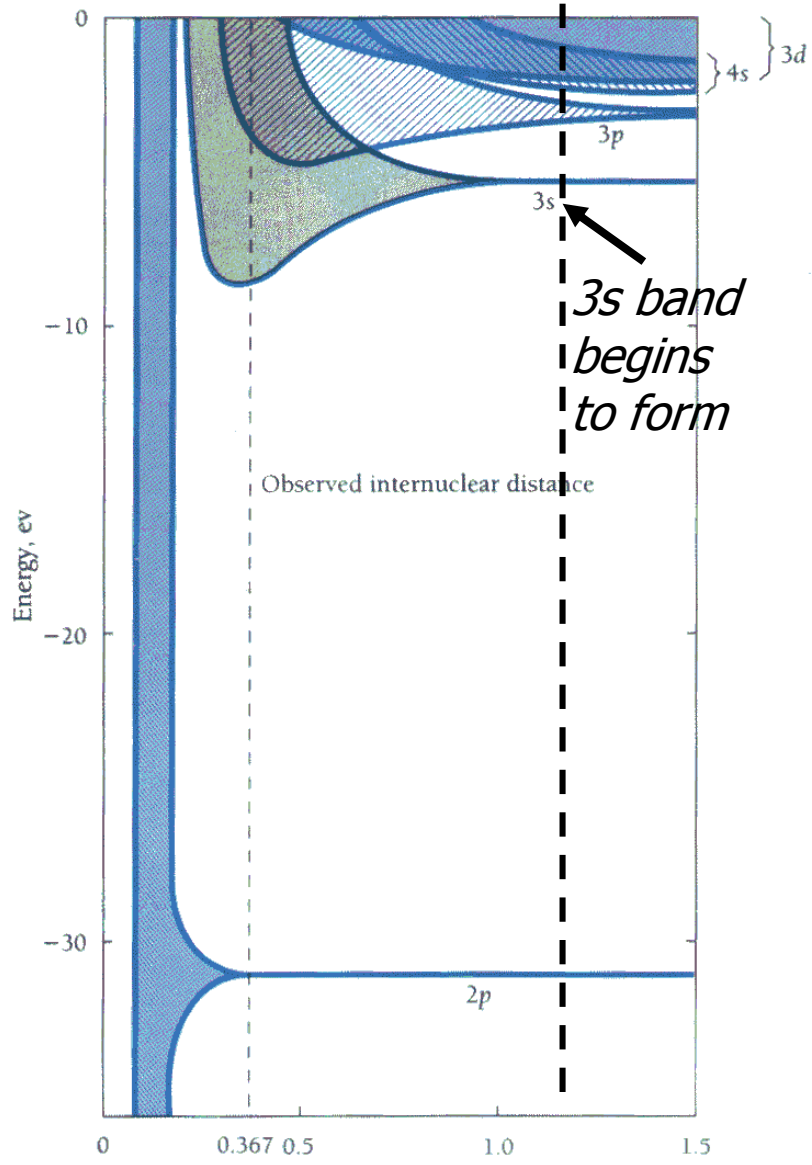
Now let's take a closer look at the energy levels in solid sodium. Remember, the 3s is the outermost occupied level

When sodium atoms are brought within about 1 nm of each other, the 3s levels in the individual atoms overlap enough to begin the formation of the 3s band.

The 3s band broadens as the separation further decreases

Na

$1s^2 2s^2 2p^6 3s^1$



3s band begins to form

Sommerfeld model of free electrons (1928)

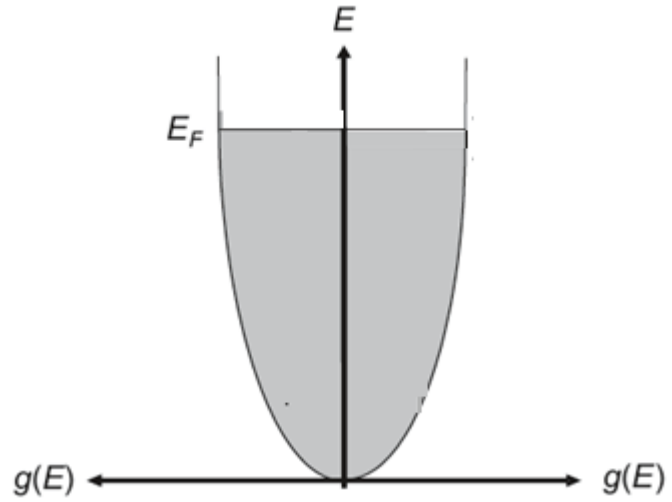
1) We are in the non relativist case.

2) We don't consider the full subshells $\Sigma L_i=0$ *and* $\Sigma S_i=0$ *until the subshell 3p (included). It is a have a positive ion.*

3) We consider the itinerant electrons as a gas (the electrons inside the subshell 3d and the last subshell 4s).

4) The itinerant electrons have a kinetic energy only.

5) It is a first approximation.



Heisenberg uncertainty principle (1927)

$$\Delta p * \Delta r \geq \hbar/2$$

1)The Pauli exclusion principle and the uncertainty principle limit the number of electrons with a low velocity.

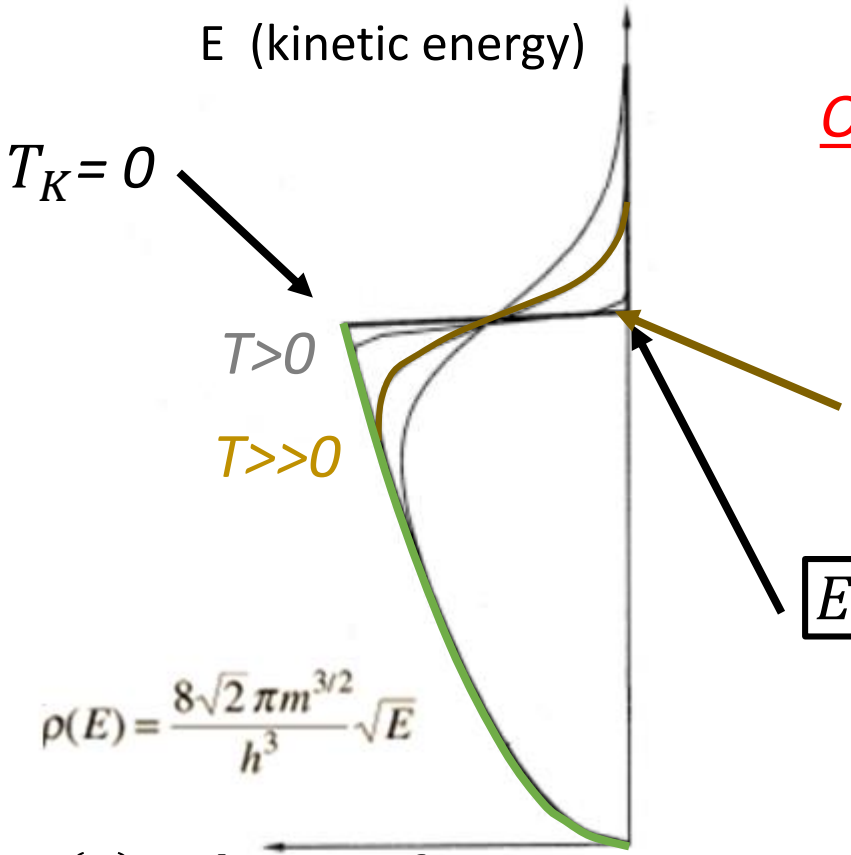
2) If you increase the number of electrons , you must increase their velocity because all the states with a lower energy are busy…

