chapter 2: magnetism in metals (lecture #3)

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Dresden, November, 1st, 2021

homework

Further work

✓ Check Hund‘s rules!

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…last slide shown by Laura Corredor Bohorquez…..

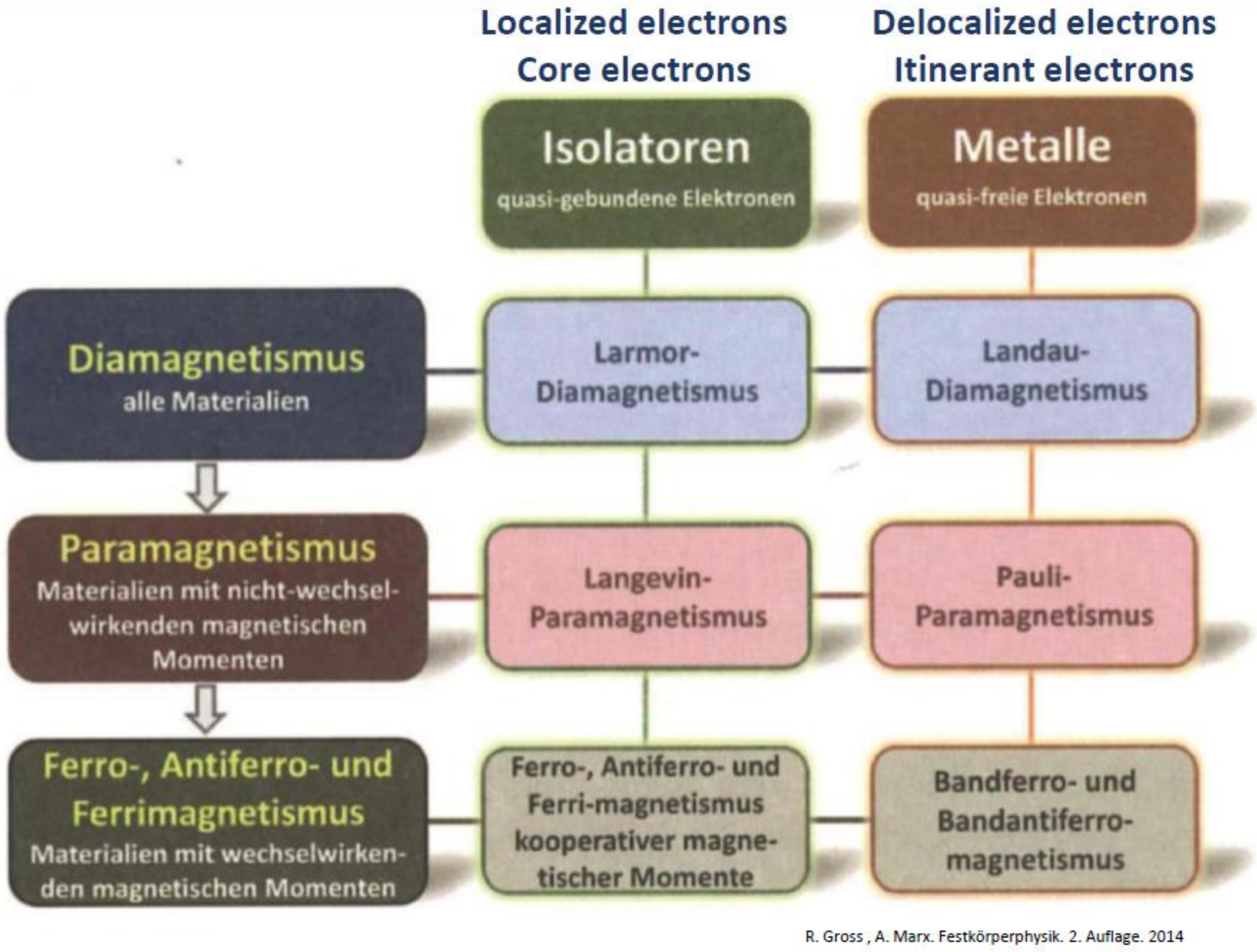
reminder and to start with:

how to approach the magnetic properties of a material

example: $Bi_{25}FeO_{39}$ (mineral: sillenite)

localized electrons or itinerant electrons?

example: $Bi_{25}FeO_{39}$ (mineral: sillenite)



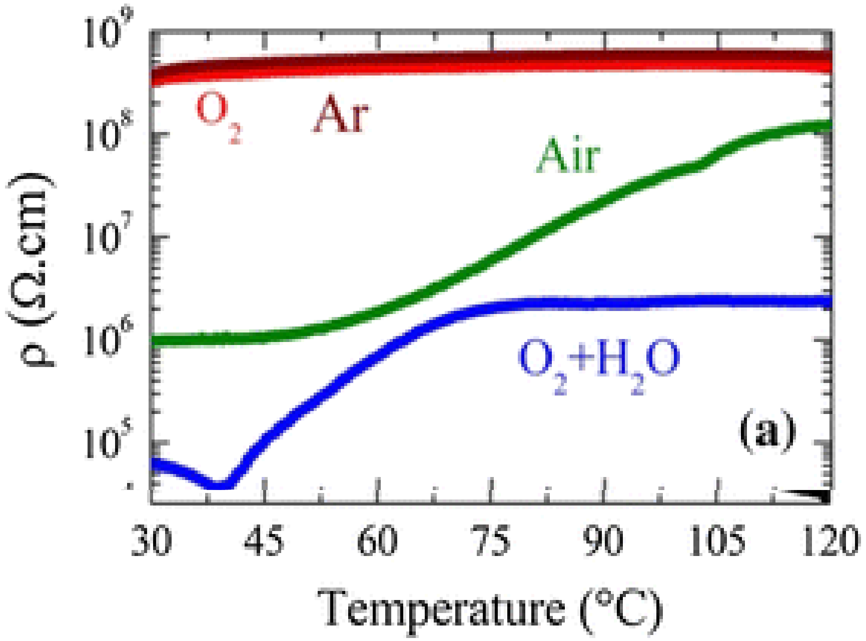
…courtesy Laura Corredor Bohorquez…..

a mineral--- probably localized

localized electrons or itinerant electrons?

example: $Bi_{25}FeO_{39}$ (mineral: sillenite)

resisitivity



+ high resistivity values

+ evolution of resisitivity as function of temperature (for oxygen and argon)

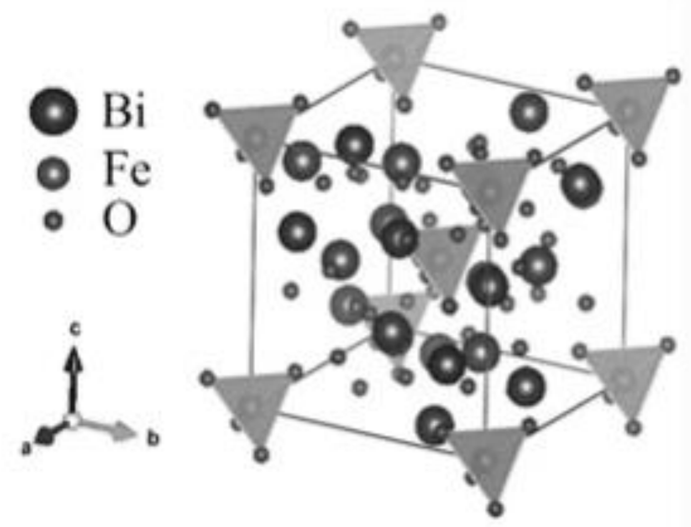
→ indicate localized electrons

F. E. N. Ramirez *et al.*, J. Mater. Science **51**, 10982 (2016)

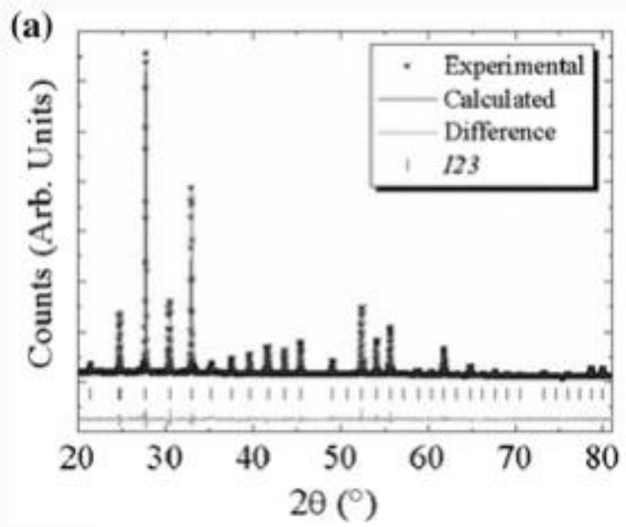
calculate magnetic properties of material with localized electrons

example: Fe^{3+} in $Bi_{25}FeO_{39}$ ferrite (mineral: sillenite)

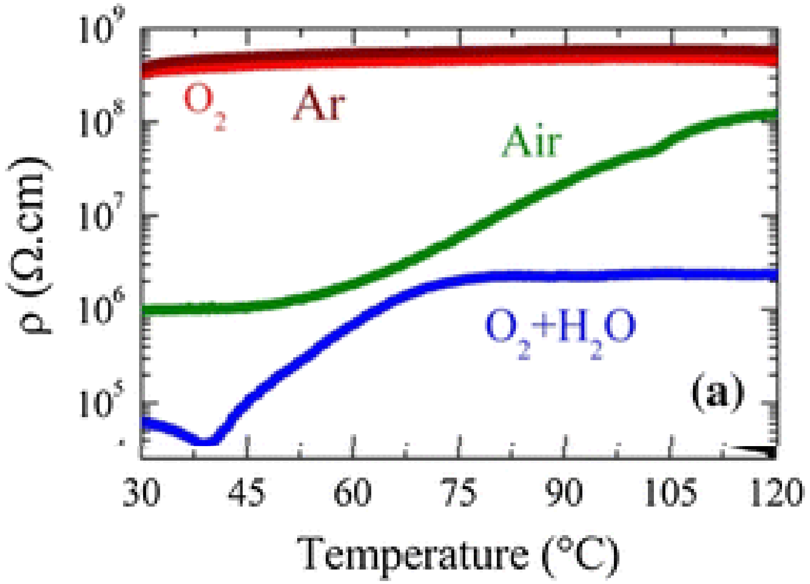
crystallographic structure
cubic space group symmetry (*I23*)



powder x-ray diffraction



resisitivity



high resistivity
→ insulating behaviour
→ localized electrons

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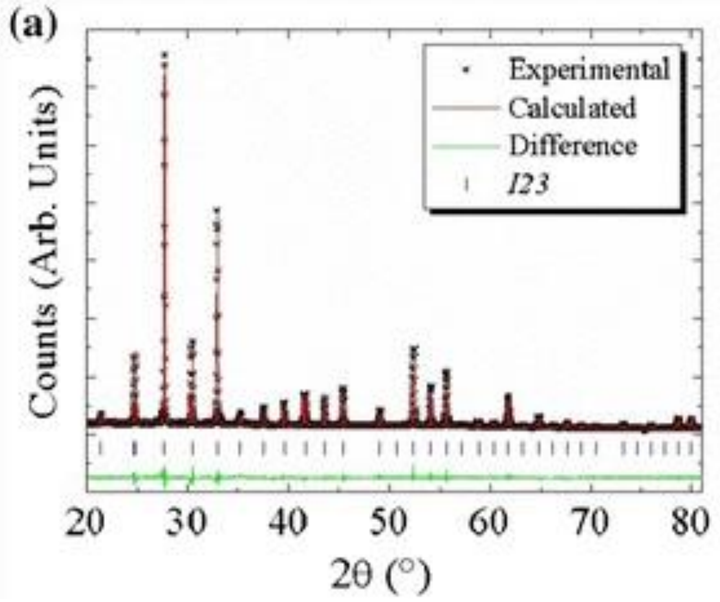
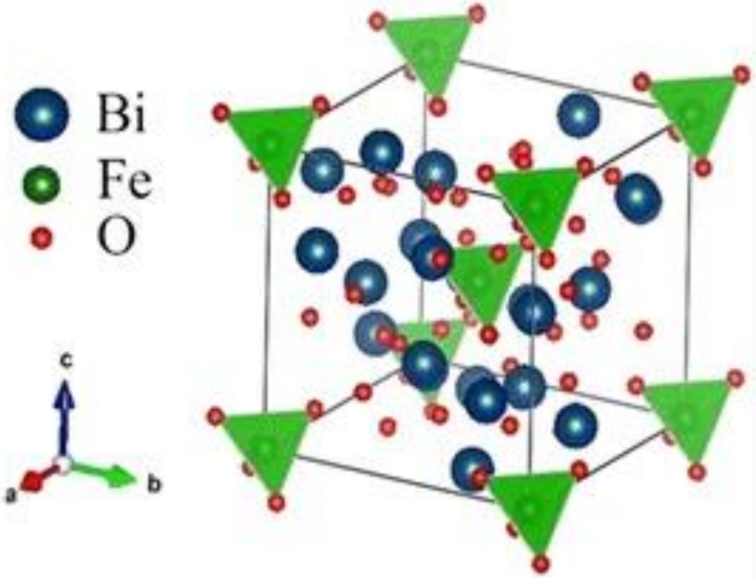
localized electrons and structure?

example: $Bi_{25}FeO_{39}$ (mineral: sillenite)

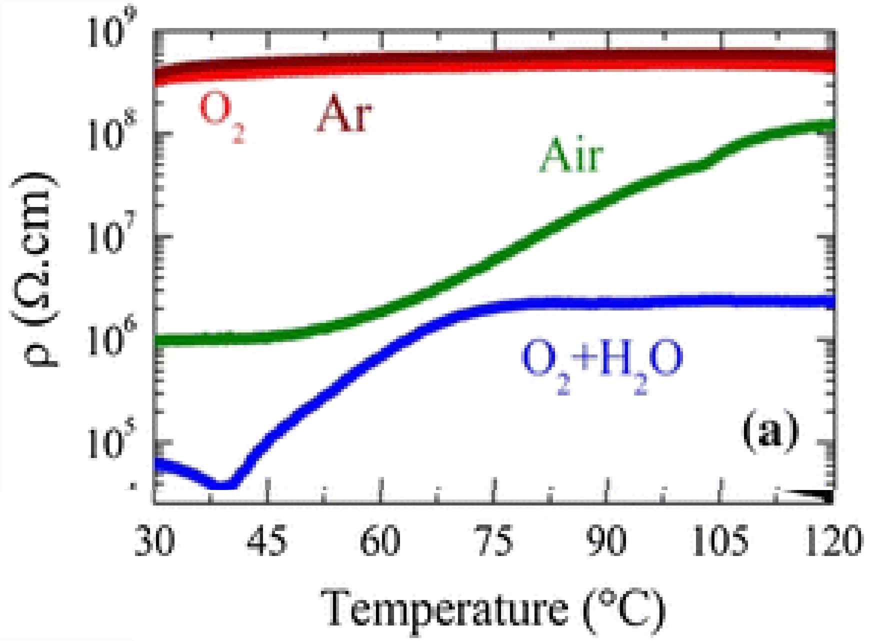
powder x-ray diffraction



crystallographic structure
cubic space group symmetry (*I23*)



resisitivity



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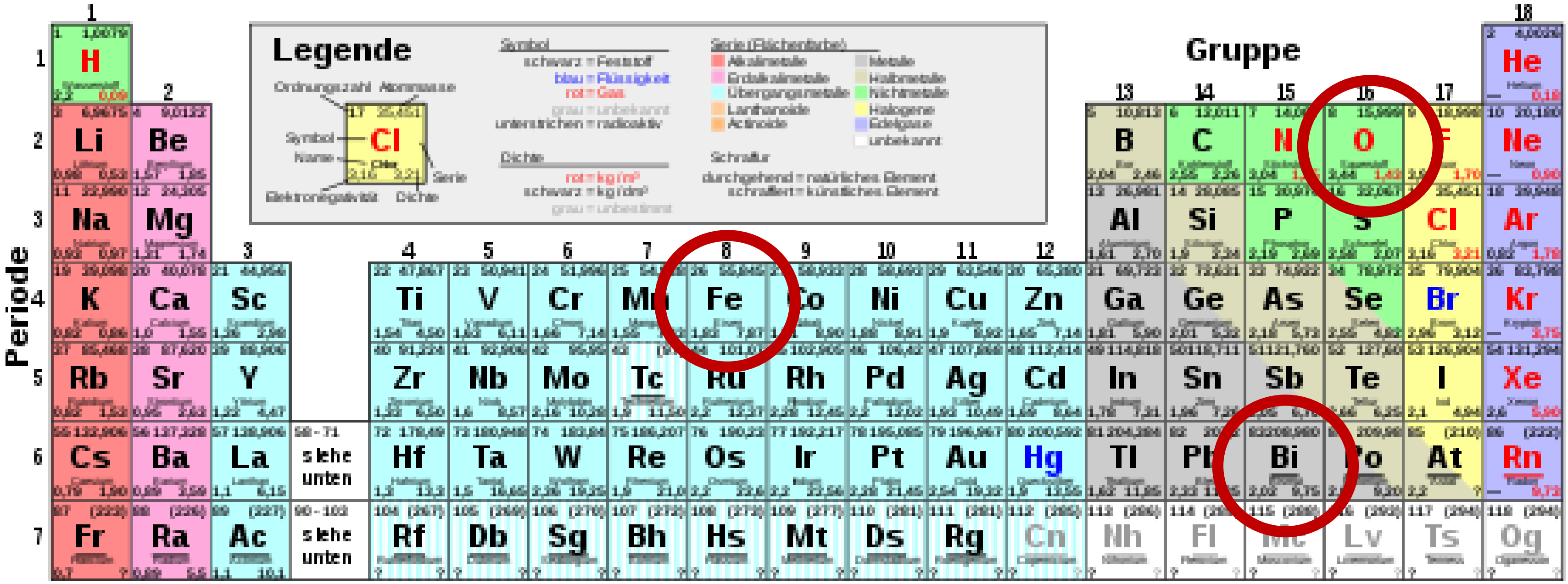
what do you think is the next step???

electronic configurations

Example: $Bi_{25}FeO_{39}$ ferrite



https://de.wikipedia.org/wiki/Periodensystem

elements

O → $1s^2\ 2s^2\ 2p^4$

Bi → [Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^3$

Fe → [Ar] $3d^6\ 4s^2$

ions

O^{2-} → $1s^2\ 2s^2\ 2p^6$

Bi^{3+} → [Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^0$

Fe^{3+} → [Ar] $3d^5\ 4s^0$

O: -II → 39 x (-II) = -78
Bi: +III → 25 x (+III) = + 75

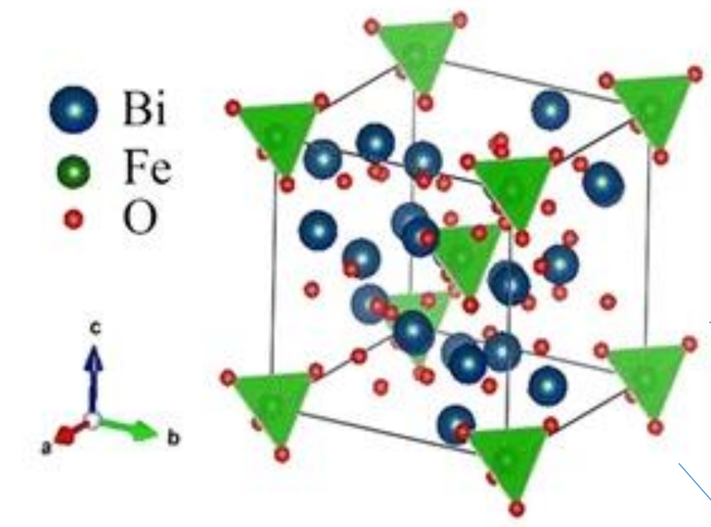
→ Fe: +III

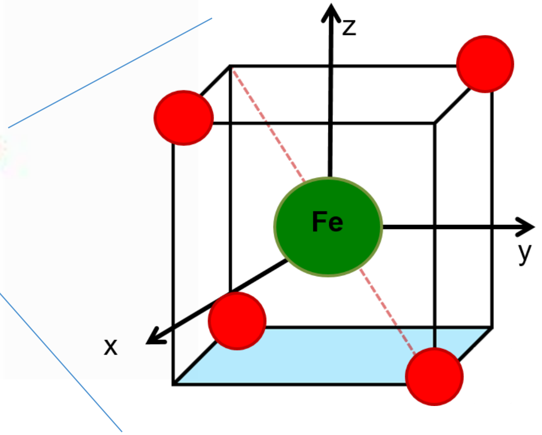
what do you think is the next step???

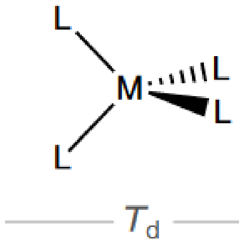
crystal field??

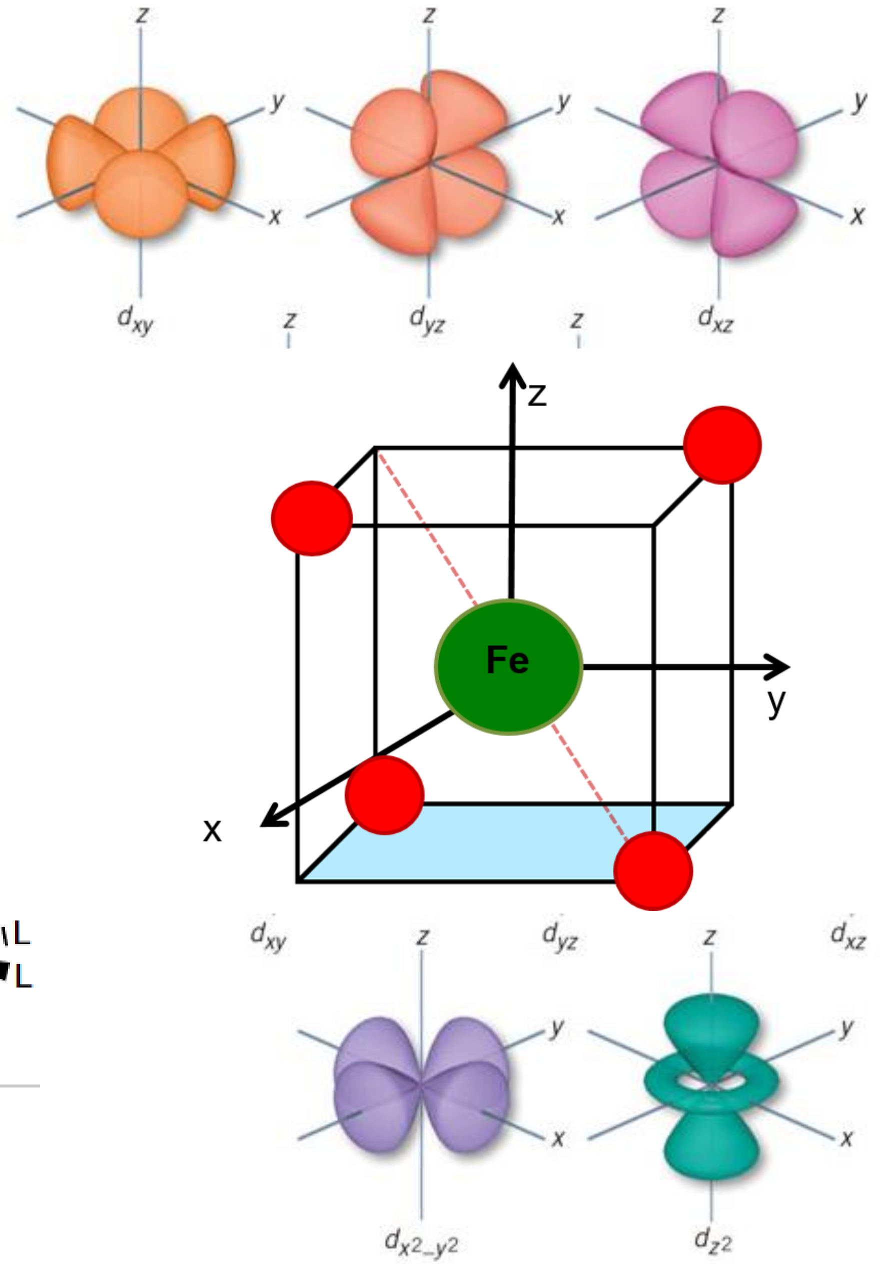
example: $Bi_{25}FeO_{39}$ (mineral: sillenite)

crystallographic structure
cubic space group symmetry (*I23*)









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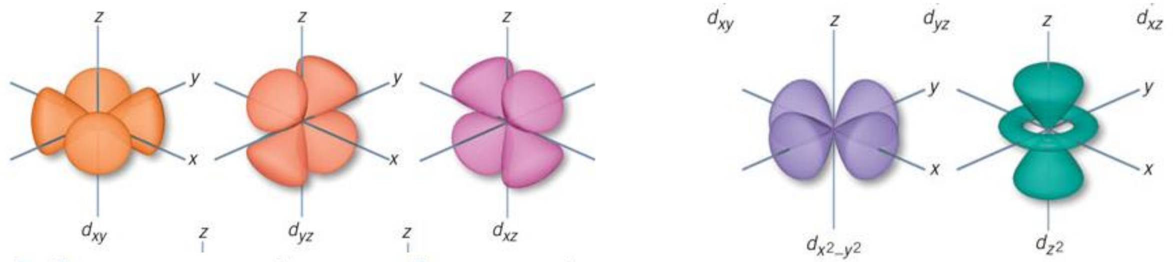
http://openstudy.com/study#/updates/4fc4d292e4b0964abc872b53

crystal field??

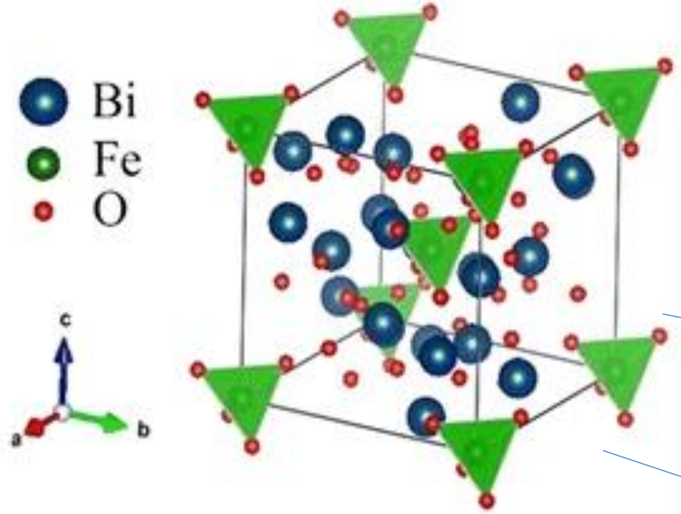
example: $Bi_{25}FeO_{39}$ (mineral: sillenite)

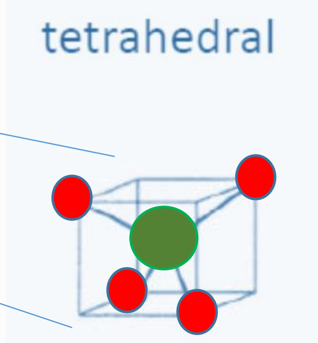


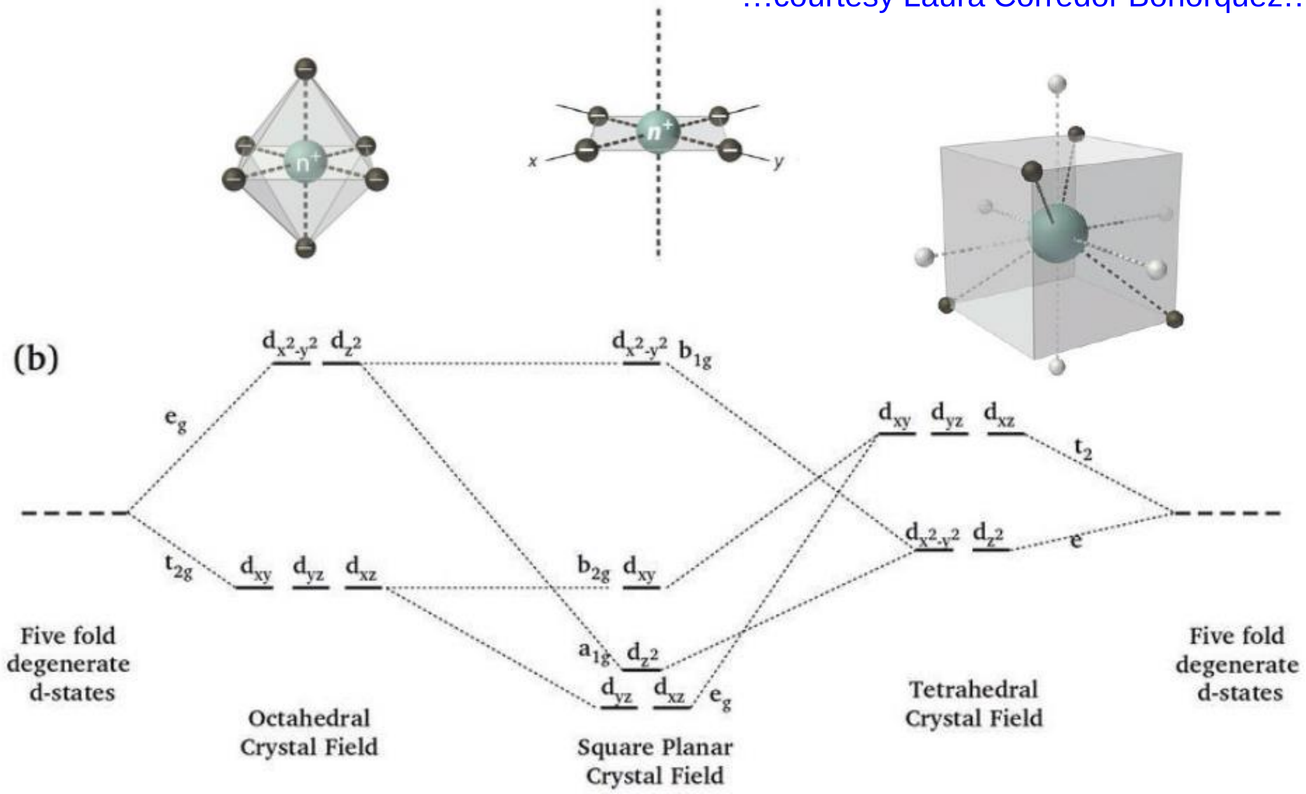
Crystal fields: an atom is not alone

crystallographic structure
cubic space group symmetry (*I23*)

…courtesy Laura Corredor Bohorquez…..







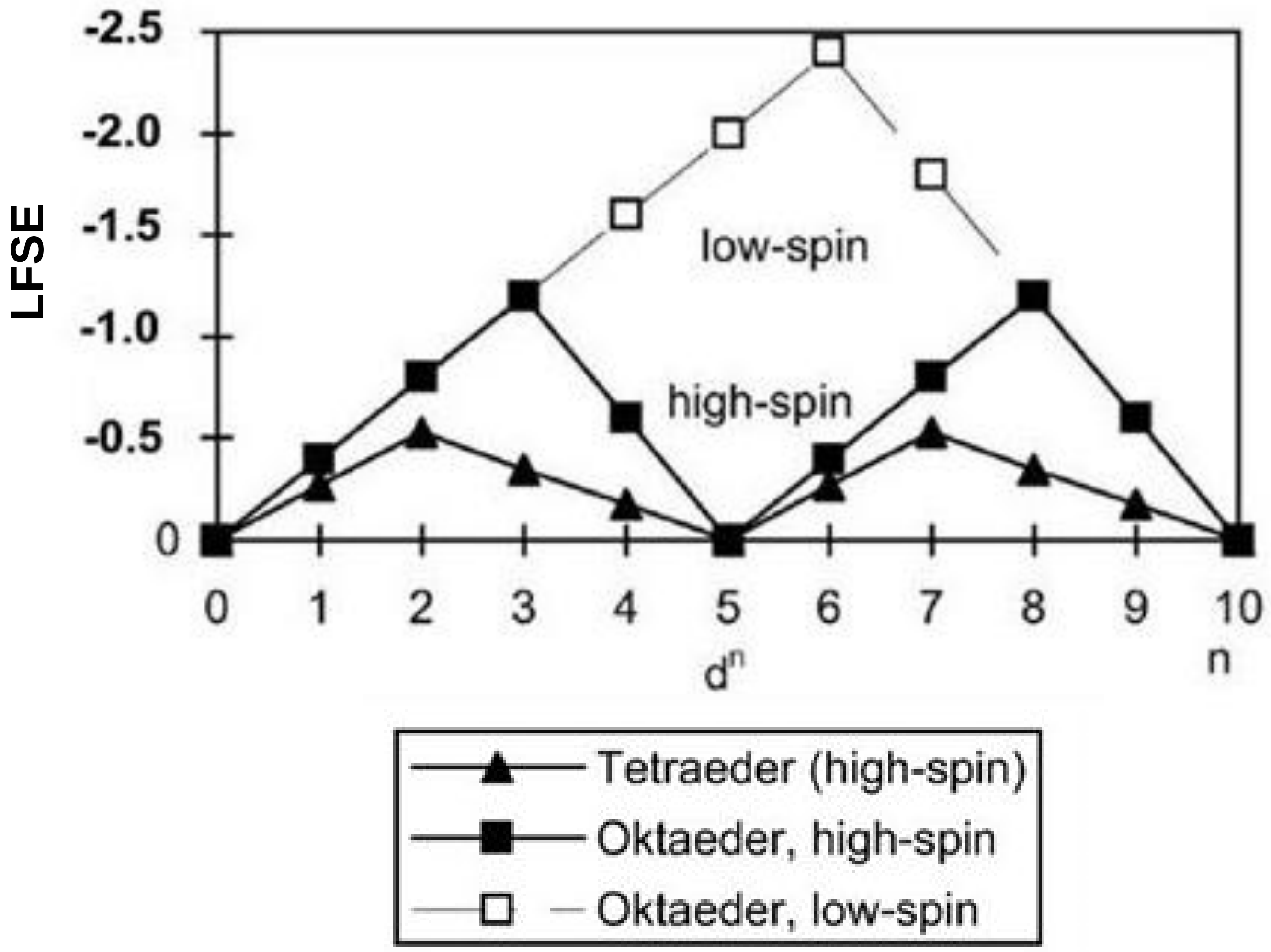
F. E. N. Ramirez *et al.*,
J. Mater. Science **51**, 10982 (2016)

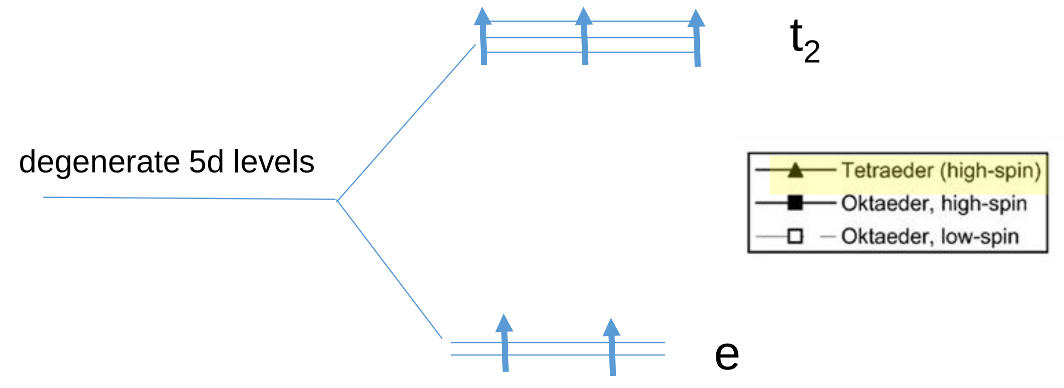
https://doi.org/10.1016/j.jpcs.2018.04.009

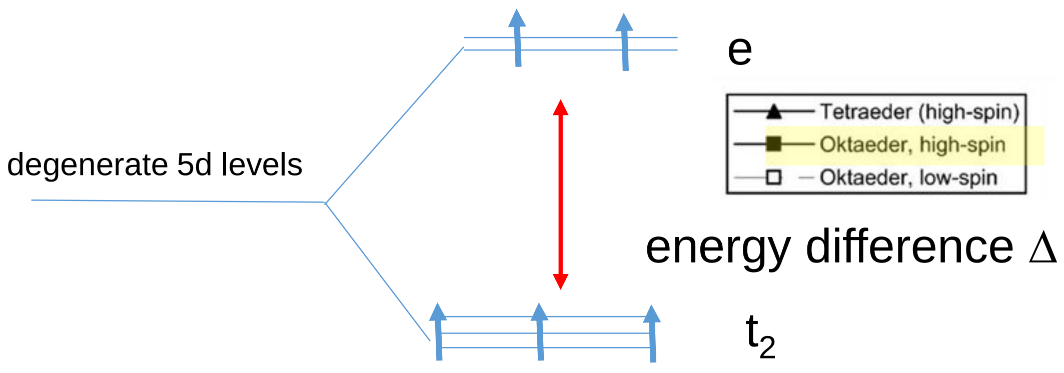
https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Modules_and_Websites_(Inorganic_Chemistry)/Crystal_Field_Theory/Crystal_Field_Theory

putting electrons in orbitals

LFSE: (**L**igandenf**eld**s**tabilisierungs**e**nergie; crystal field energy)







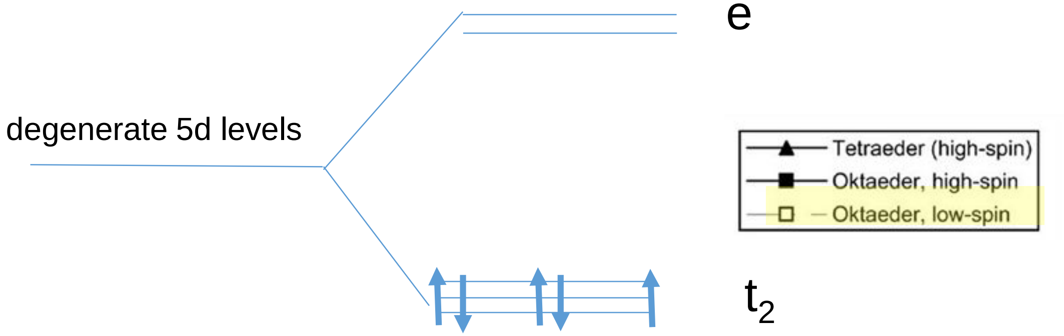
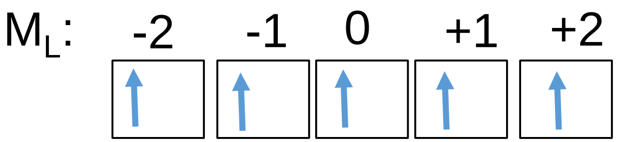
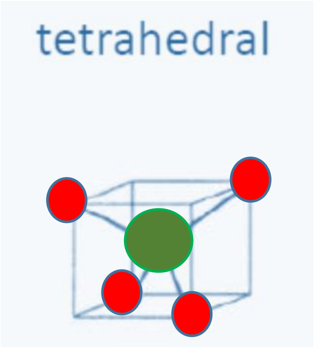