Fermi-Dirac distribution (Sommerfeld model)

- *Each state can hold 2 electrons of opposite spin (Pauli's principle).*
- ***Near zero degree Kelvin the free electrons have a kinetic energy.***

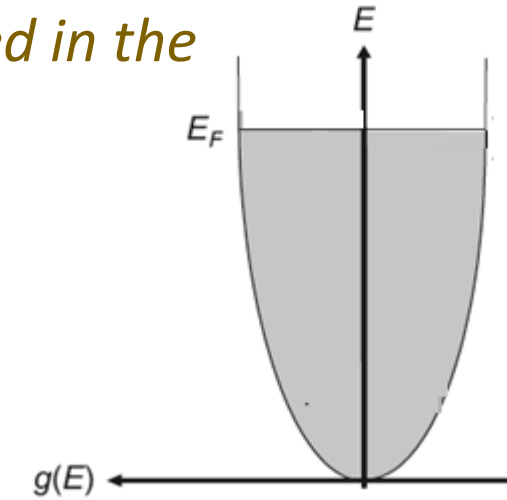
For a transition metal, the augmentation of temperature is created by the nucleus vibrations . These vibrations obey to a Bose-Einstein distribution.

Only the free electrons near the Fermi are sensitive to the temperature (Fermi-Dirac distribution).



The spin of these particles is oriented in the sense that the external field.

$E_F\ (Fermi\ energy)$



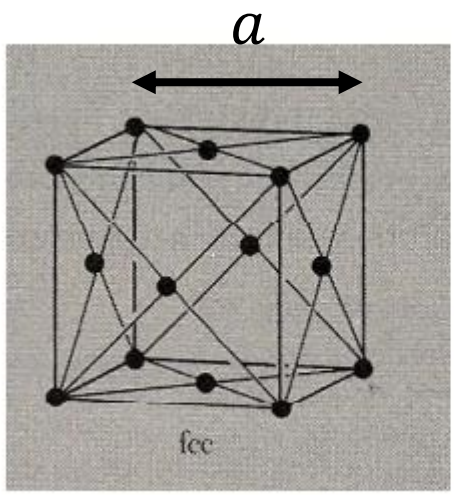
$T \approx 0K$

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2 \eta_e\right)^{2/3}$$

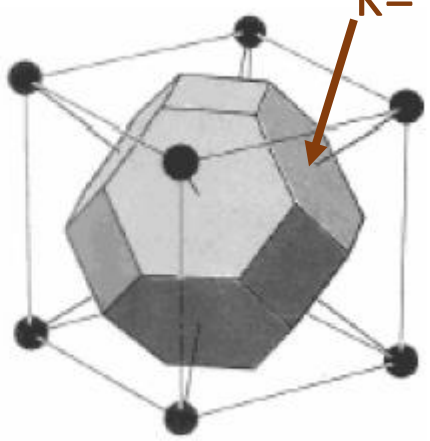
Fermi Parameters for some metals (Sommerfeld model)

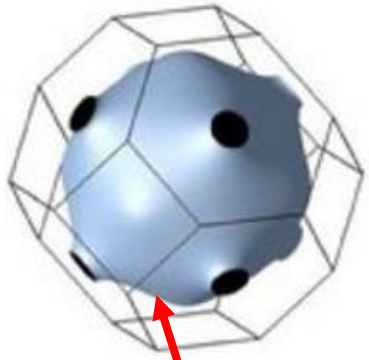
Element	Molar volume	electrons	density	Fermi energy calculated	Fermi temperature	Fermi velocity	electrons cm-3
	m^3/mol		g/cm^3	E_F[eV]	T_F[10^3K]	10^8 cm^{-1}	
Scandium	15,00×10-6	21	2.985				4.01 10^22
Titanium	10,64×10-6	22	4.506				5.67 10^22
Vanadium	8,32×10-6	23	6.01				7.20 10^22
Chromium	7,23×10-6	24	7.19				8.33 10^22
manganese	7,35×10-6	25	7.31	10.9	12.7	1.96	8.19 10^22
Fe	7,09×10−6	26	7.874	11.15	12.94	1.98	8.49 10^22
Co	6,67×10-6	27	8.9	11.7	13.58	2.03	9.01 10^22
Ni	6,59×10-6	28	8.902	11.74	13.62	2.03	9.14 10^22
Cu	7,11×10-6	29	8.96	7.04	8.17	1.57	8.47 10^22
Zn	9,16×10-6	30	7.14	9.47	10.9	1.82	6.57 10^22

Fermi surface for Ag Bloch model 1946 (crystallography)