Figure:
Courtsesy of Prof. Dr. Berthold Kersting, Uni Leipzig
https://nanopdf.com/download/in-d-o_pdf

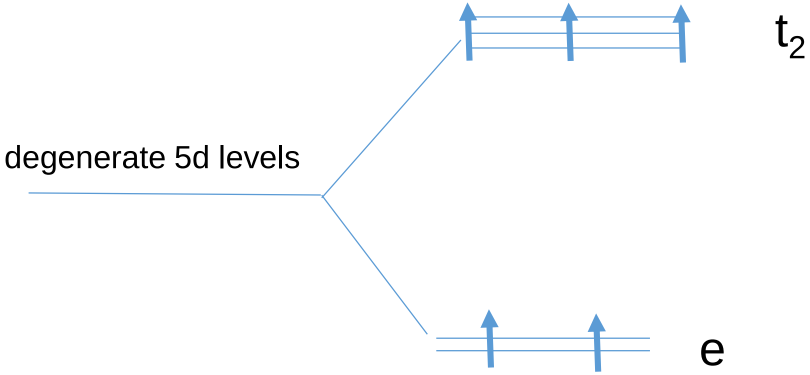
ground state of Fe^{3+} in $Bi_{25}FeO_{39}$ ferrite

Fe^{3+} with $3d^5$ electrons





tetrahedral crystal field
(symmetry T_d)



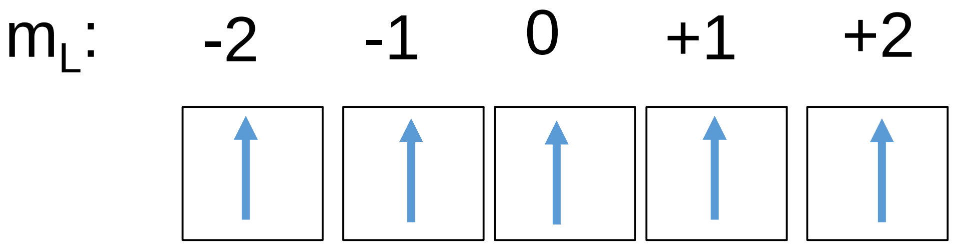
what do you think is the next step???

ground state, term symbol of Fe^{3+} in $Bi_{25}FeO_{39}$ ferrite

(Russel-Saunders coupling + Hund‘s rules)

Fe^{3+} with $3d^5$ electrons

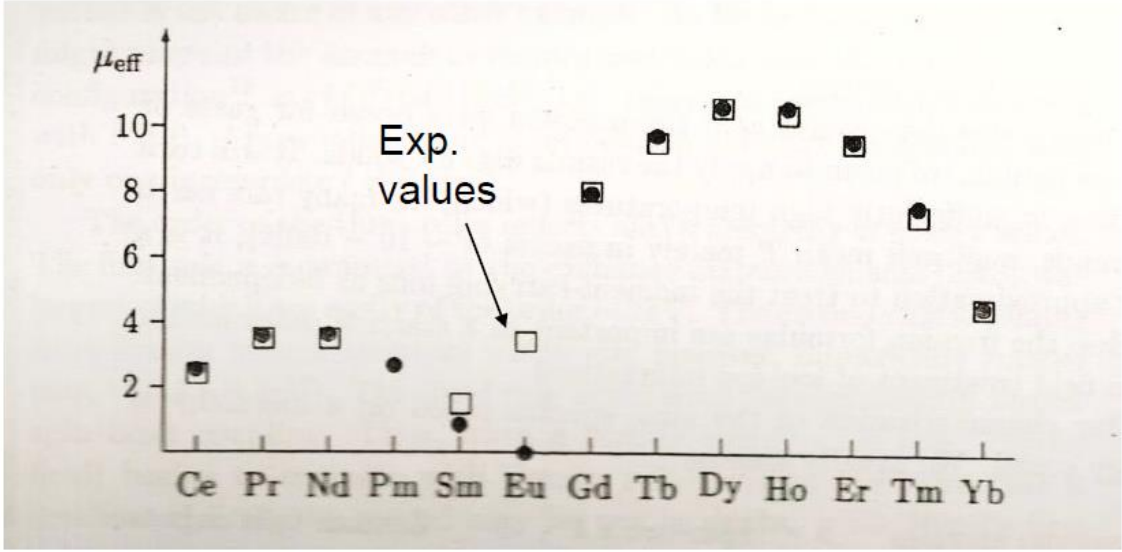
S= 5/2; L= 0; J=5/2, ground term $^{2S+1}L_J \rightarrow$ $^6S_{5/2}$



- **general:** orbital moment is quenched for 3*d* electrons; **spin only values** for effective moment
- **reason:** interaction with crystal field is stronger than spin-orbit interaction (violates Hunds- rule)
- (side remark: not relevant for present case where L=0)

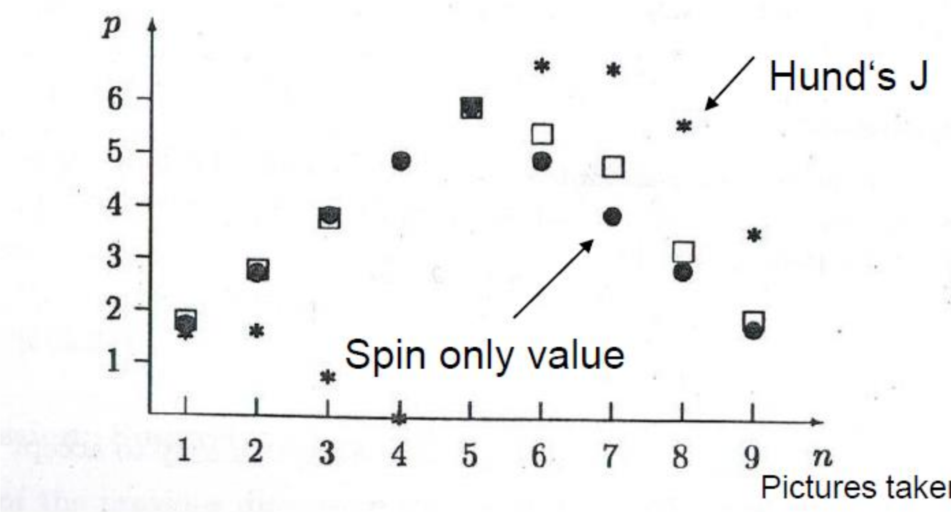
limitations of Hund‘s rules

Effective moments derived by fits with Curie law



Rare earth elements: Using J derived by Hund‘s rules gives very good estimates for μ_{eff}

→ **Weak crystal field acting on inner f electrons**



Transition metals: Using J drived by Hund‘s rules contradicition with experiment!

→ **Crystal field effects, Quenching of orbital moment L**

Pictures taken from:Fazekas, electron correlation and magnetism, page 49-51

magnetic properties in paramagnetic state

Fe^{3+} with $3d^5$ electrons

calculation: **spin only values** for effective moment

experiment: linear fit to $1/\chi$ with $1/\chi = \frac{C}{T-\theta}$

$$\mu_{eff} = 2\mu_B \sqrt{S(S+1)} \approx 5.9\ \mu_B$$

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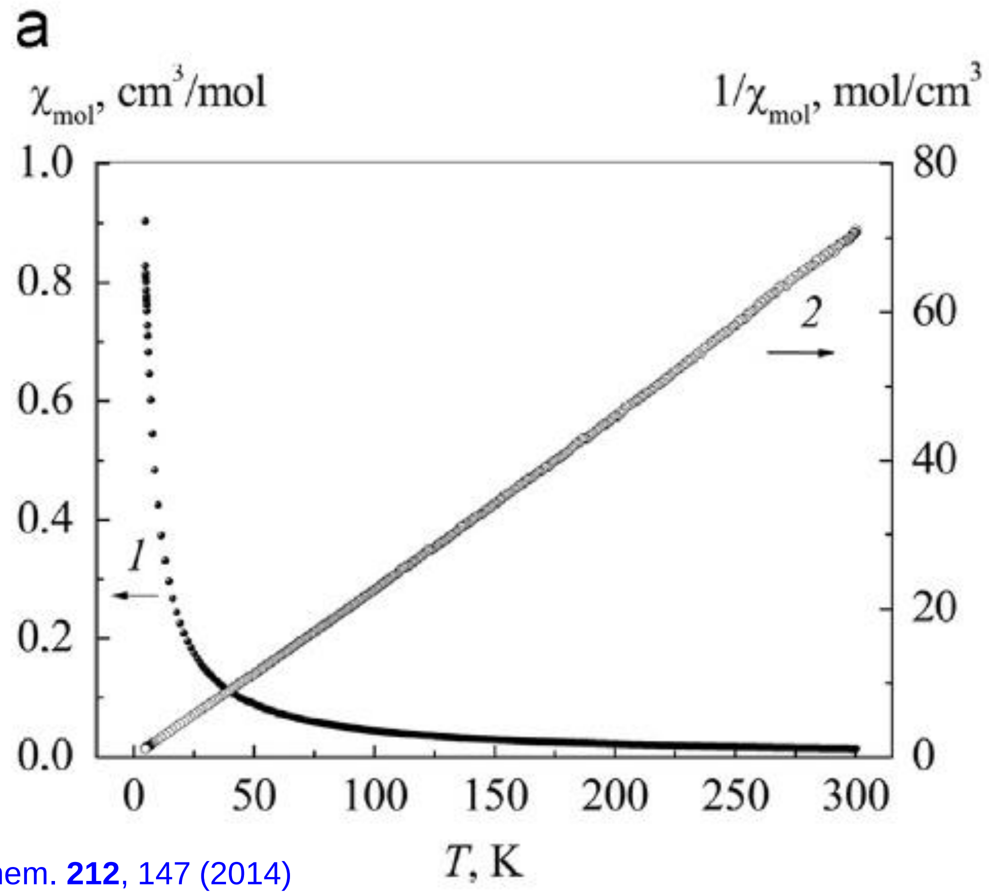


A.A. Zatsiupa, J. Solid State Chem. **212**, 147 (2014)

magnetic susceptibility, effective magnetic moment in $Bi_{25}FeO_{39}$

Fe^{3+} with $3d^5$ electrons

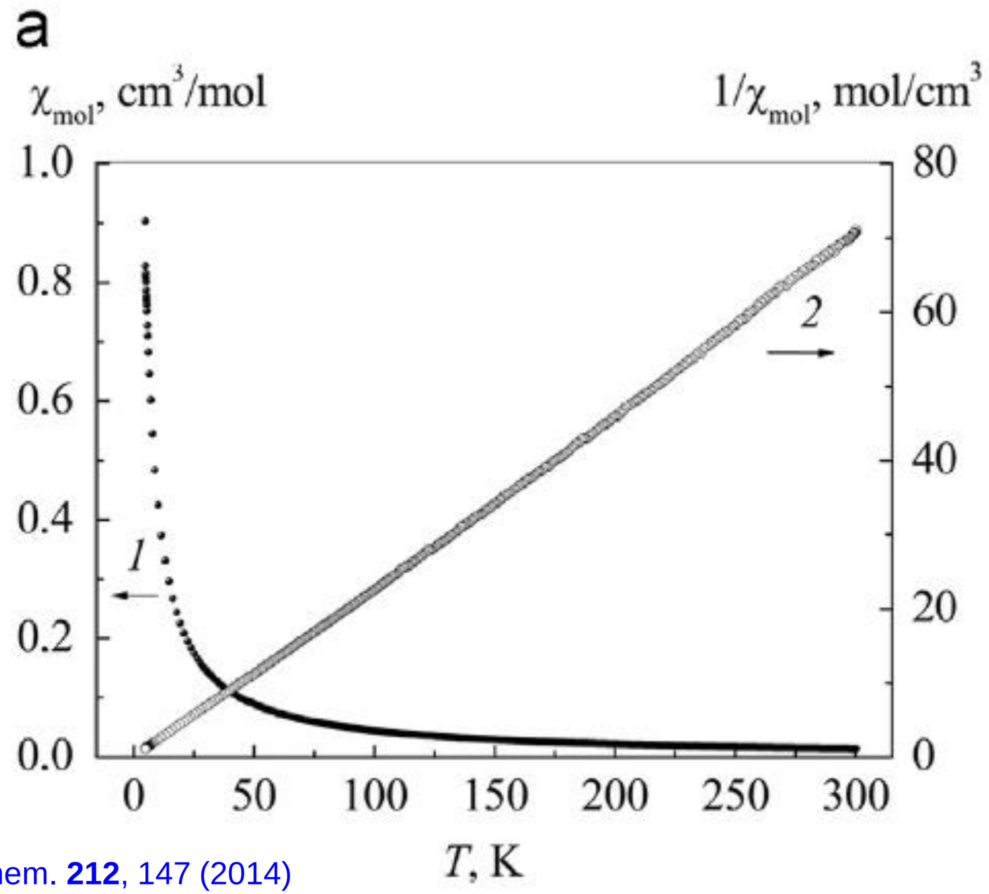
calculation: spin only values for effective moment

$$\mu_{eff} = 2\mu_B \sqrt{S(S+1)} \approx 5.9\ \mu_B$$

experimental values:

- measured effective moment about 5.82 μ_B
- θ_{CW} is +4 K → fm interaction

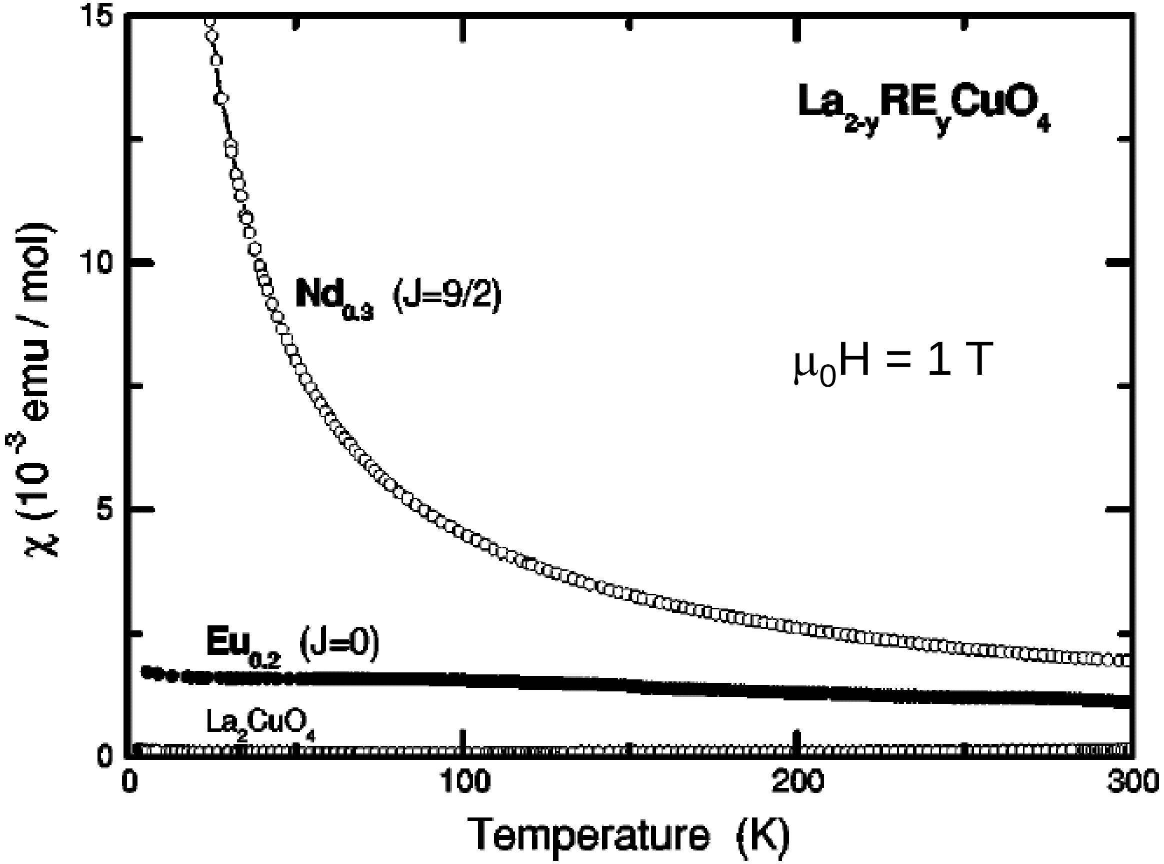
experiment: linear fit to $1/\chi$ with $1/\chi = \frac{C}{T-\theta}$



A.A. Zatsiupa, J. Solid State Chem. **212**, 147 (2014)

another example

low T→ alignment along field is energetically favoured



$$\chi_{para} = \frac{C}{T} = \frac{N\mu_0\mu_{eff}}{V3k_B} 1/T$$

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

Curie law

high T→ „entropy wins“

home work:
derive ground term

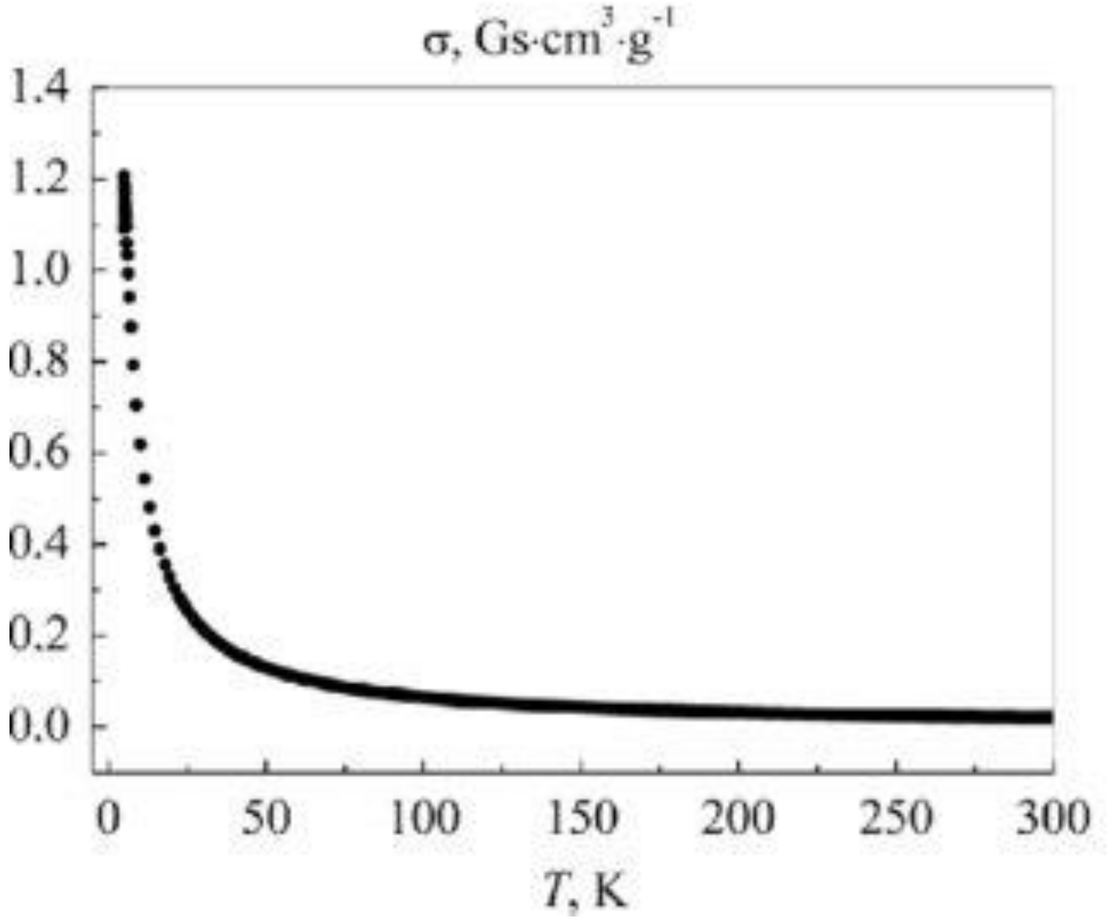
FIG. 3. Static magnetic susceptibility (H=1 Tesla) of pure and RE-doped La_2CuO_4 with $RE_y = Nd_{0.3}$ and $Eu_{0.2}$.