Crystalline structure for Ag



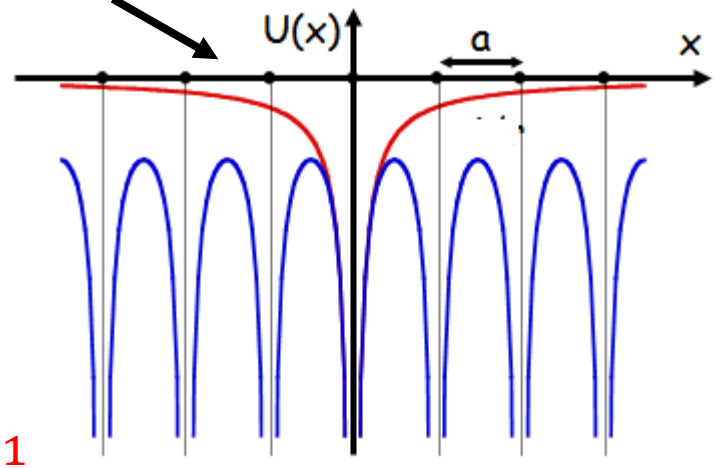


Fermi surface

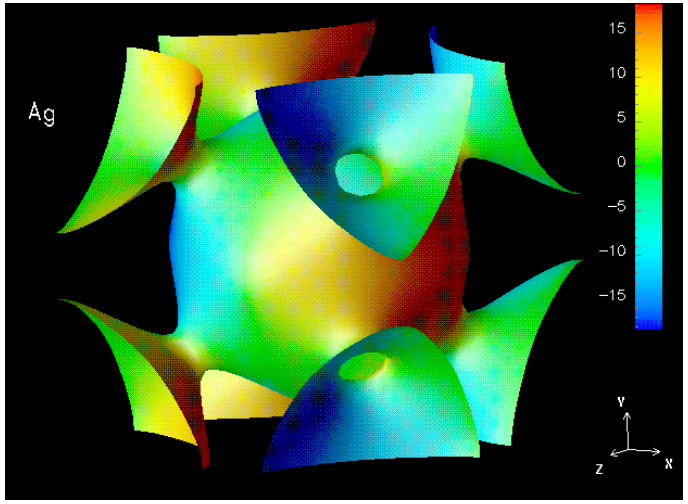
$k_F = 12.\ 10^9\ m^{-1}$

k= $\frac{4\pi}{a}$ = 39.2 $10^9 m^{-1}$

Atomic nucleus



The reference for k is the radius of the atom



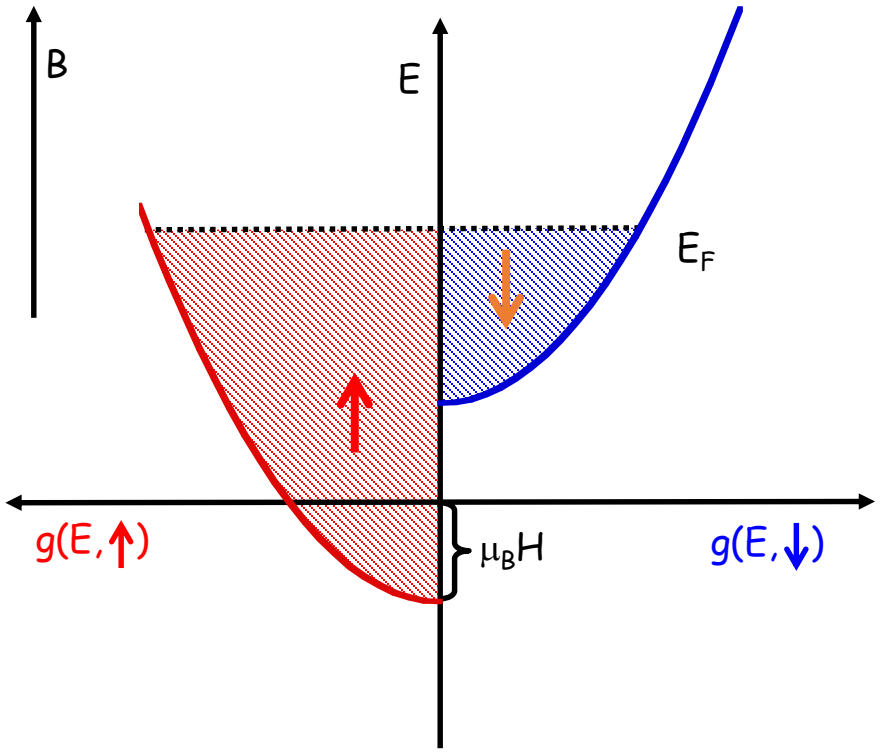
$p * \lambda = h$

$p = \hbar * k$

A velocity in a direction isn't possible if the wavelength is already occupied by a distance between two atoms.

$\frac{p}{\hbar}$ = k< $4\pi/a$

Free Electrons for the metals in a Magnetic Field (Pauli paramagnetism)



"The difference between paramagnetism and Pauli paramagnetism is that the latter applies to a metal because it describes the tendency of free electrons in an electron gas to align with an applied magnetic field." Inna Vishik (Standford)

Magnetic Spin – Susceptibility
Low temperature

$$\chi_P = \frac{M}{H} = \frac{3\eta_e \mu_0 \mu_B^{\ 2}}{2E_F}$$

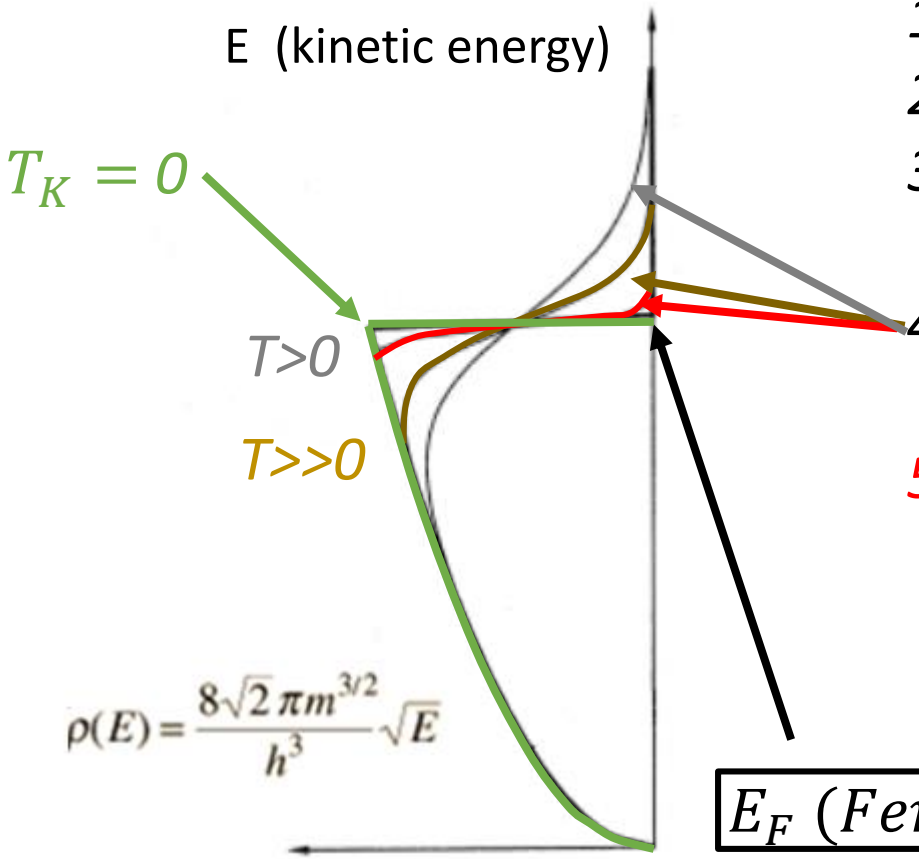
(Pauli Paramagnetism)

W. Pauli
Nobel Price 1945

Titanium	Pauli magnetic susceptibility (χ_{mol})	$33.4\ 10^{-6}\ cm^3/mol$
Vanadium	Pauli magnetic susceptibility (χ_{mol})	$84.2\ 10^{-6}\ cm^3/mol$

Paramagnetism for free electrons.

Fermi gas of electrons without an external magnetic field.
The electrons are free (no subshell)



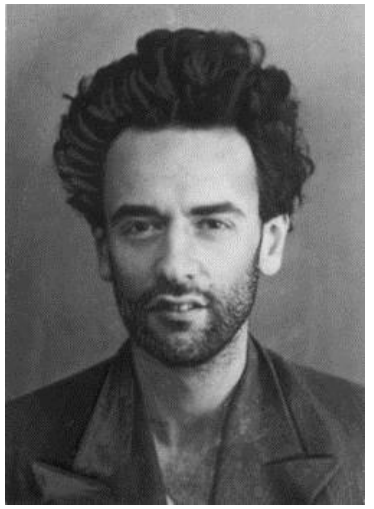
1) The order of the Fermi kinetic energy is high T ≈10 000 K.
2) The reference temperature is ≈ 300K.
3) The thermal energy can increase the kinetic energy only for a very small number of particles.
4) The spin of these particles is oriented in the sense that the external field.
5) The paramagnetism is created by these electrons…

$$\chi_{Pauli} \sim \chi_{curie}\left(\frac{T}{T_F}\right) \sim \chi_{Pauli}\ 10^{-2}$$

T≈ 0K

T≈ 300K

Landau diamagnetism (1930) $T \approx 0K$



1) A gas of free electrons in a magnetic field.
2) Free electrons move along spiral trajectories.
3) Lenz's law.
4) Diamagnetic effect.
5) The energy of the free electrons depend of
A) The kinetic energy is principally limited by the energy of Fermi.
B) The quantification of the energy created by the circular movement of the electrons

$$E_l = (l + \tfrac{1}{2})\hbar\omega_c.$$

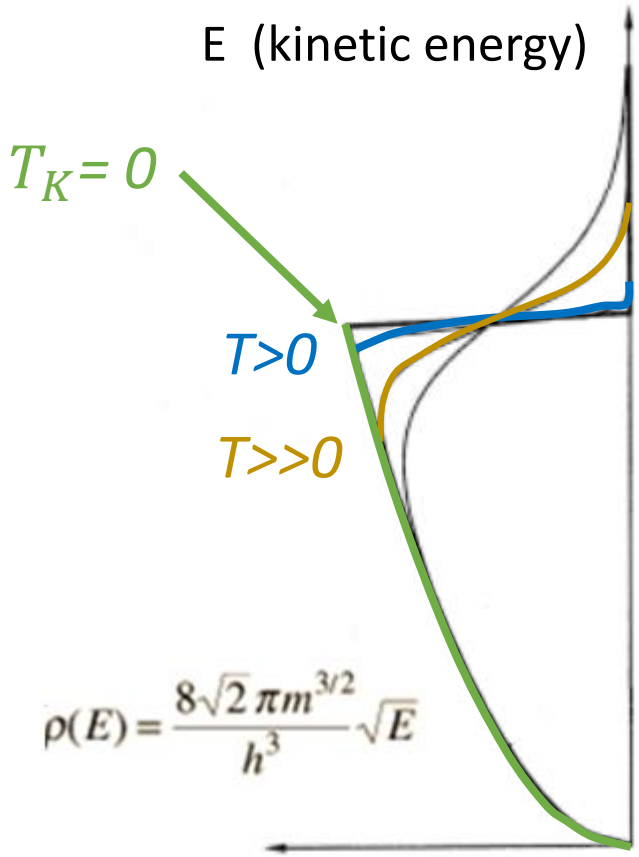
$$M_{Landau} = -\frac{N\mu^2}{2k_B T_F} B$$

$$\chi_{Landau} = -\frac{\chi_{Pauli}}{3}$$

Titanium	*Landau diamagnetic susceptibility (χmol)*	$-11.1\ 10^{-6}\ cm^3/mol$
Vanadium	*Landau diamagnetic susceptibility (χmol)*	$-28.6\ 10^{-6}\ cm^3/mol$

Landau diamagnetism $T \approx 0K$

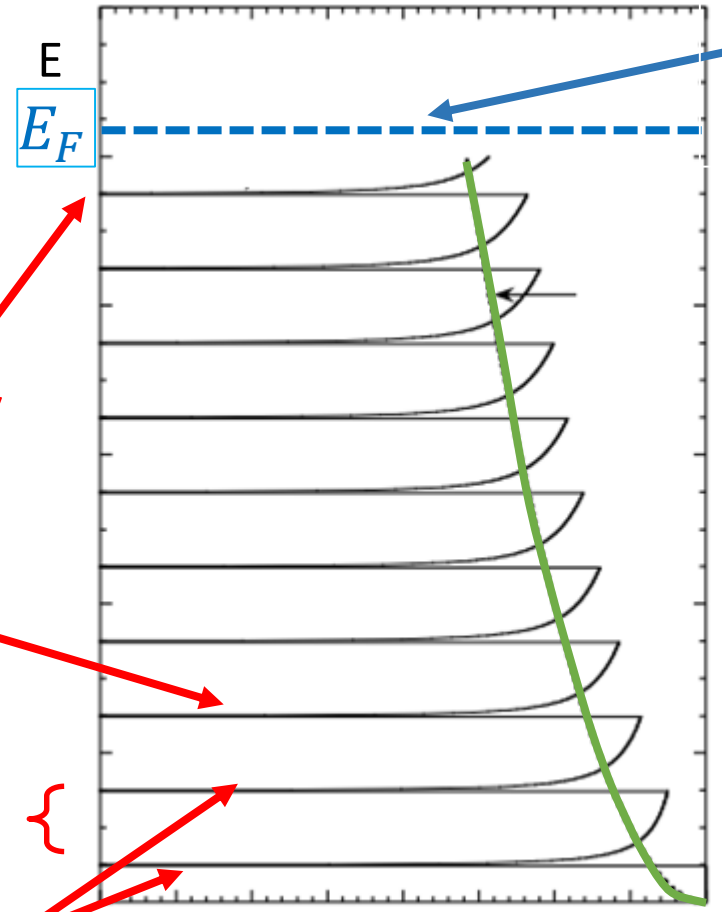
Fermi gas of electrons without an external magnetic field.



$\rho(E) = density\ of\ states$

Fermi gas of electrons with an external magnetic field.