PHYSICAL REVIEW B **70**, 214515 (2004)

Dzyaloshinsky-Moriya spin canting in the low-temperature tetragonal phase of $La_{2-x-y}Eu_ySr_xCuO_4$

M. Hücker,[1] V. Kataev,[2,4] J. Pommer,[2] U. Ammerahl,[3] A. Revcolevschi,[3] J. M. Tranquada,[1] and B. Büchner[4]

ferromagnetic order at T< 5 K



https://www.researchgate.net/publication/260215366_Magnetization_Magnetic_Susceptibility_Effective_Magnetic_Moment_of_Fe3_Ions_in_Bi25FeO39_Ferrite/figures?lo=1

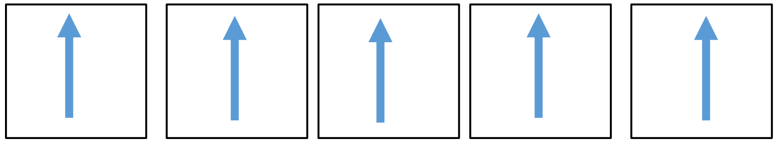
what do you think is the next step???

magnetic properties in ordered state

Fe^{3+} with $3d^5$ electrons

calculation: saturation magnetization in ordered state

m_L: -2 -1 0 +1 +2



m_{Sat} (0 K) = 5 μ_B

important: Integer number!

experiment: saturation magnetization in ordered state can be derived from magnetization curve at lowest temperature

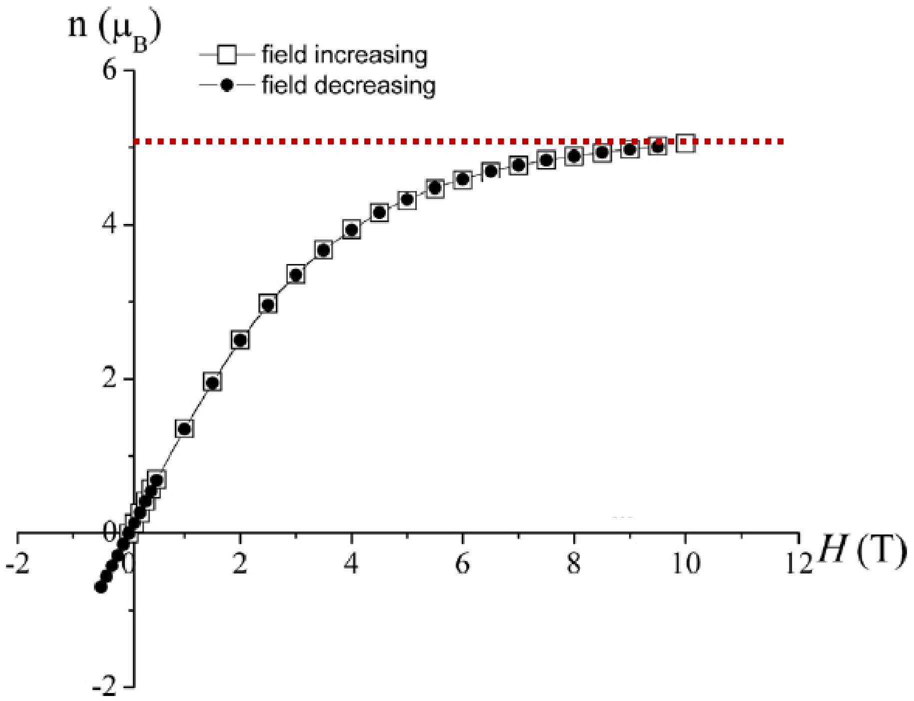


Fig. 3. The dependence of the magnetization (n, μ_B) on the magnetic field for one formula unit of $Bi_{25}FeO_{39}$ at 5 K.

A.A. Zatsiupa, J. Solid State Chem. **212**, 147 (2014)

magnetic properties in ordered state

Fe^{3+} with $3d^5$ electrons

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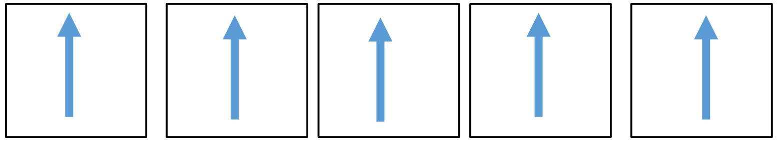
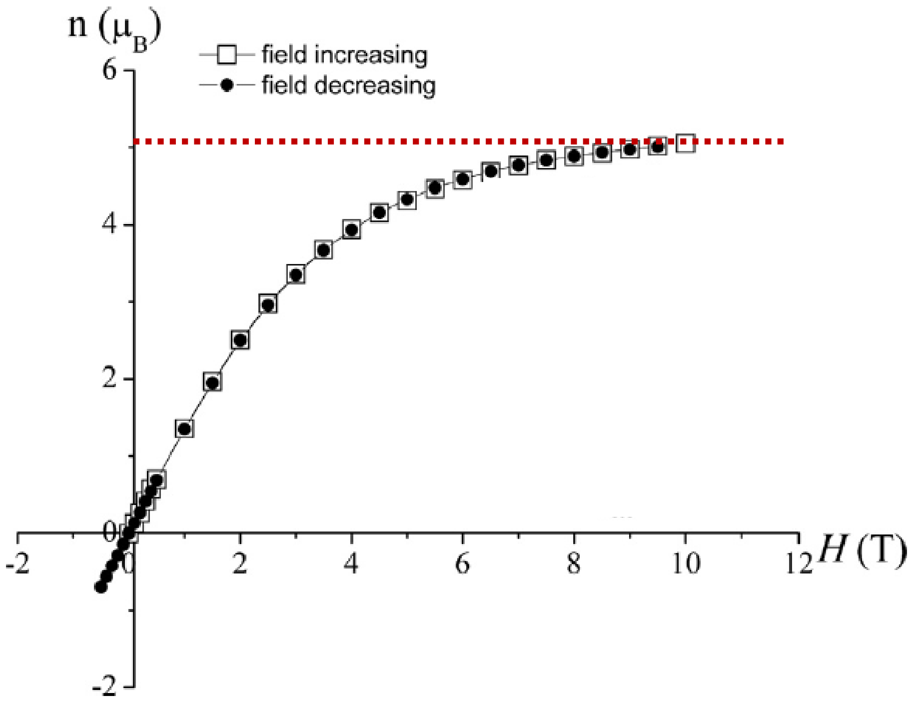


m_{Sat} (0 K) = 5 μ_B

Important: Integer number!

experimental value: ordered moment about 5.04 μ_B

experiment: saturation magnetization in ordered state can be derived from magnetization curve at lowest temperature



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A.A. Zatsiupa, J. Solid State Chem. **212**, 147 (2014)

pretty good agreement with calculated values for Fe^{3+} in $Bi_{25}FeO_{39}$

questions???

2.0 magnetism in metals

example: metallic Fe, Co, Ni, Gd

15. Magnetic Phenomena and Their Interpretation—Classical Approach 355

Table 15.1. Saturation Magnetization at 0 K and Curie Temperature (T_C) for Some Ferromagnetic Materials.

Metal	M_{S0} (A/m)	M_{S0} (Maxwells/cm^2)	T_C (K)
Fe	1.75×10^6	2.20×10^4	1043
Co	1.45×10^6	1.82×10^4	1404
Ni	0.51×10^6	0.64×10^4	631
Gd	5.66×10^6	7.11×10^4	289

Table 16.1. Magnetic Moment, μ_m, at 0 K for Ferromagnetic Metals.

Metal	μ_m
Fe	2.22 μ_B
Co	1.72 μ_B
Ni	0.60 μ_B
Gd	7.12 μ_B

Important: NON-Integer number!

how to derive NON-Integer numbers of moment in saturation at 0 K?!

do we deal with „half of an electron“????

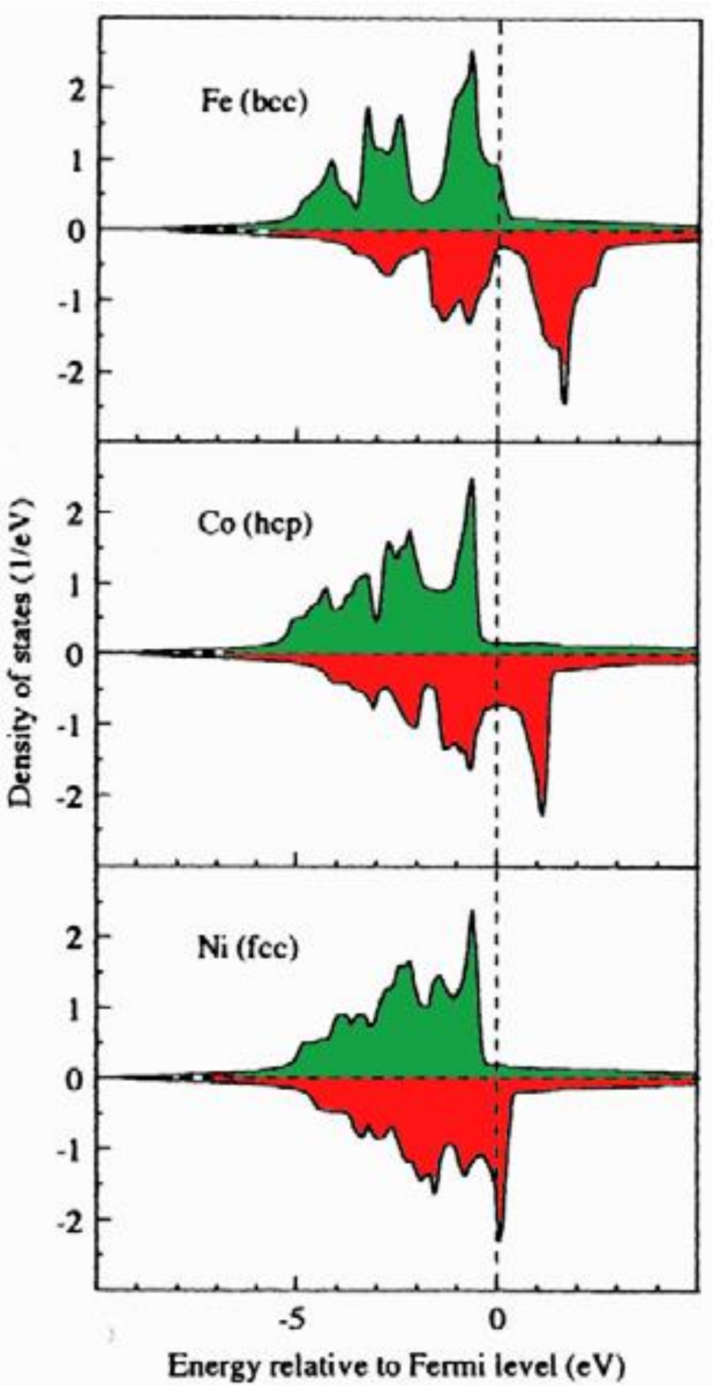
ideas???

why???

… it is the metallic state that is responsible

spin resolved density of states (DOS)

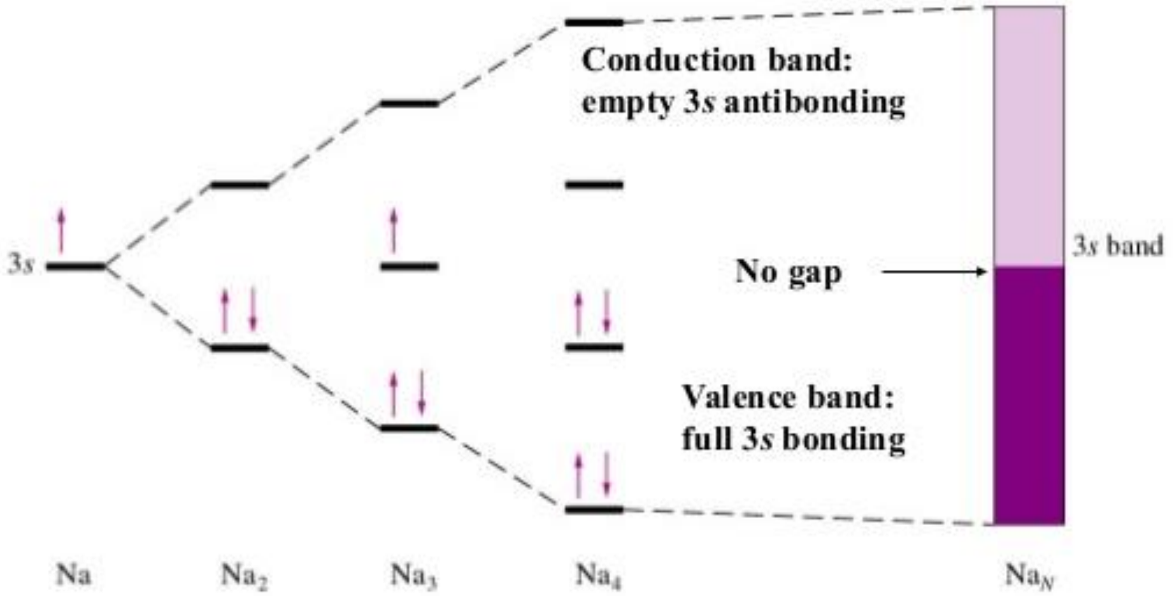
to get a description about DOS,
we need to consider a model for a free electron in a metal

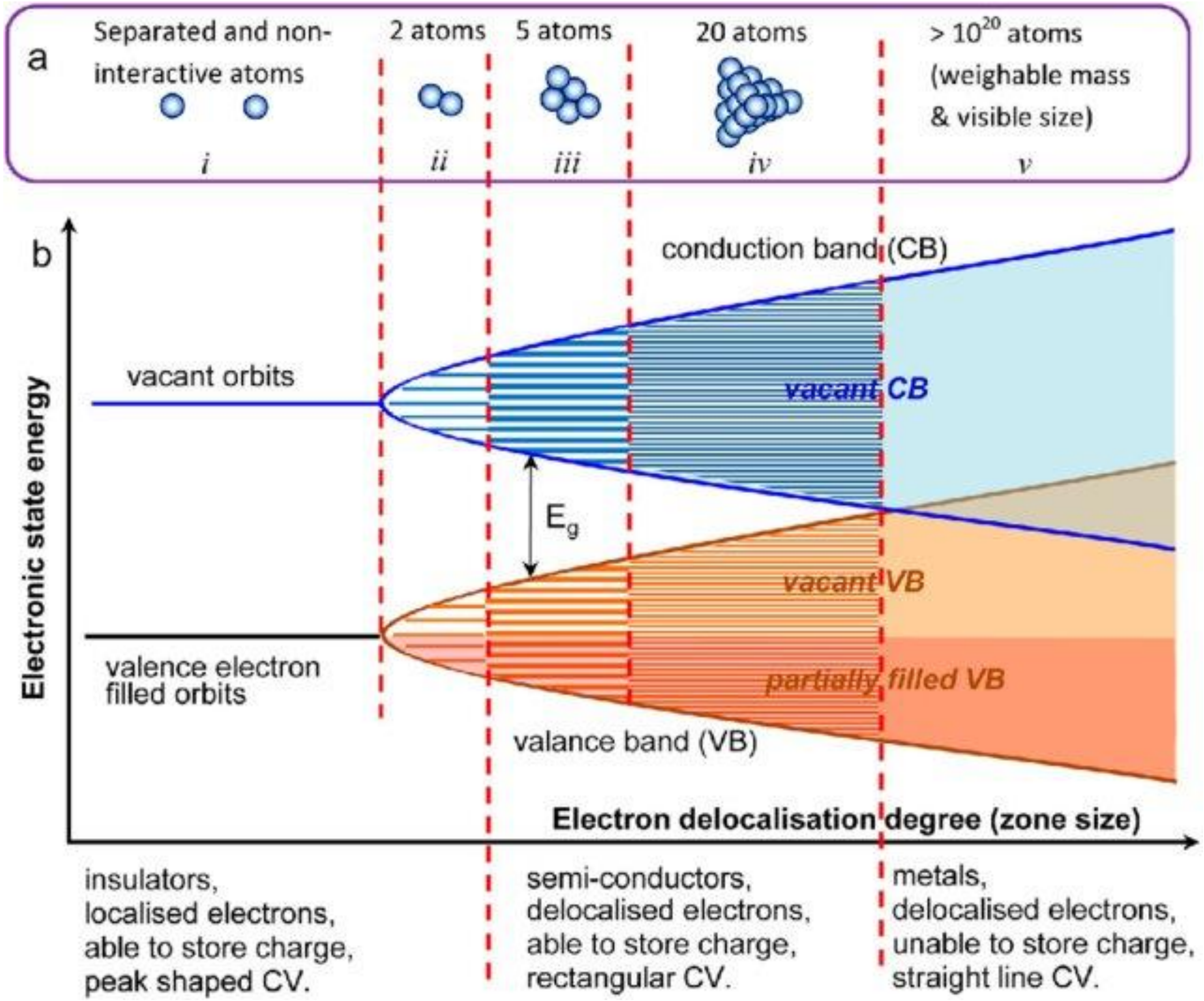


http://www.wmi.badw.de/teaching/Lecturenotes/magnetismus/Kapitel-5.pdf

from localized states to bands

formation of metallic Na according to band theory





https://www.slideshare.net/KamalKhan822/solids-conductors-insulators-semiconductors

https://www.researchgate.net/profile/George_Chen10

what do our electrons now in such a band???

ideas???