The oscillations are impossible



B

Kinetic energy + oscillator energy

$\frac{5}{2}\omega_c$

$\omega_c = \frac{e\,H}{mc}$ {

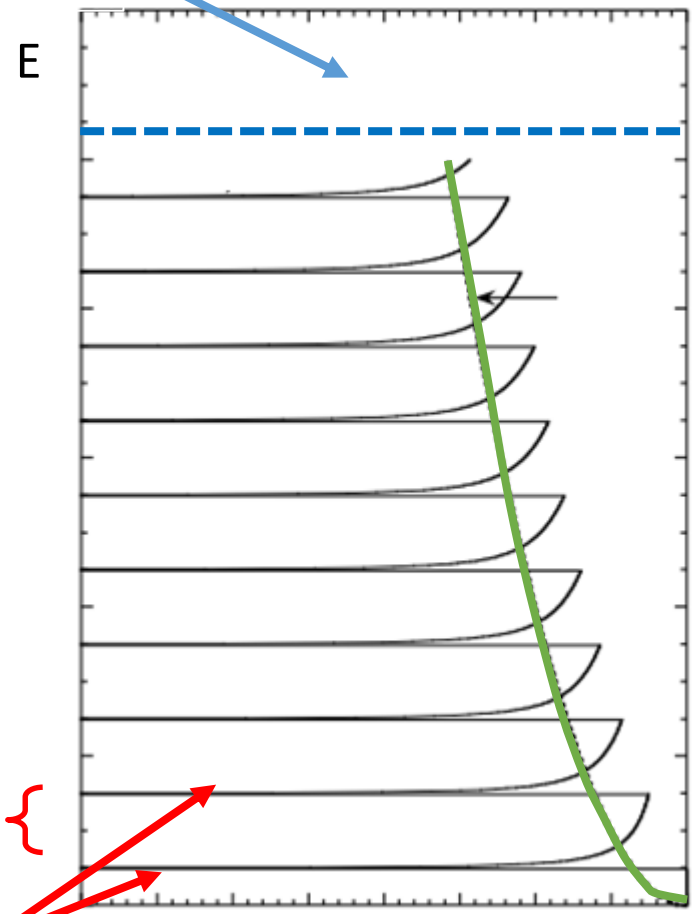
Cyclotron frequencies

$\rho(E) = desity\ of\ states$

Scan in energy when we modify B

Haas-van Halphen effect (1930) $T \approx 0K$

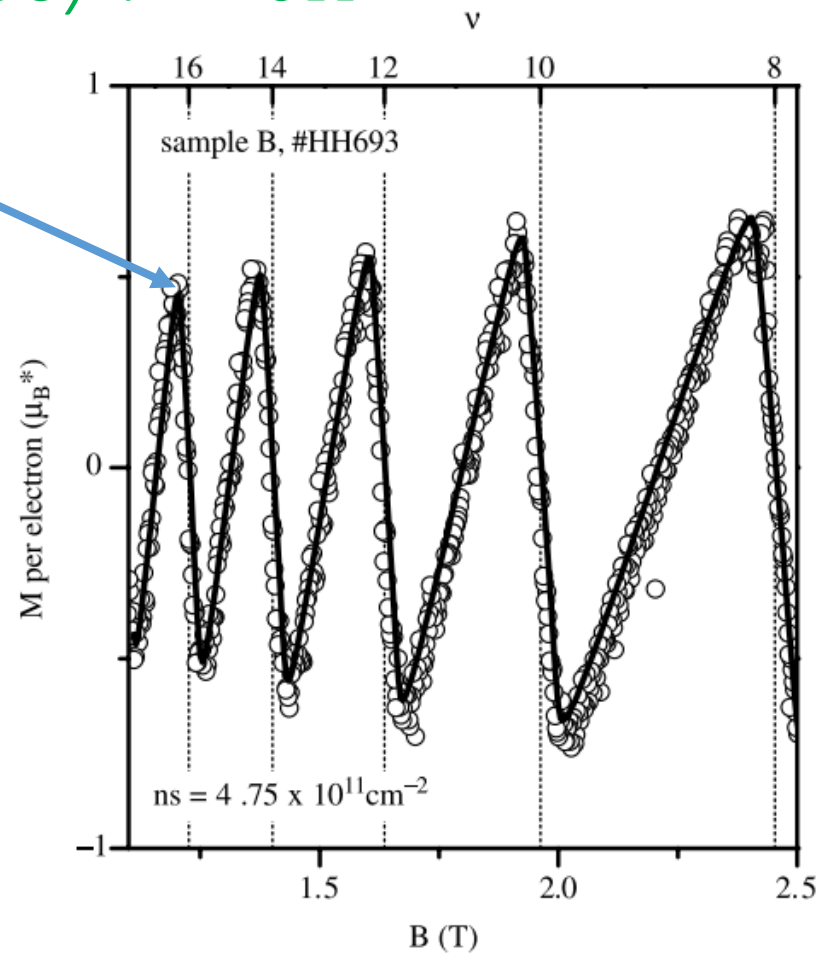
The oscillations are impossible



$\omega_c \uparrow if\ H \uparrow$

$$\omega_c = \frac{e\,H}{mc}$$

Cyclotron frequencies

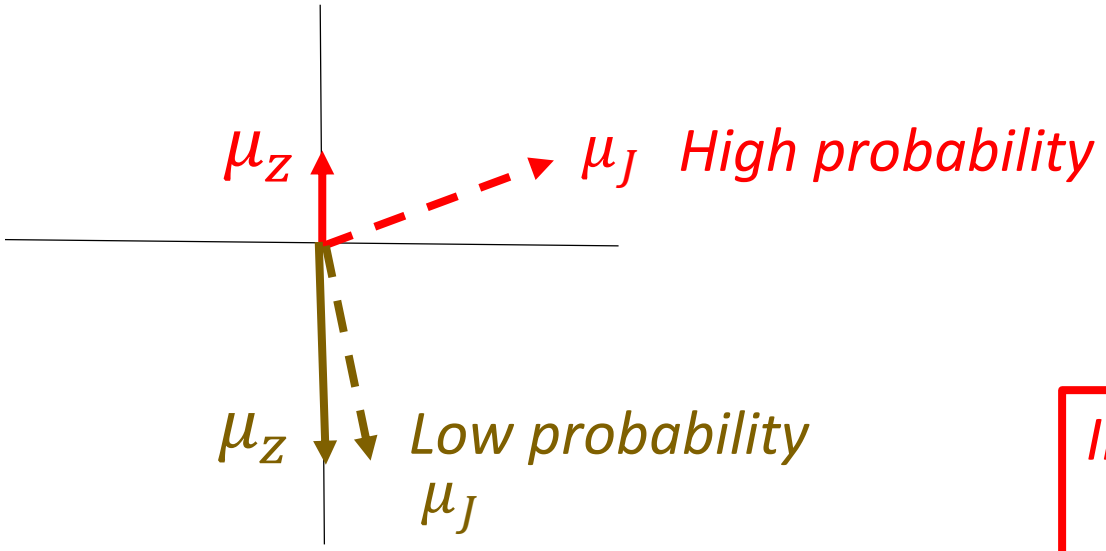


1) *The cyclotron frequencies increase with the magnetic field.*
2) *The diamagnetic field increase with the energy.*
3) *The diamagnetic field stopped with the E_F.*
4) *The diamagnetic field increase again with the next cyclotron frequency.*

Brillouin-Langevin paramagnetism (statistical physics)

1) *Each atom is independent.*
2) *For each atom, the total magnetic moment μ_J(orbitals + spin) is the same for each atom. It is calculate with the quantum mechanics.*
3) *The distribution of the magnetic moments obey to the Boltzmann distribution.*
4) *We calculate < total magnetic moment > for one atom and we multiply by N.*
5) *We use the Z axis as reference.*

B ↑



$$\mu_J = g_J \mathrm{J}\, \mu_b$$

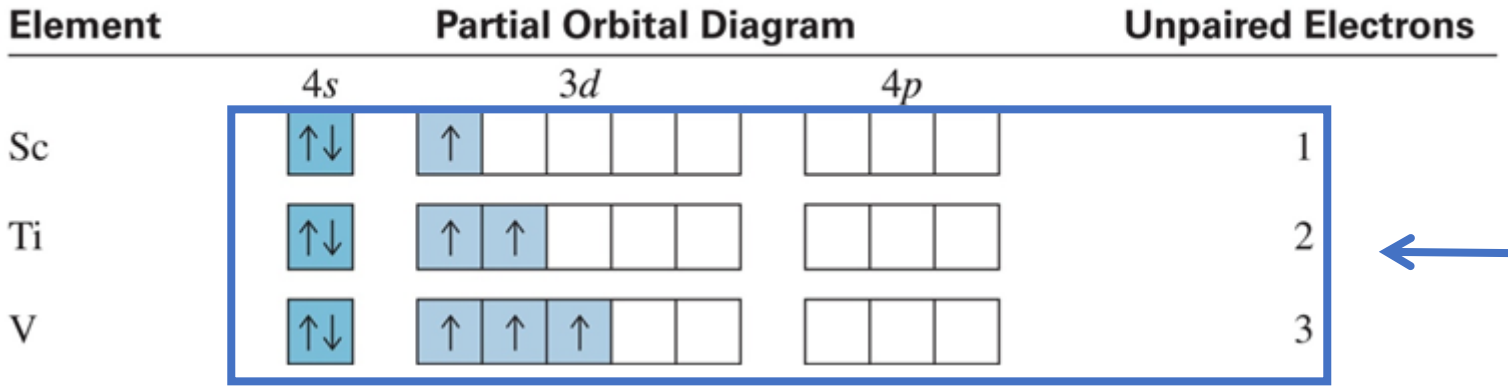
$$\mu_z = g_J \mathrm{m}\, \mu_b$$

In quantum mechanics the number of orientations is limited

Paramagnetism (quantum mechanics)

Scandium	Electrical resistivity	55×10^{-8} Ω m (at 20 °C)
	Magnetic susceptibility (χmol)	+ 3.956 10^{-9} m^3/mol
	Electronegativity	Pauling scale: 1.36
Titanium	Electrical resistivity	40×10^{-8} Ω m (at 20 °C)
	Magnetic susceptibility (χmol)	+1.919 10^{-9} m^3/mol
	Electronegativity	Pauling scale: 1.54
Vanadium	Electrical resistivity	20×10^{-8} Ω m (at 20 °C)
	Magnetic susceptibility (χmol)	+3.199 10^{-9} m^3/mol
	Electronegativity	Pauling scale: 1.63

1) The valence electrons are more located in the 3d subshell 4S.
2)The number of electrons with the same spin orientation is limited.



Paramagnetic

Remark:
Electronegativity *is a chemical property that describes the tendency of an atom to attract electrons.*

http://www.periodictable.com/

Langevin diamagnetism

$< r^2 > \approx 1$

$$\chi \approx -0.99\ 10^{-5}\ Z \left(\sum_{i=1}^{Z} \frac{1}{Z} <0 \left[\frac{r_i^2}{a_0^2} \right] 0> \right)$$

$\approx$ Borh radius

Atom radius

Copper

Electrical resistivity	16.78 nΩ·m (at 20 °C)
Electronegativity	Pauling scale: 1.90
Magnetic susceptibility	-6.86×10^{-11} m^3/mol

Zinc

Electrical resistivity	59.0 nΩ·m (at 20 °C)
Electronegativity	Pauling scale: 1.65
Magnetic susceptibility(χ_{mol})	-1.45×10^{-10} m^3/mol

1)The number of electrons with the same spin orientation is limited.

2) The external field modify the external orbit.

3) By the law Lenz the electrons create a magnetic field in opposition wit the external field.

4) The diamagnetism is localized in the atoms.

Element	Partial Orbital Diagram (4s, 3d, 4p)	Unpaired Electrons
Cu	↑ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ☐ ☐ ☐	1
Zn	↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ☐ ☐ ☐	0

Diamagnetic

http://www.periodictable.com

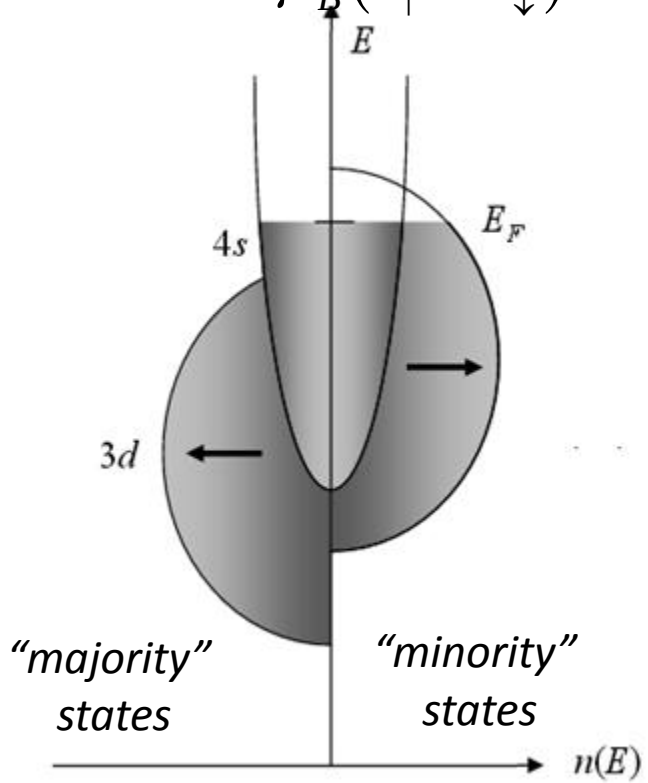
Landau diamagnetism (1930)

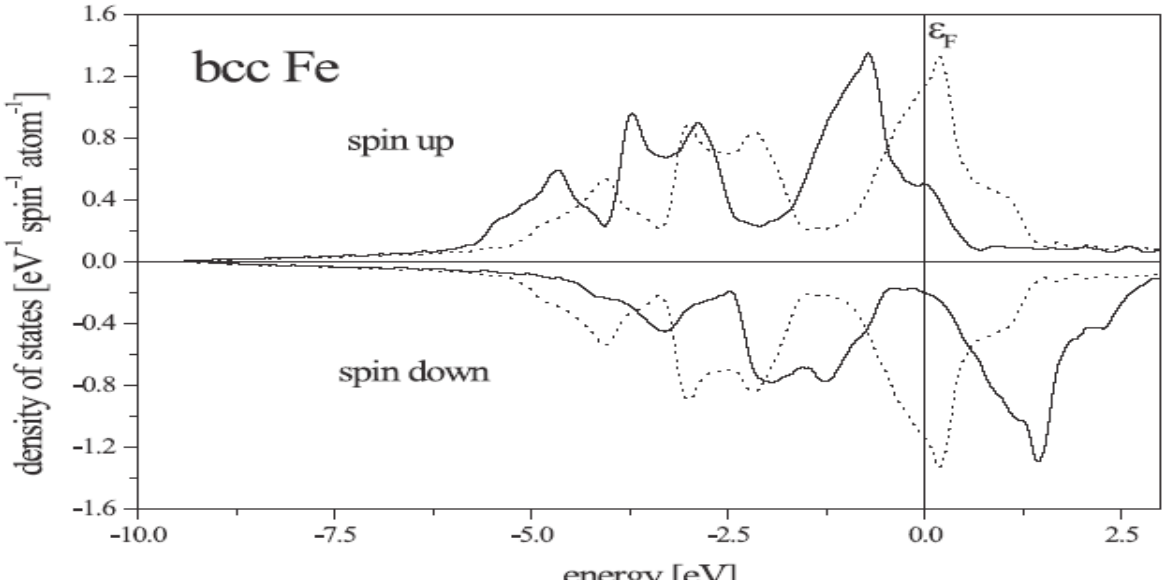
1) A gas of free electrons in a magnetic field.
2) Free electrons move along spiral trajectories
3) Lenz's law
4) Diamagnetic effect

$$M_{Landau} = -\frac{N\mu^2}{2k_B T_F} B \qquad M = M_{Pauli} + M_{Landau} = \frac{N\mu^2}{2k_B T_F} B$$