3.1 Fermi-gas of free electrons in metals

assumptions:

1) electrons are free
atom ions and e^- do not interact (but atom ions set boundary conditions)

2) electrons are independent
e^- do not interact

3) no lattice contribution
→Bloch's theorem:
- unbound electron moves in a periodic potential as a free electron in vacuum
- electron mass may be modified by band structure and interactions→ effective mass m*

4) Pauli exclusion principle applies
each quantum state is occupied by a single electron
→ Fermi–Dirac statistics

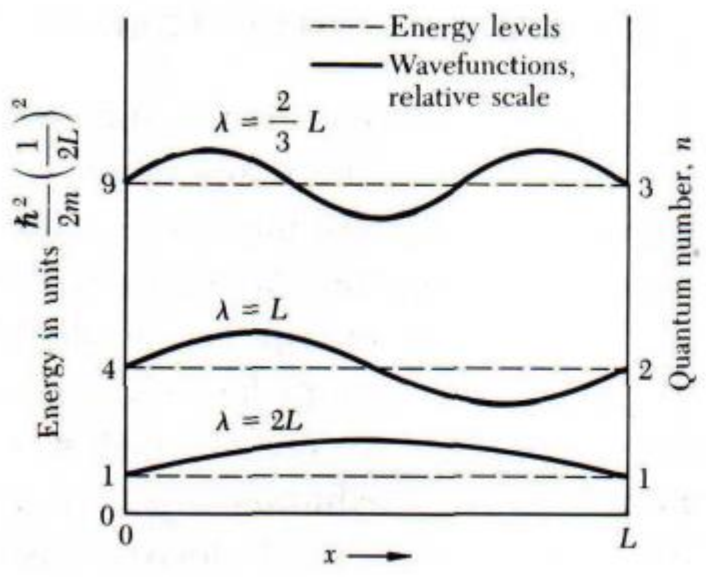
→ **description similar to „particle in a box“ problem**

free electron gas (simplified approach)

description by „particle in a box“ problem (here: 2-dim)

Schrödinger equation (3-dim)

$$-\frac{\hbar^2}{2m}\nabla^2\varphi = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2}\right) = E\varphi,$$



solution

(condition $\phi(0) = \phi(L) = 0$ allows only special values for k)

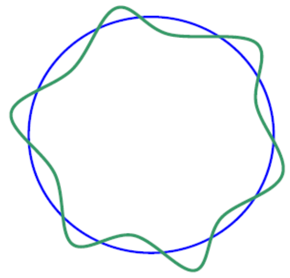
$$\varphi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}$$

plane waves with wave vector $\mathbf{k} = (k_x, k_y, k_z)$

k = π /L, 2 π /L, 3 π /L…

normalization to volume of box

- Periodic BC



k = ±2 π /L, ±4 π /L, ±6 π /L…

corresponds to the Eigenvalues for the energy

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2).$$

typically, materials have a certain number of electrons….

in a localized material, we distribute the electrons at distinct energy states

we start with to occupy states from the lowest ones in energy (LUMO)

and in metals???
ideas???

Fermi energy (short & simplified)

Gedankenexperiment: a metal has N number of electrons

→ we fill up states to a certain maximum wave vector (viz. until all electrons “are spent”)

→ we define this maximum wave vector as k_F

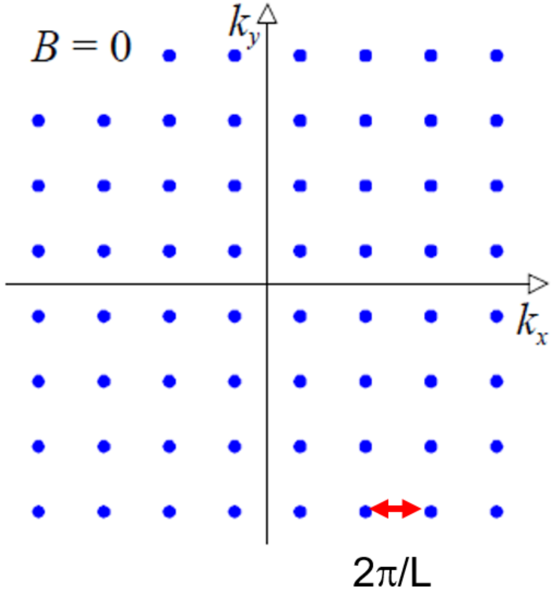
→ the energy of the highest energy electron at $T = 0$ K is defined as the Fermi-energy E_F

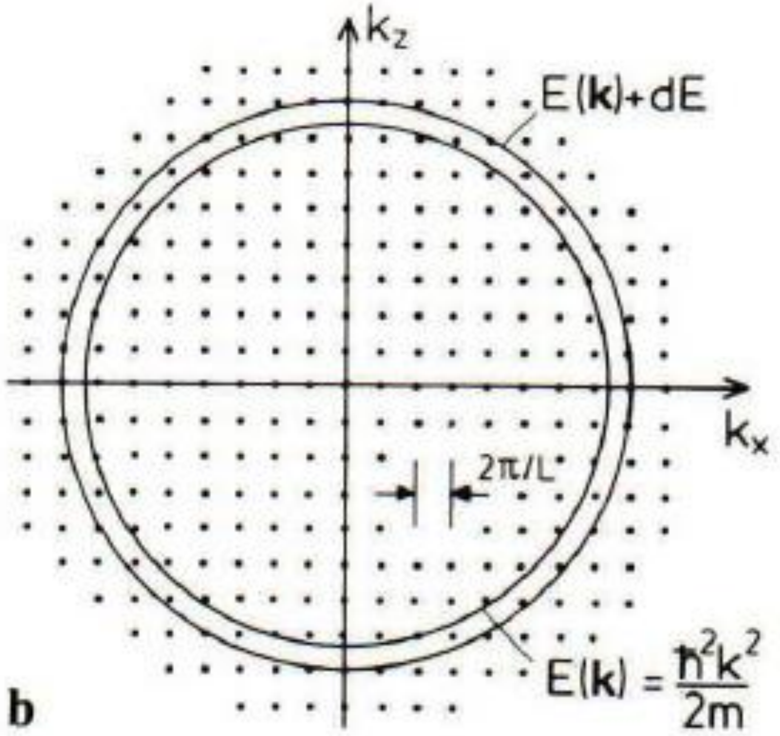
http://www.wmi.badw.de/teaching/Lecturenotes/magnetismus/Kapitel-5.pdf

electronic states in k-space

electronic states are dots in **k**-space with distance 2π/L with L^3 the volume of the sample

electronic states are plane waves $\varphi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}$





plane with constant energy

spherical shell

Gedankenexperiment:
spherical shell is considered as evanescently thin

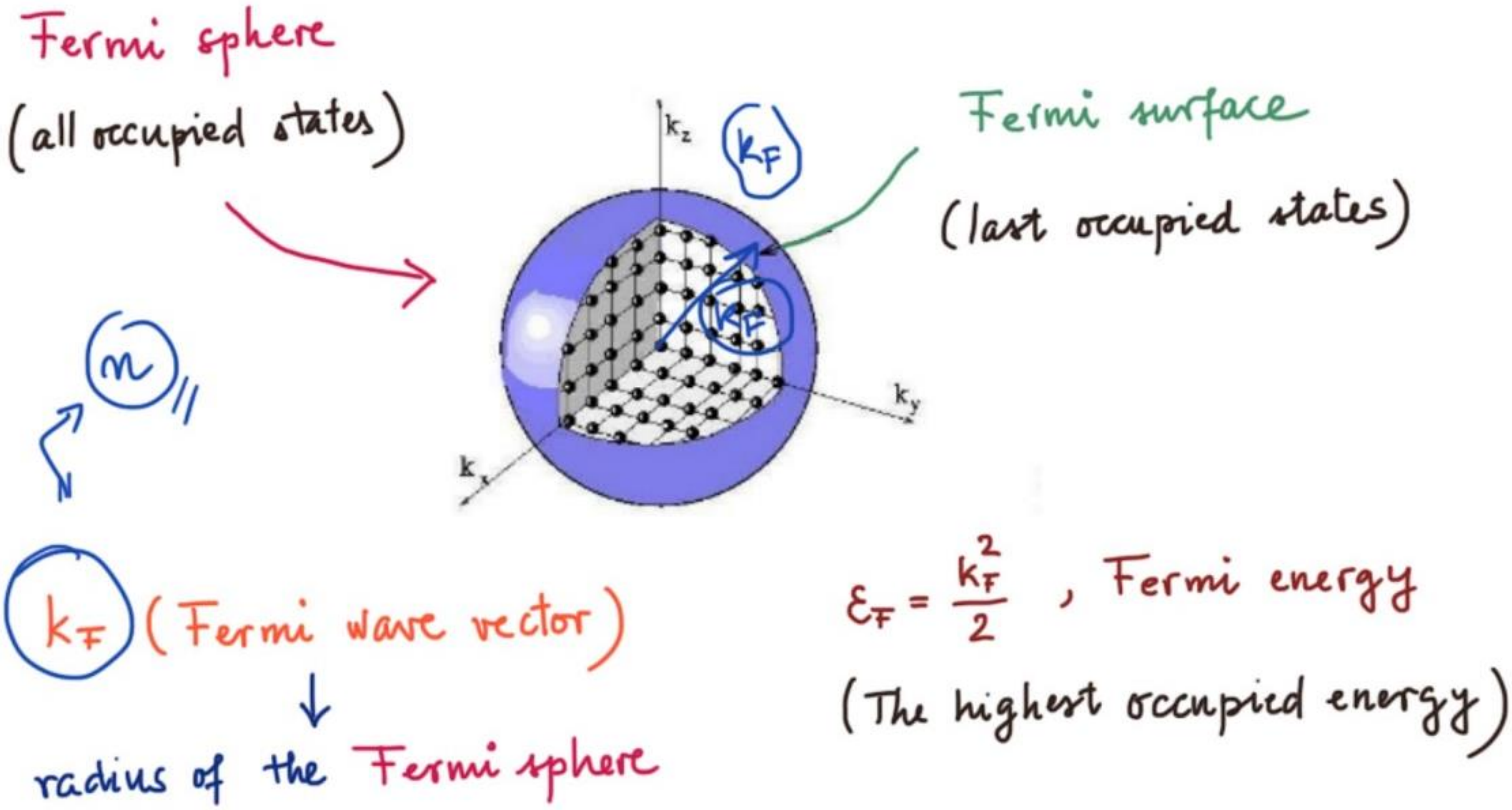
- radius k
- width dk
- shell volume 4pk^2dk
- volume of one state $(2\pi/L)^3$

how many states N do we have in a volume d**k**=$dk_x\ dk_y\ dk_z$??

https://phy.ntnu.edu.tw/~changmc/Teach/SS/SSG_note/mchap06.pdf

If all states are filled: Fermi surface (model)

N number of states

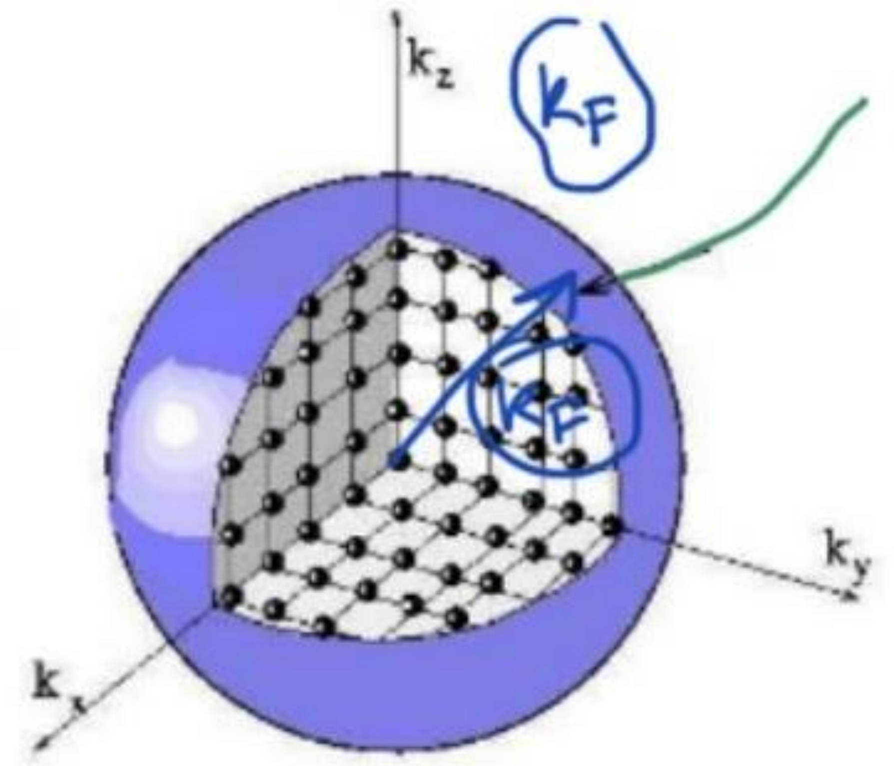


https://www.youtube.com/watch?v=qlq6Qh4QcIc

plane waves in k-space

electronic states are dots in **k**-space with distance $2\pi/L$ with L^3 the volume of the box

electronic states are plane waves $$\varphi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{r}}$$



plane with constant energy

k-space: spherical shell

Gedankenexperiment: sphere is considered as evanescently thin

number of states N in volume $d\mathbf{k} = dk_x\, dk_y\, dk_z$

how many states do we have??

https://www.youtube.com/watch?v=qlq6Qh4QcIc

ideas???

number of states (short & simplified) at T = 0 K

number of states N in volume d**k**=dk_x dk_y dk_z

with spherical polar coordinates in k-space $$\mathrm{d}\mathbf{k} = k^2 \sin\theta \, \mathrm{d}k \, \mathrm{d}\theta \, \mathrm{d}\phi, \qquad (0 \le k < \infty, 0 \le \phi < 2\pi, \text{ and } 0 \le \theta \le \pi)$$

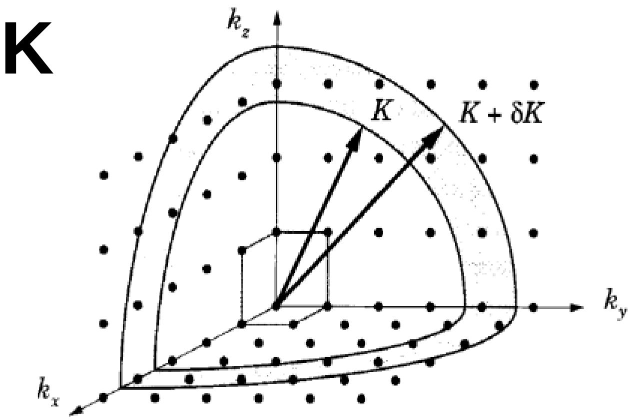
integration over polar and azimuth angle $$N(\mathbf{k}) \, \mathrm{d}\mathbf{k} = \frac{2}{(2\pi)^3} \mathrm{d}\mathbf{k} = \frac{1}{\pi^2} k^2 \, \mathrm{d}k$$

$$N = 2 \, \frac{\frac{4\pi}{3} k^3}{(\frac{2\pi}{L})^3} = \frac{V k^3}{3\pi^2}$$

Pauli principle (fermions)
→ spin degeneracy is 2

increase *k* by *dk* → changes number of states by *dN*

density of states (short & simplified) at T = 0 K



increase *k* by *dk* → changes number of states by *dN*

$$dN = \frac{Vk^2}{\pi^2} dk \equiv g(E) dE .$$ with g(E) the density of states (number of states per energy intervall *dE)*

replace *dk* by *dE* using $E = \hbar^2 \mathbf{k}^2 / 2m$ → $dk = \frac{1}{2\hbar}\sqrt{\frac{2m}{E}} dE$

$$g(E) dE = \frac{Vk^2}{2\pi^2\hbar}\sqrt{\frac{2m}{E}} dE ,$$ with g(E) the density of states DOS

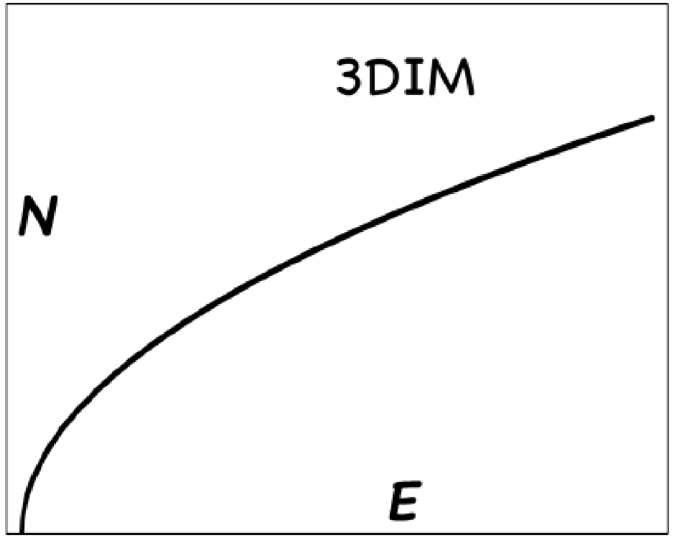
https://phy.ntnu.edu.tw/~changmc/Teach/SS/SSG_note/mchap06.pdf

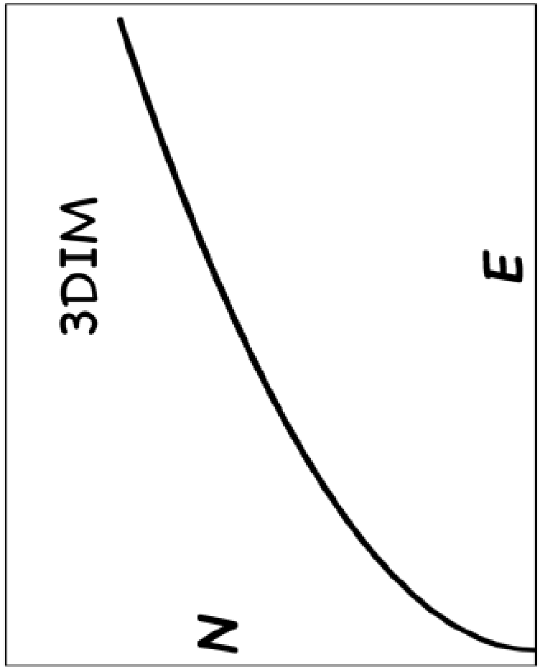
density of states (short & simplified)

$$g(E)dE = \frac{Vk^2}{2\pi^2\hbar}\sqrt{\frac{2m}{E}}dE\,,$$

with g(E) the density of states DOS

$$\text{DOS} \propto k^2 \propto E^{1/2}$$





density of states at Fermi energy

T = 0 K, total number of eletrons in volume V :

$$N = \int_0^{E_F} g(E)dE = \frac{V}{3\pi^2}\left(\frac{2mE_F}{\hbar^2}\right)^{3/2} \propto E_F^{3/2}$$

Fermi-energy E_F

$$E_F = \frac{\hbar^2}{2m}(3\pi^2 N/V)^{2/3}$$

Fermi-wave vector k_F

$$k_F = \sqrt{\frac{2mE_F}{\hbar^2}} = \left(3\pi^2\frac{N}{V}\right)^{1/3}.$$

why do we care about the Fermi energy???