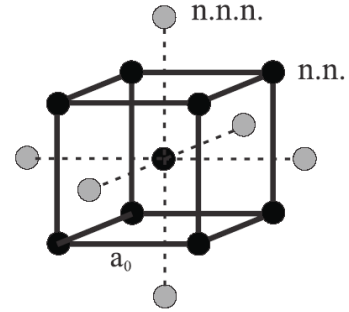
Ferromagnetism (Solid state physics)

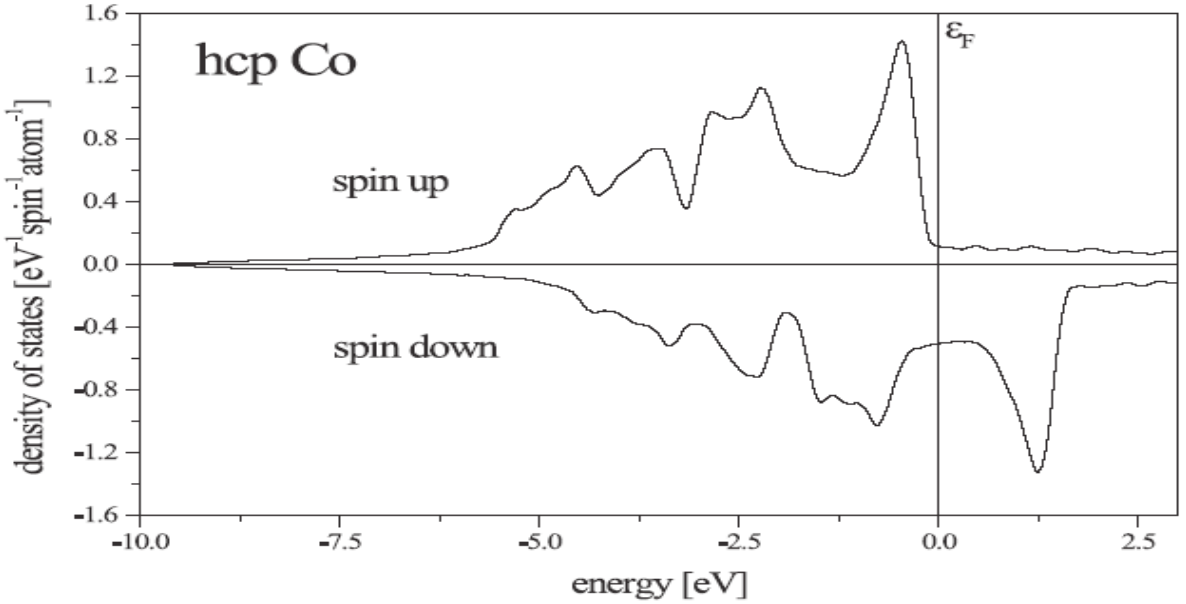
$$M = \mu_B\left(n_\uparrow - n_\downarrow\right)$$





Fe: weak ferromagnet (almost)