DOS at Fermi energy

$$g(E_F) = \frac{3}{2}\frac{N}{E_F} = \frac{mk_F}{(\pi\hbar)^2}V\,.$$

$g(E_F) \propto m$

disclaimer:
sometimes m is not the mass of the free electron,
but modified by bandstructure effects and electronic interactions → m*

$\Longleftrightarrow$ measure m* to learn about band structure and interactions…

questions???

→ homework: revisit QM

what we have learned (so far)

- in localized materials→ distinct states
- itinerant materials→ DOS, bands
- DOS $\propto k^2 \propto E^{1/2}$

now: apply knowledge to real stuff

Fermi distribution function to account for temperature ≠ 0 K

$$f(E,T) = \frac{1}{\exp(\frac{E-\mu)}{kT}+1}$$

μ := chemical potential
μ (T)

$$\mu(T=0K)=\varepsilon_F$$
$$\mu(T>0K)\neq\varepsilon_F$$

we define the Fermi energy E_F at all temperatures:

$$\int_0^{E_F} f(E,0)\,g(E)\,dE = N.$$

for T = 0 K, $E_F = \mu$

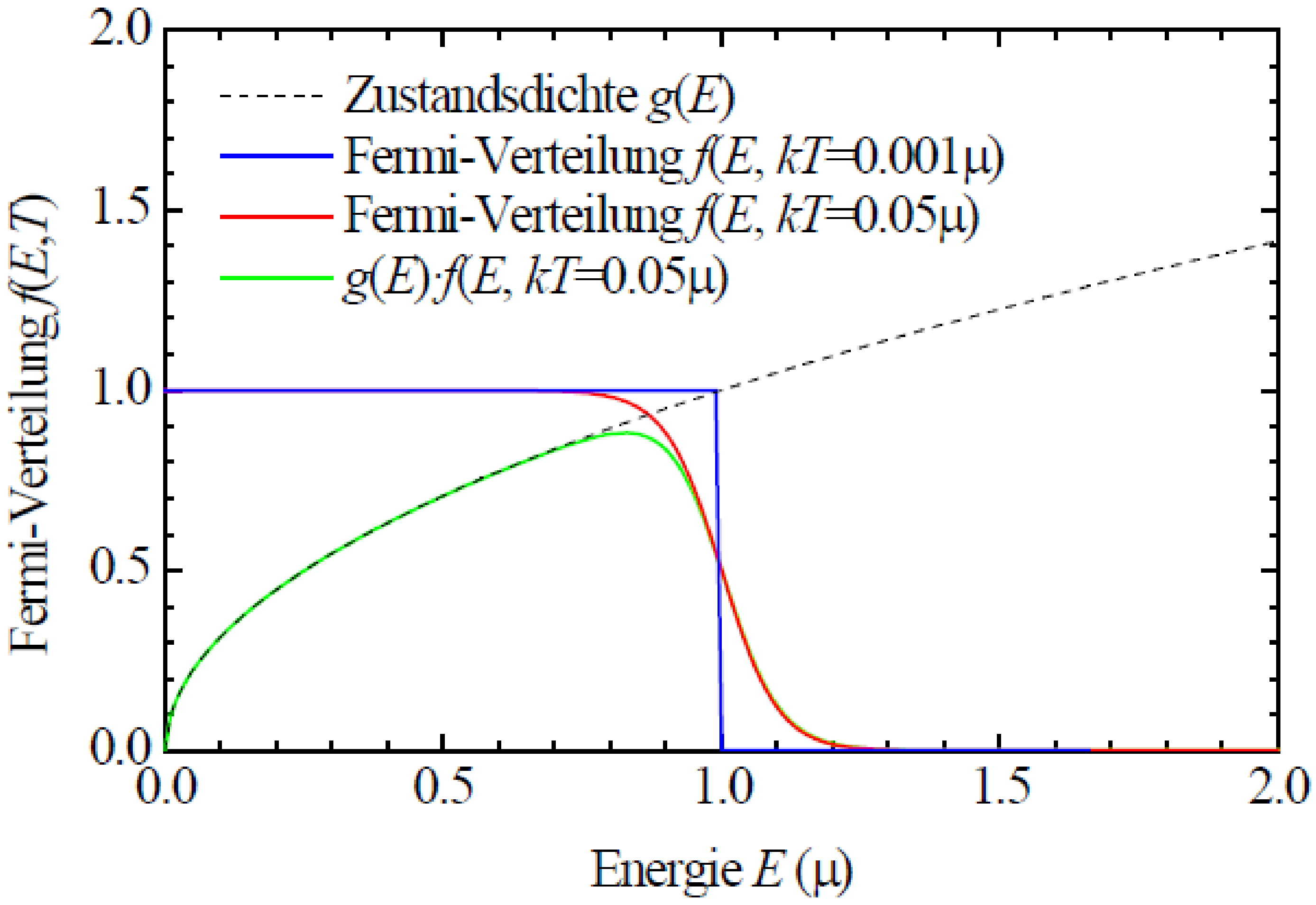
for T > 0 K → ….→ $$\mu = E_F\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2 + O\left(\frac{kT}{E_F}\right)^4\right].$$

visualisation of distribution of states for different temperature?

Fermi distribution or DOS „in reality“

$$f(E,T) = \frac{1}{\exp(\frac{E-\mu)}{kT}+1}$$

μ := chemical potential



----- DOS g(E) $\propto E^{1/2}$

Fermi distribution f(E, kT=0.001μ)→ close to T= 0 K ($E_F \approx \mu$)

Fermi distribution f(E, kT=0.05μ)→ finite T

g(E) x f(E, kT=0.05μ)→ occupied states at finite T

http://www.wmi.badw.de/teaching/Lecturenotes/magnetismus/Kapitel-5.pdf

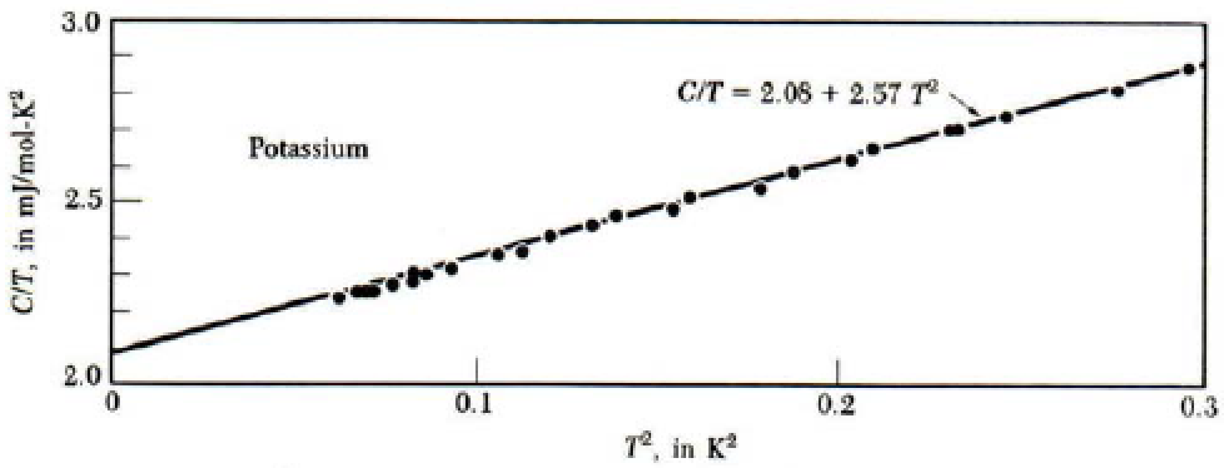
DOS from, e.g., specific heat experiments

electronic contribution

phonic contribution (lattice)

- In general $C_V = C_e + C_p$

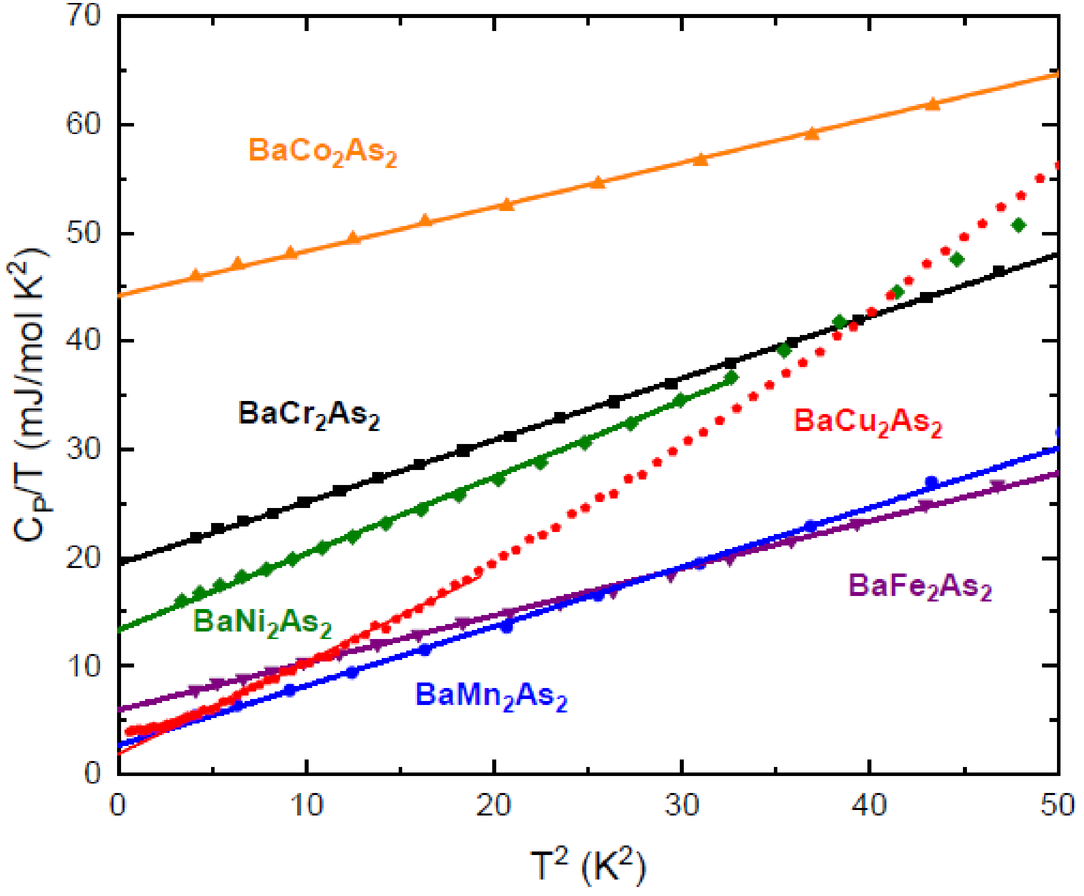
$$= \gamma T + AT^3$$



C_e is important only at very low T

https://phy.ntnu.edu.tw/~changmc/Teach/SS/SSG_note/mchap06.pdf

structure modifications and electronic correlations in the series BaT_2As$_2$ (T = Cr, Mn, Fe, Co, Ni, Cu)



$$C_P(T) = \gamma T + \beta T^3 + o(T^3)$$

$$\gamma = \frac{\pi^2}{3} k_B \rho(E_F) = \frac{k_B^2}{3\hbar^2} V k_F m^*$$

$$\frac{\gamma_{exp}}{\gamma_{theory}} = \frac{m^*}{m_b}$$

S. Selter, F. Scaravaggi *et al.* Inorg. Chem. (2020)

from discussion (simplified):

no full information about DOS from gamma if:

- semiconducting or insulating ground state (here: $BaMn_2As_2$)
- spin density wave gap is present (afm) (here: $BaFe_2As_2$)
- superconductivity present (sc gap)

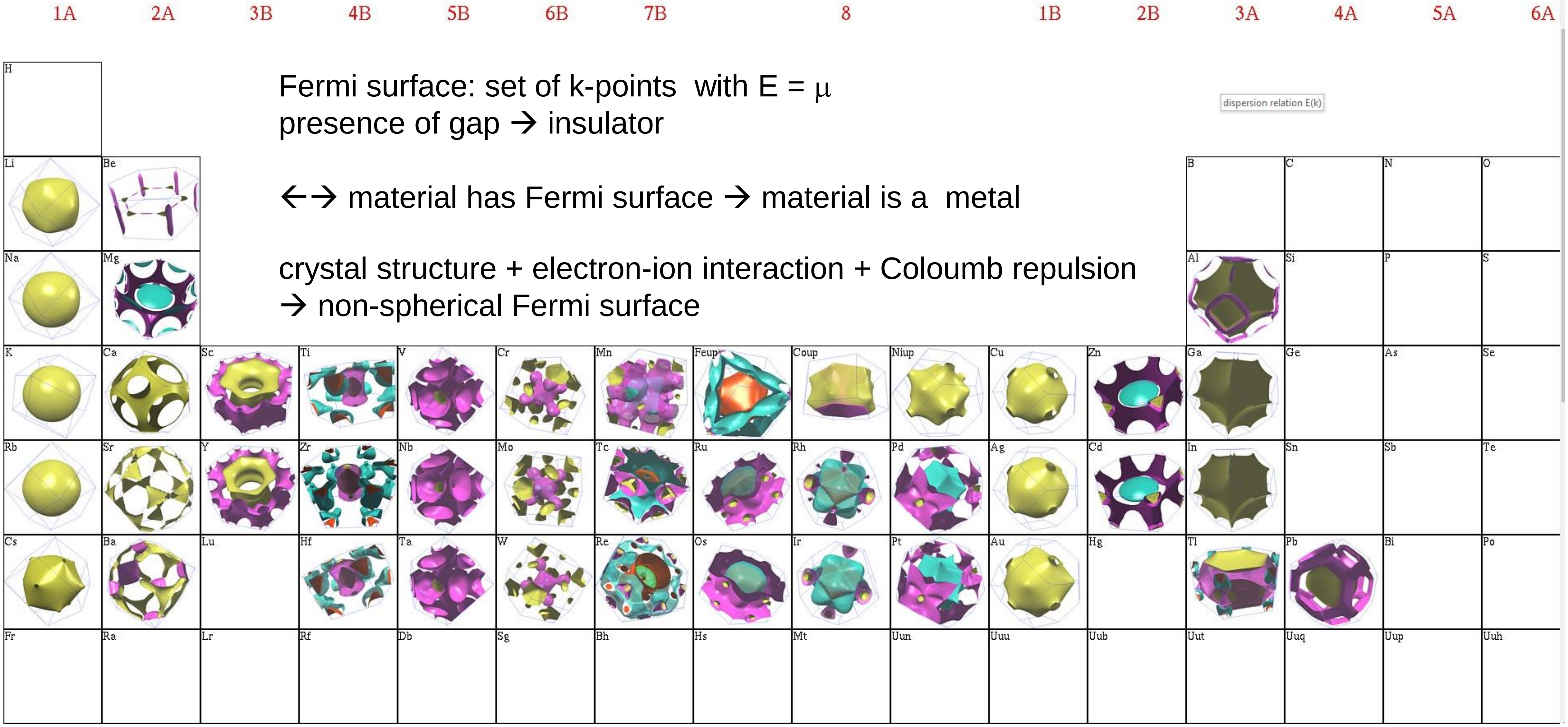
Fermi surface for real metals

[Physica Scripta](#)
INVITED COMMENT • OPEN ACCESS
Life on the edge: a beginner's guide to the Fermi surface
S B Dugdale

Fermi surface: set of k-points with E = μ
presence of gap → insulator

←→ material has Fermi surface → material is a metal

crystal structure + electron-ion interaction + Coloumb repulsion
→ non-spherical Fermi surface



http://www.phys.ufl.edu/fermisurface/periodic_table.html

now: free electron plus magnetic field

free electron gas in magnetic field

Consider a single atom which contains Z electrons in an external magnetic field ***B***:

…courtesy Laura Corredor Bohorquez…..

$$\mathcal{H}_0 = \sum_{i=1}^{Z} \left(\frac{p_i^2}{2m} + V_i \right) \quad \longrightarrow \quad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$$

$$\mathcal{H}_1 = \mu_B \left(\boldsymbol{L} + g\boldsymbol{S} \right) \cdot \boldsymbol{B} + \frac{e^2}{8m} \sum_{i=1}^{Z} \left(\boldsymbol{B} \times \boldsymbol{r}_i \right)^2 = \mathcal{H}_1^{\text{para}} + \mathcal{H}_1^{\text{dia}}$$

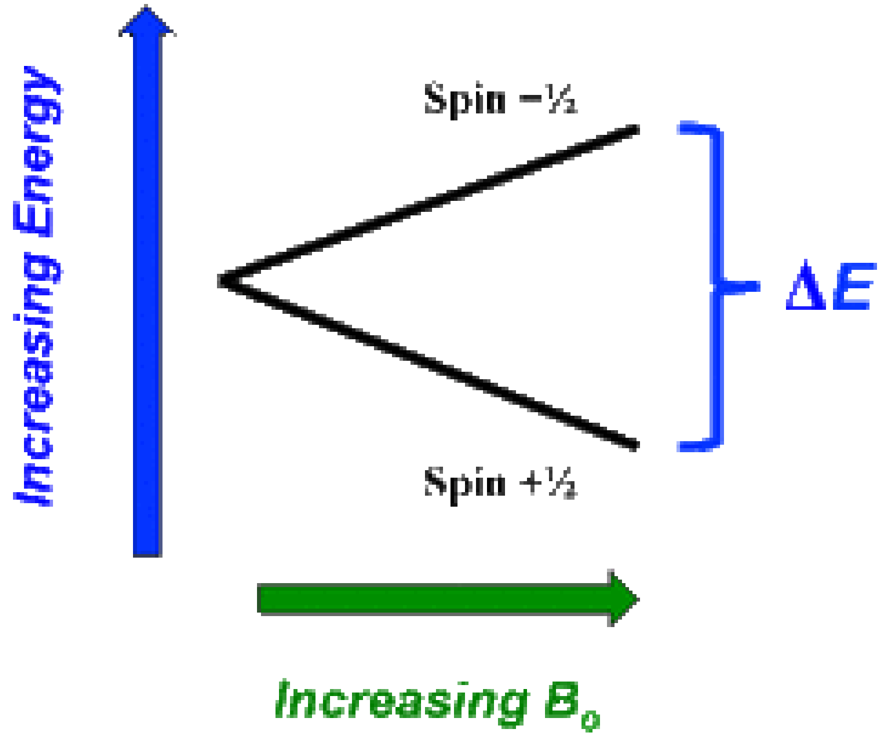
$$\hat{H} = \underbrace{\frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2}_{\text{Landau diamagnetism}} \pm \underbrace{\mu_B B}_{\text{Pauli paramagnetism}}$$

3.2 Pauli paramagnetism

→ free electron plus magnetic field

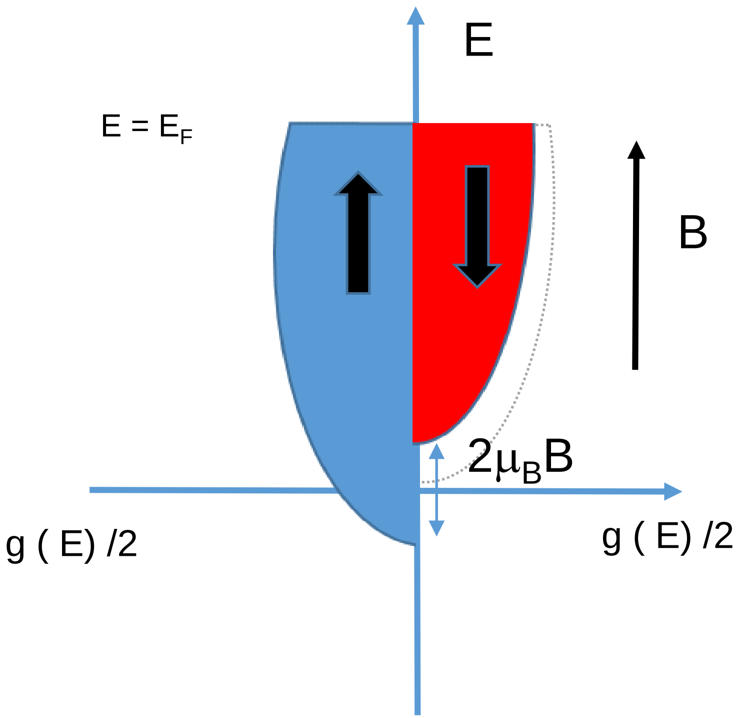
Zeemann splitting

for localized states in magnetic field
splitting in (2L+1) states



$\Delta E = \gamma \hbar B_0$

for a metal in magnetic field



http://mriquestions.com/energy-splitting.html

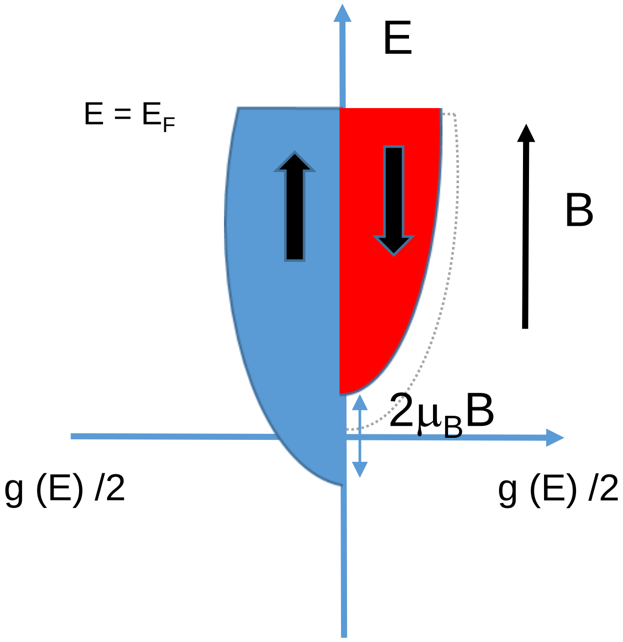
origin of Pauli paramagnetism

simplification: no orbital contribution, T = 0 K

if conductions electrons are weakly interacting and delocalized (Fermi gas)
→ magnetic response originates in interaction of spin with magnetic field

Zeemann splitting in magnetic field in a metal

$$\hat{H} = \underbrace{\frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2}_{\text{Landau diamagnetism}} \pm \underbrace{\mu_B B}_{\text{Pauli paramagnetism}}$$



$$E = \frac{\hbar^2 \mathbf{k}^2}{2m} \pm \mu_B B$$

with $N(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$ and $E = \frac{\hbar^2 \mathbf{k}^2}{2m} \pm \mu_B B$

we yield $\left(\frac{N(E)}{2}\right)^{\downarrow,\uparrow} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E \pm \mu_B B}$

temperature independent

how small is the field contribution?

Example: Cu

E_F: 7 eV
μB : 5*10^{-5} eV/T

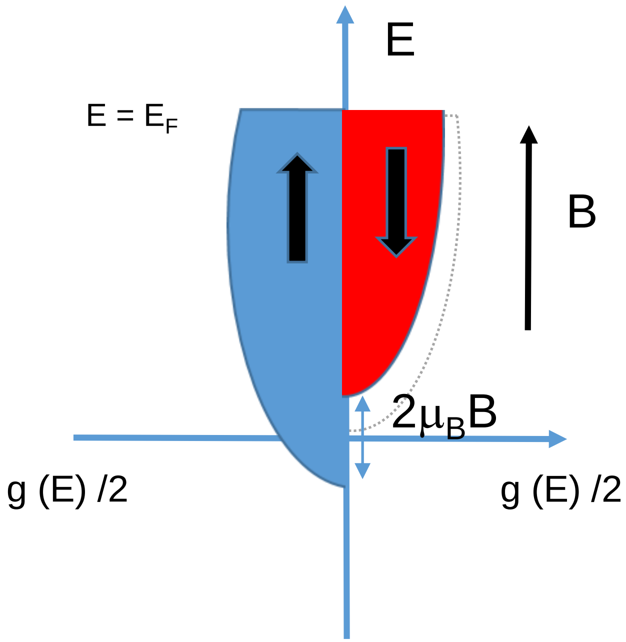
Pauli paramagnetism

$$E = \frac{\hbar^2 \mathbf{k}^2}{2m} \pm \mu_B B \qquad \left(\frac{N(E)}{2}\right)^{\downarrow,\uparrow} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E \pm \mu_B B}$$

number of „extra“ electrons per volume unit $n^{\uparrow} = N(E_F)\,\mu_B\,\mathbf{B}$

number of „deficit“ electrons per volume unit $n^{\downarrow} = N(E_F)\,\mu_B\,\mathbf{B}$

difference in electron density $$\Delta n \equiv n^{\downarrow} - n^{\uparrow} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \left\{ \int_{-\mu B}^{\infty} f(E,T)\sqrt{E+\mu_B B}\, dE - \int_{+\mu B}^{\infty} f(E,T)\sqrt{E-\mu_B B}\, dE \right\}$$



$$\Delta n = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \int_{E_F-\mu_B B}^{E_F+\mu_B B} \sqrt{E}\, dE$$

$$\mu_B B << E_F: \Rightarrow \cdot \int_{E_F-\mu_B B}^{E_F+\mu_B B} \sqrt{E} \Rightarrow \sqrt{\boldsymbol{E_F}}$$

$$\Delta n = \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_F}}_{N(E_F)/2} \cdot 2\mu_B B = N(E_F) \cdot \mu_B B$$

why are we interested in the difference in electron density?

magnetization for a metal in magnetic field

$$\longrightarrow \quad M = \mu_B \cdot \Delta n = N(E_F) \cdot \mu_B^2 B$$

$$\chi_{Pauli} = \mu_0 \frac{\partial M}{\partial B} \approx \mu_0 \mu_B^2 N(E_F) = \frac{3N\mu_0\mu_B^2}{2E_F}$$

temperature independent, very weak

→ correction for T > 0 K ~ $(T/T_F)^2$ << 1 (we started with the trick that T = 0 K)

→ example: Cu has T_F of 81,000 K

what we should know about Pauli paramagnetism

- metals: only electrons at Fermi energy contribute

- localized system: all unpaired electrons contribute

→ paramagnetism in localized systems much stronger than in metals

- in metals, spin of electrons leads to Pauli susceptibility χ_P

- χ_P is temperature independent

side note: measurement of χ_P in metals by NMR so-called Knight shift
(viz. measure of interaction of nuclear moment with conduction electrons, comparison to non-magnetic system)
→ access to DOS at E_F

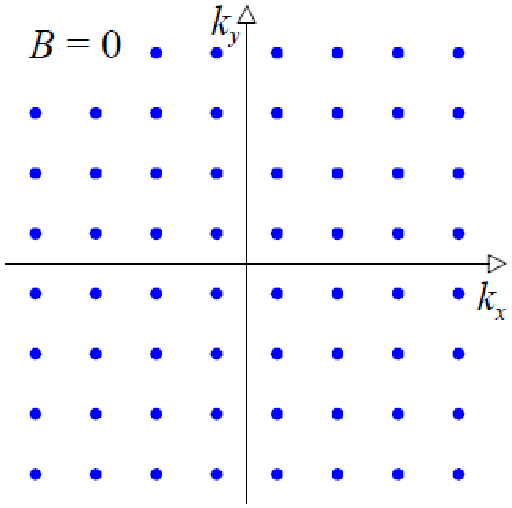
3.3 Landau diamagnetism

$$\hat{H} = \underbrace{\frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2}_{\text{Landau diamagnetism}} \pm \underbrace{\mu_B B}_{\text{Pauli paramagnetism}}$$

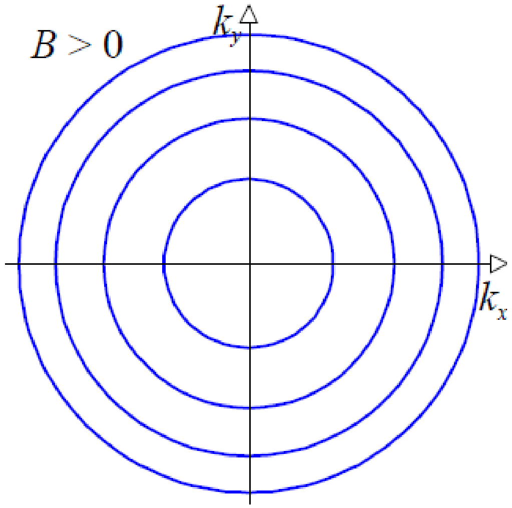
or, what about the orbital contribution to magnetism in metals ???

Landau levels (tubes)

no magnetic field:
discrete states



with magnetic field:
k-vectors condense on tubes paralell to field



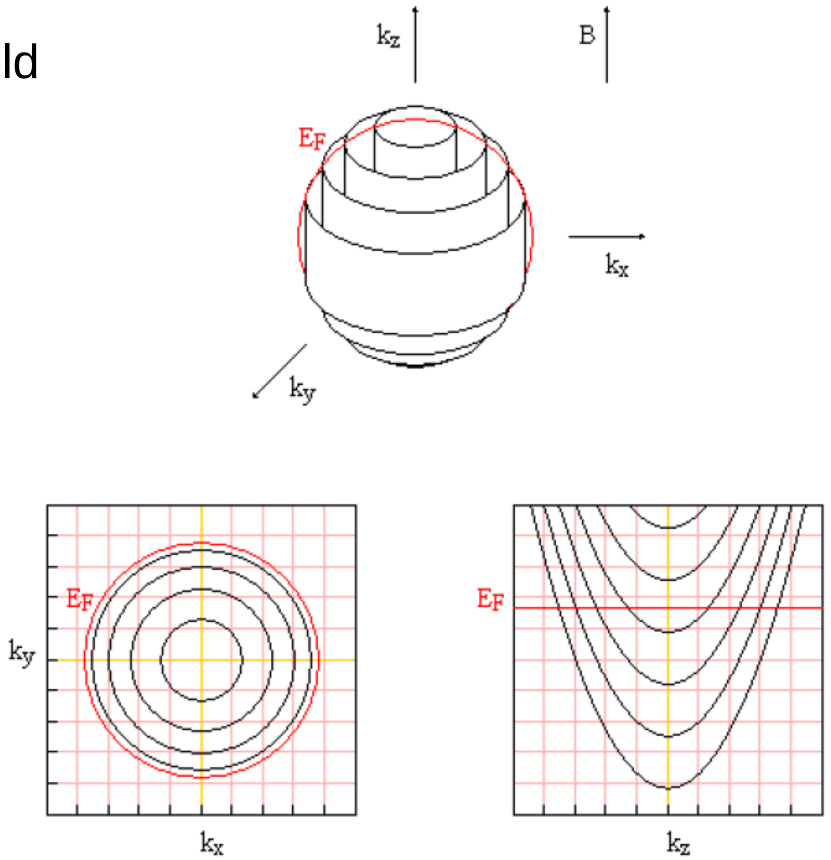


Bild 5.5: Landau-Röhren im **k**-Raum. Die Fermi-Energie E_F ist rot eingezeichnet.

(Quelle: http://buckminster.physics.sunysb.edu/intlearn/landau/landau.html)

http://www.wmi.badw.de/teaching/Lecturenotes/magnetismus/Kapitel-5.pdf

2.3 Landau diamagnetism

$$\hat{H} = \underbrace{\frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2}_{\text{Landau diamagnetism}} \pm \underbrace{\mu_B B}_{\text{Pauli paramagnetism}}$$

$$\mathcal{H}_0 = \sum_{i=1}^{Z}\left(\frac{p_i^2}{2m} + V_i\right)$$ no magnetic field

with magnetic field **B**= (0,0,B) **p** = -iħ∇ becomes **p** = −iħ∇+e**A**

→ weak counteracting field that forms when the electrons' trajectories are curved due to the Lorentz force

$$\hat{H} = \frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2 = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2 + 2p_y eBx + e^2B^2x^2\right) =$$

$$= \frac{1}{2m}\left(p_x^2 + (p_y + eBx)^2 + p_z^2\right)$$

…some mathematics…. and wave functions as plane waves in y,z direction $\psi(x,y,z) = e^{ik_z z}\, e^{ik_y y}\, \psi_x(x)$

$$\left(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_c^2(x-x_0)^2}_{\text{harmonic oscillator}} + \underbrace{\frac{\hbar^2 k_z^2}{2m}}_{\text{plane wave}}\right)\psi_x(x) = E\,\psi_x(x).$$

energy Eigenvalues for harmonic oscillator

$$E_n^{\text{Landau}} = \left(n+\frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}.$$

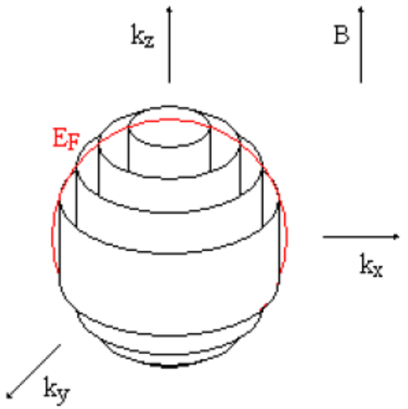
$$\overbrace{\frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 k_z^2}{2m}}^{\text{plane waves in y,z direction}} = \overbrace{\left(n+\frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}}^{\text{quantized states along }\mathbf{B}}$$

$$k_x^2 + k_y^2 = \left(n+\frac{1}{2}\right)\frac{2m\omega_c}{\hbar}.$$

Landau susceptibility of conduction electrons

application of magnetic field→ quantized Landau levels→ changes energetic state

thermodynamics: magnetic field induced change of energy→ magnetization



Calculation is not easy.

$$\chi_{Landau} = -\frac{e^2 k_F}{12\pi^2 mc^2}$$

$$= -\frac{1}{3}\chi_{Pauli} \quad \text{for free electron gas}$$

with

$$\chi_{\text{Pauli}} = \mu_0 \frac{\partial M}{\partial B} = \mu_0 \mu_{\text{B}}^2 g(E_{\text{F}}) = \frac{3N\mu_0\mu_{\text{B}}^2}{2E_{\text{F}}}$$

tentative assumption: all metals are paramagnets as $\chi_{\text{Pauli}} >> \chi_{\text{Landau}}$

disclaimer: bandstructure effects may matter since $N(E_F) \sim m^*/m_e$

for most metals $m^* \sim m_e$ → most metals are paramagnets

occupation of Landau levels

application of magnetic field

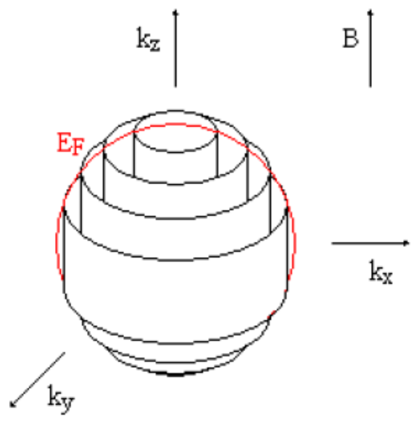
→ formation of Landau levels

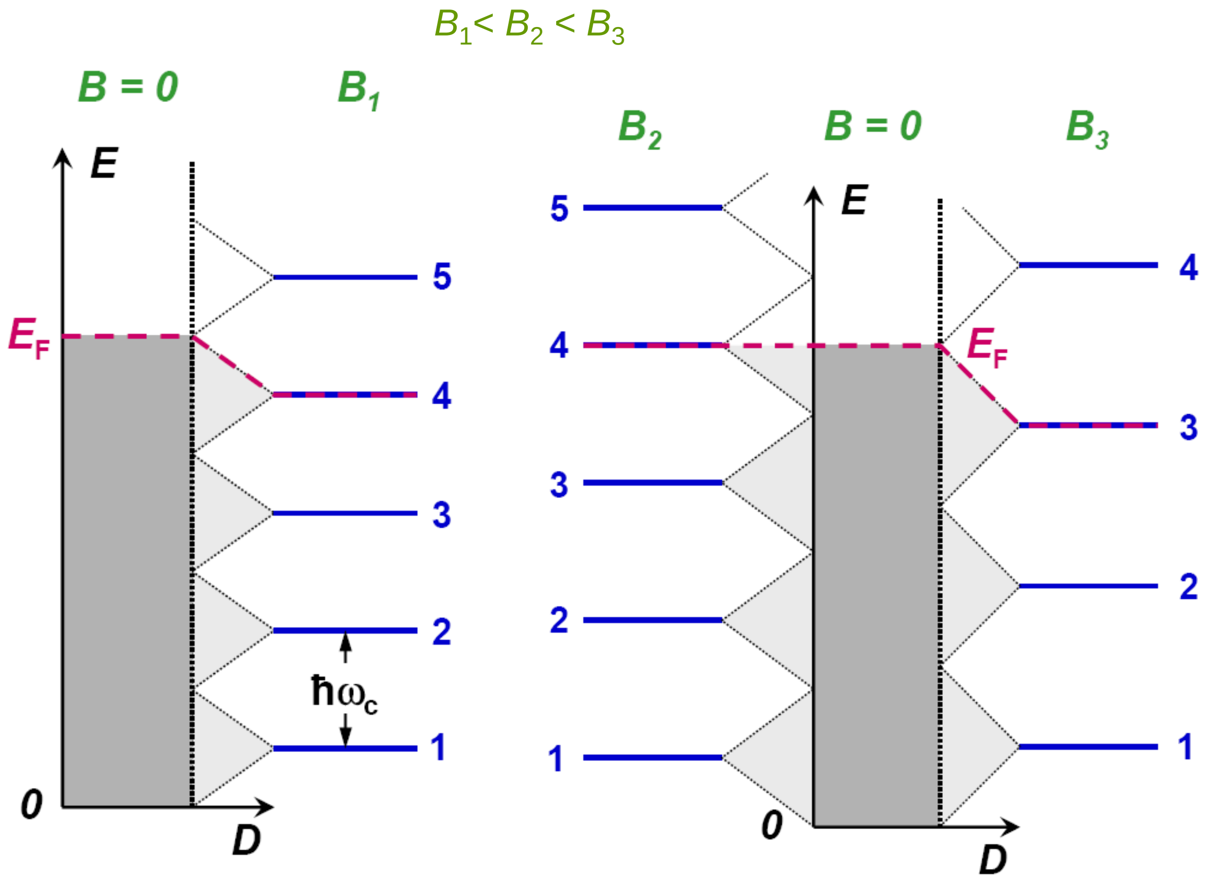
→ Fermi sphere becomes stack of cylinders normal to B

→ radius of cylinders ∝ H

→ cylinders expand with increasing H

→ orbits/tubes are pushed out of the FS one by one





Fermi surface and field

Landau tubes

→ number of states at E_F are highly enhanced when there are extremal orbits on the Fermi surface

→ extremal orbits at regular interval of 1/B

- Successive H's that produce orbits with the same area:

$S_n = (n+1/2)\ 2pe/\hbar c\ H$ S:= area of the extremal orbit of the Fermi surface (m^{-2})

$S_n' = (n-1/2)\ 2pe/\hbar c\ H' \quad (H' > H)$

$$\rightarrow \quad S\left(\frac{1}{H}-\frac{1}{H'}\right)=\frac{2\pi e}{\hbar c}$$

→ equal increment of 1/H reproduces similar orbits

https://phy.ntnu.edu.tw/~changmc/Teach/SS/SSG_note/grad_chap14.pdf

quantum oscillations

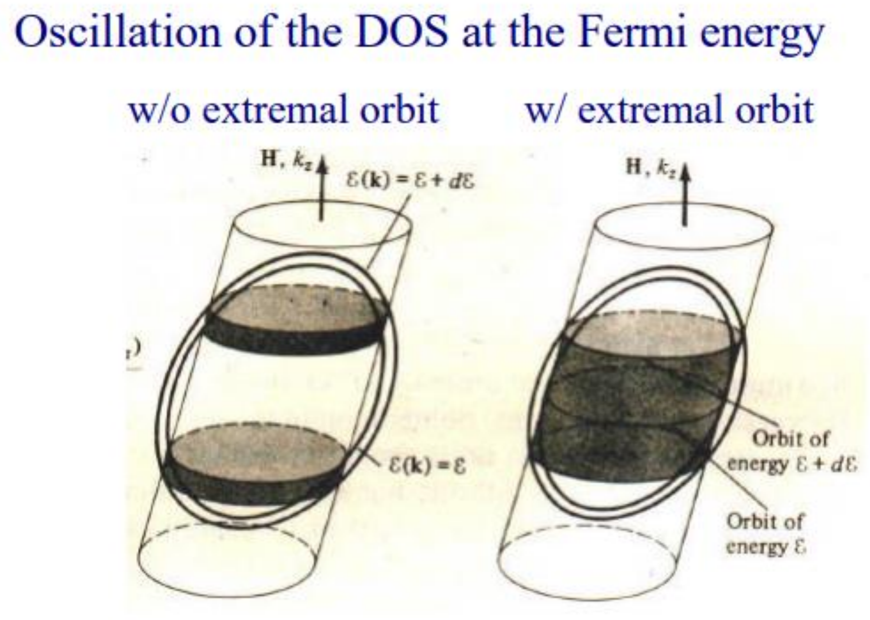
oscillatory variation of physical quantity as a function of a magnetic field strength (B)

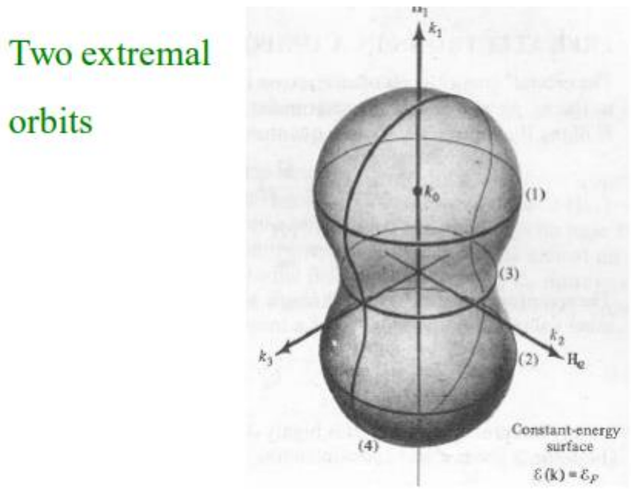
Landau tubes

→ number of states at E_F are highly enhanced when there are extremal orbits on the Fermi surface

→ extremal orbits at regular interval of 1/B

→ oscillation in 1/B can be detected in any physical quantity that depends on the DOS

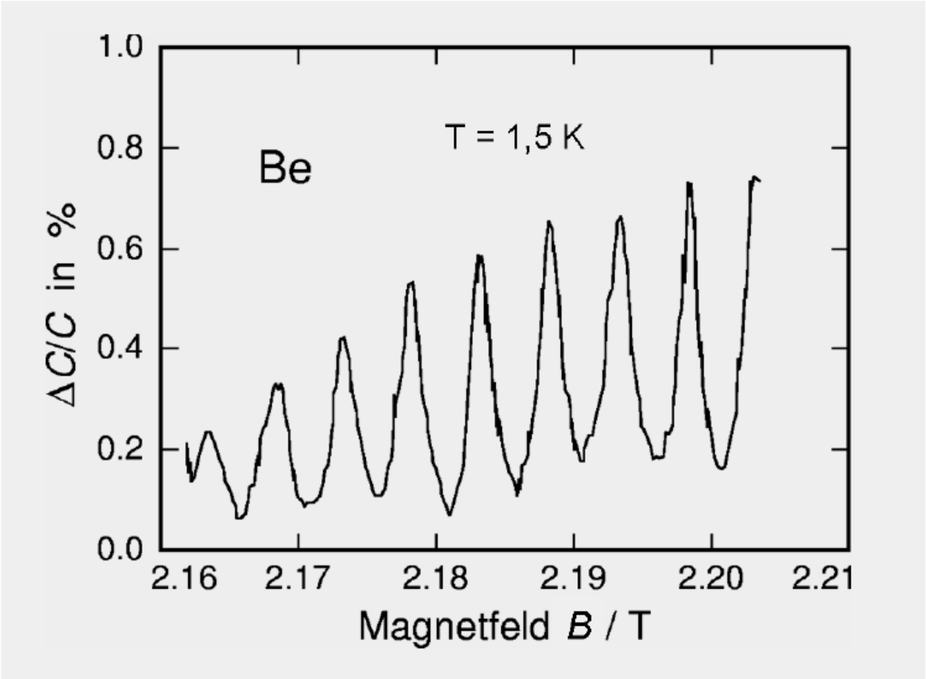




https://phy.ntnu.edu.tw/~changmc/Teach/SS/SSG_note/grad_chap14.pdf

quantum oscillations in metals

specific heat



$$C_P(T) = \gamma T + \beta T^3 + o(T^3)$$

$$\gamma = \frac{\pi^2}{3} k_B \rho(E_F) = \frac{k_B^2}{3\hbar^2} V k_F m^*$$

De Haas-van Alphen effect

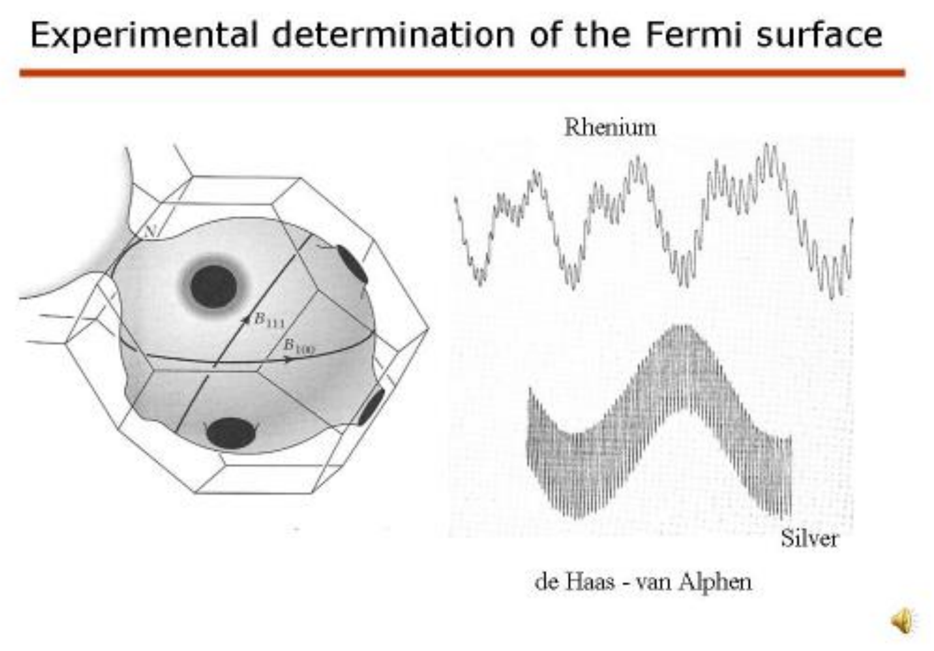
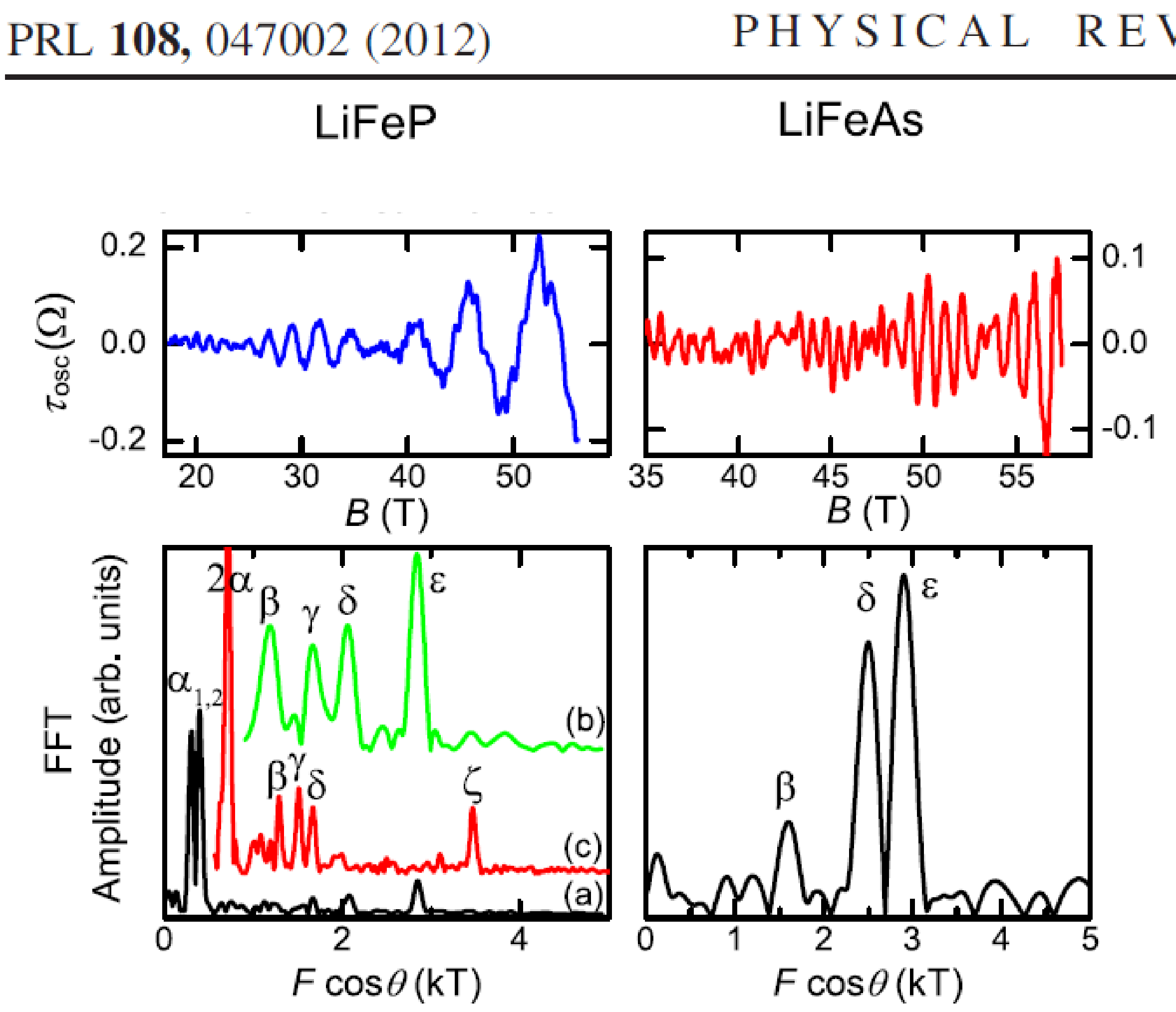


Abbildung 3: de Haas - van Alphen oscialltions

http://lampx.tugraz.at/~hadley/ss2/problems/fermisurf/s.pdf

De Haas van Alphen in LiFeAs

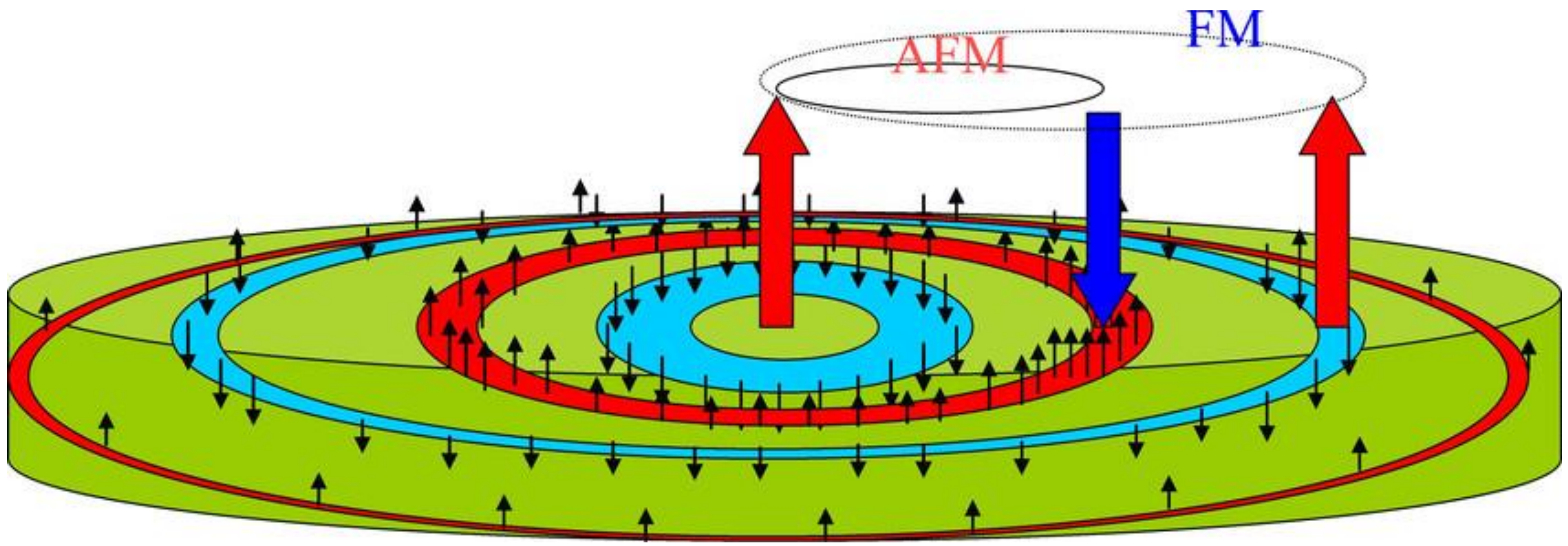


2.4 band ferromagnetism (spontanous band splitting)

Stoner criterion, s-d model (see lectures by J. Dufoleur)

2.5 RKKY interaction in metals

Ruderman–Kittel–Kasuya–Yosida.

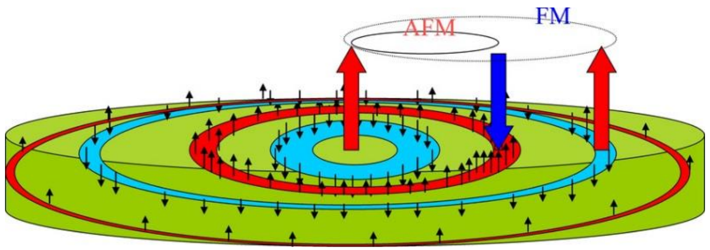


local magnetic polarizes conduction electrons which in turn couples to another local moment at distance *r*

→ interaction of free electron gas with localized moments

https://www.researchgate.net/profile/Puspamitra_Panigrahi/publication/252771578/figure/download/fig1/AS:669380048351236@1536604048549/RKKY-interaction-the-interaction-of-magnetic-spins-mediated-by-conduction-electrons.ppm

2.5 RKKY interaction in metals

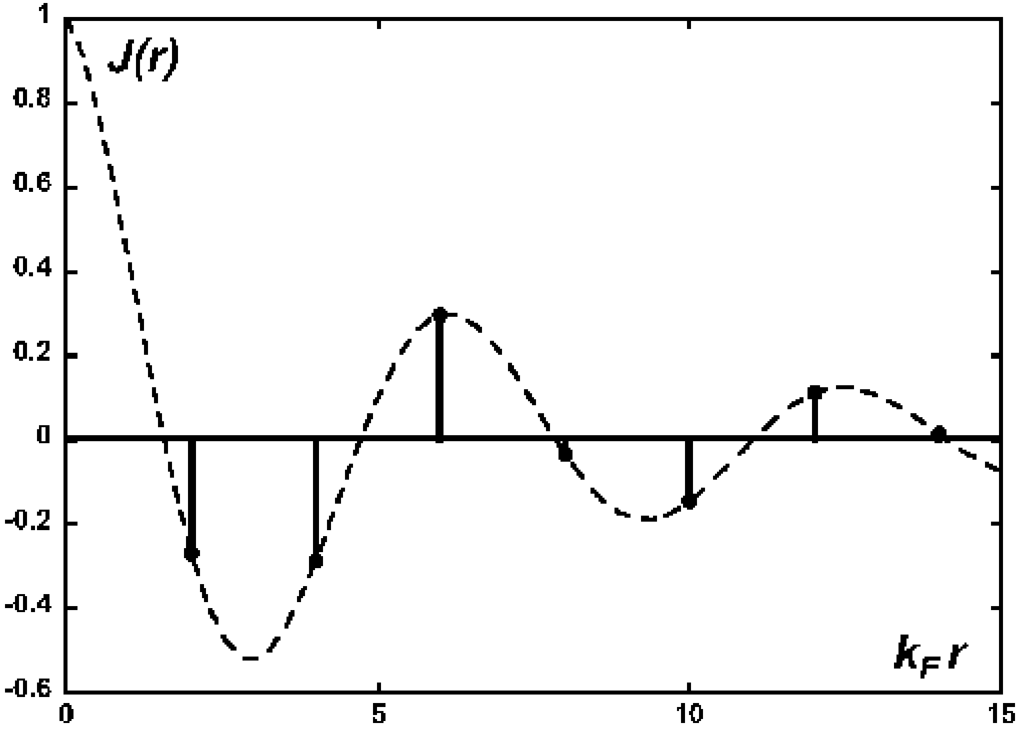


local magnetic polarizes conduction electrons which in turn couples to another local moment at distance *r*

→ indirect, itinerant exchange interaction between magnetic moments mediated by conduction electrons

- long ranged
- oscillating dependance of J_{RKKY} on r → fm or afm
- description by second-order perturbation theory

$$J_{RKKY} \propto \frac{\cos(2k_F r)}{r^3}$$



https://www.researchgate.net/profile/Puspamitra_Panigrahi/publication/252771578/figure/download/fig1/AS:669380048351236@1536604048549/RKKY-interaction-the-interaction-of-magnetic-spins-mediated-by-conduction-electrons.ppm
https://www.researchgate.net/profile/Heinz_Horner/publication/1940273/figure/fig1/AS:497194916474880@1495551913737/RKKY-interaction.png