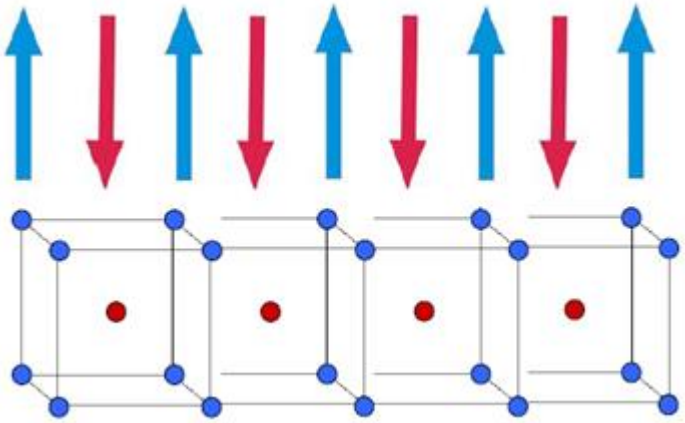


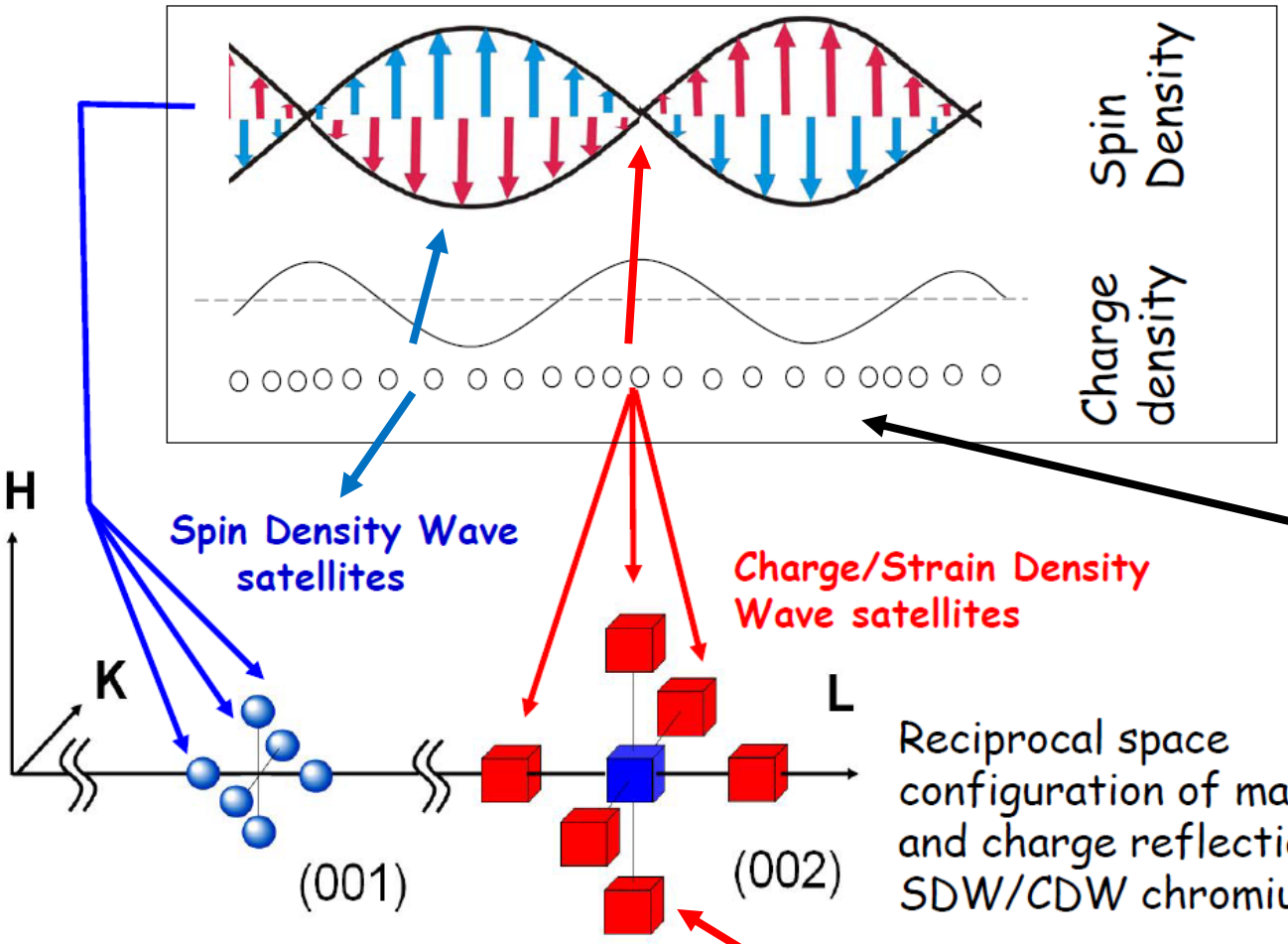


Co: strong ferromagnet

Antiferromagnetism chromium (molecular physic)

Uniform distance between the atoms.





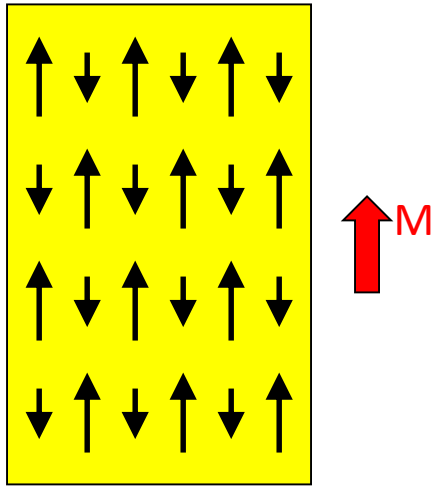
Non uniform distance between the atoms.

Reciprocal space configuration of magnetic and charge reflection of SDW/CDW chromium

Commensurate SDW (C-SDW)
Wave follows periodicity of underlying atomic lattice

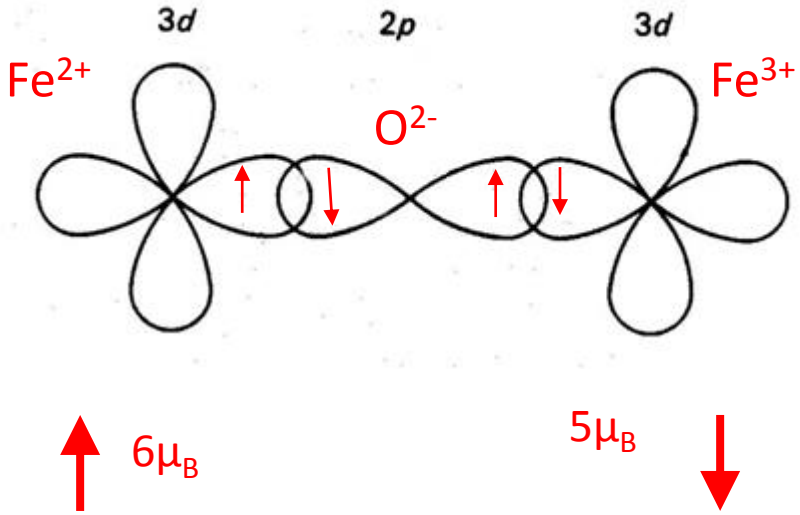
To reduce the energy , we have a alternation of the total magnetic moment (Pauli principle)

Ferrimagnetism (molecular quantum physic)

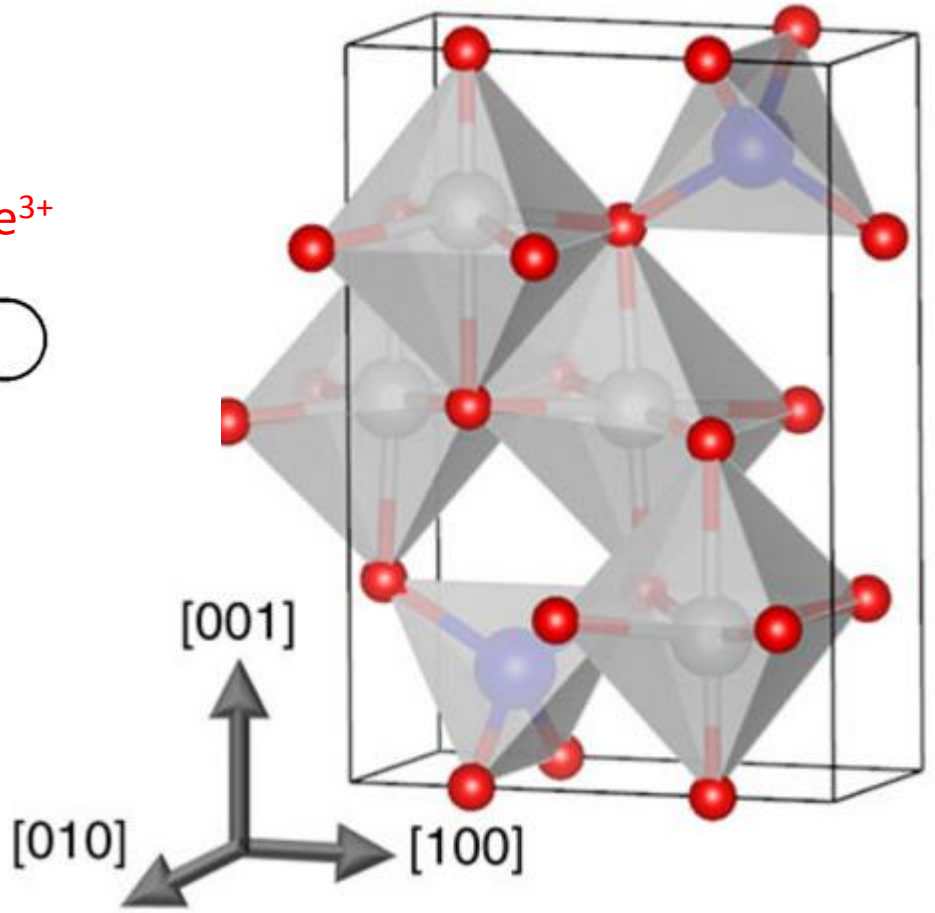


Ferrimagnets (ferrites) behave similar to ferromagnets

Super-exchange interaction



Magnetite (Fe_3O_4)



Oxygen atoms (small sphere in red)

Fe2+ (tetrahedral sphere in blue) , Fe3+ (octahedral sphere grey)