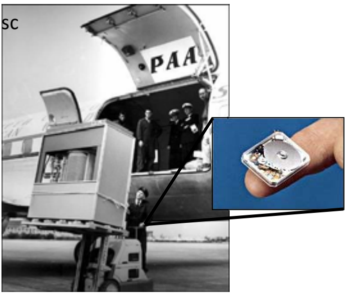
Frithjof Nolting :: Head of LSC :: Paul Scherrer Institut

Introduction to electronic correlation

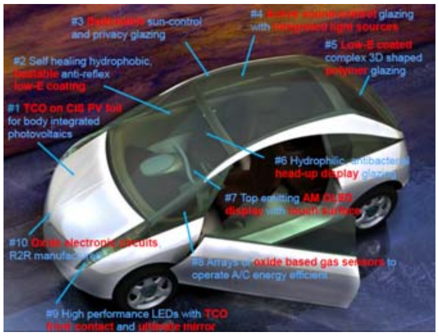
PSI Master School 2017

Basic research – electronic devices

Hard disc



Cars, sensors, displays



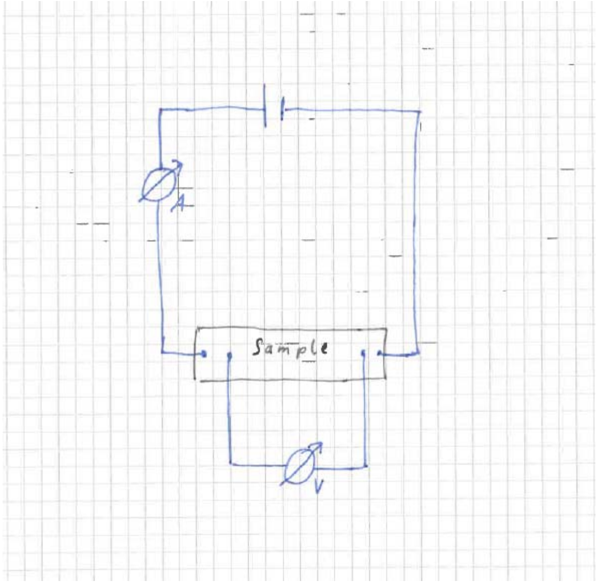
Modern communication devices are full of fascinating physics and advanced materials

Aim of the lecture

Brief reminder about condensed matter physics – electronic structure as basis for the following lectures

- Resistivity
- Electron bands
- Superconducivity
- Magnetism
- Other example of strongly correlated electron systems

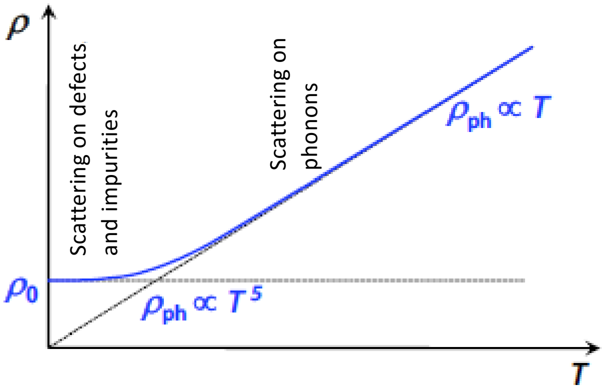
How do we measure the resistance of a sample



Why do we measure the resistance?

Resistance

Scattering is responsible for resistance



$$\rho = \frac{m}{ne^2}\left(\tau_{\rm imp}^{-1} + \tau_{\rm el-el}^{-1} + \tau_{\rm el-ph}^{-1}\right)$$

Matthiessen rule

Can all electrons contribute to the transport?

Drude Model

electron like a classical gas of free particles

acceleration by electric field (all electrons are accelerated)

scattering on atoms

no electron interaction

$$J_q = -en v_D = \frac{ne^2\tau}{m} E = ne\mu E$$

μ: mobility

V_D: drift velocity

τ: scattering time

Drude model: all electrons

Sommerfeld: just the ones at fermi but they have higher velocity

Sommerfeld-Model

gas of fermions

Pauli principle

Schrödinger Equation

density of states

Electron density in k-space

$$-\frac{\hbar^2}{2m}\nabla^2 \Psi(\mathbf{r},\sigma) = E\,\Psi(\mathbf{r},\sigma)\,.$$

Schroedinger equation

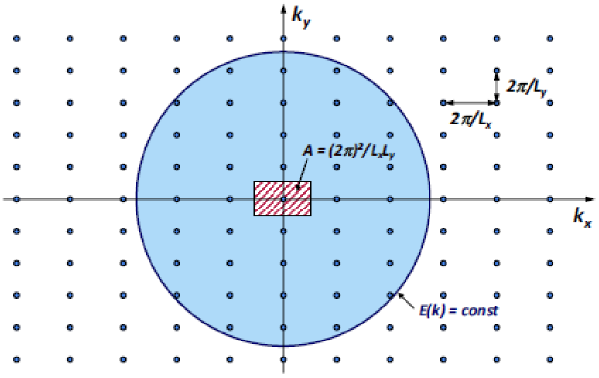
$$\Psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{\imath \mathbf{k}\cdot\mathbf{r}}$$

Electron waves

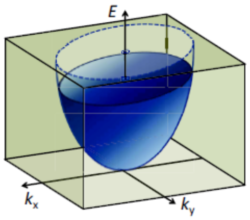
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}\,.$$

Dispersion

Boundary condition: Box

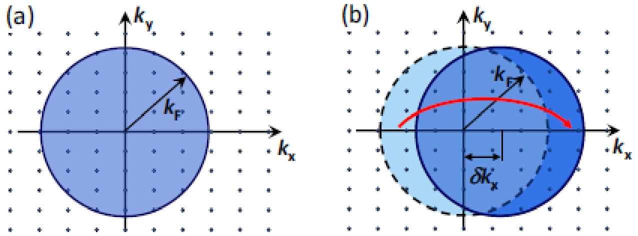


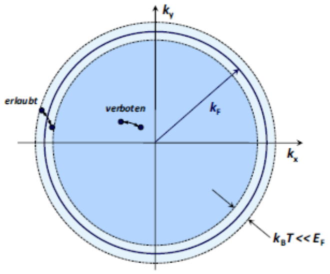
Allowed states in k-space (2 dimensional)



Source: Gross und Marx, Festkörperphysik

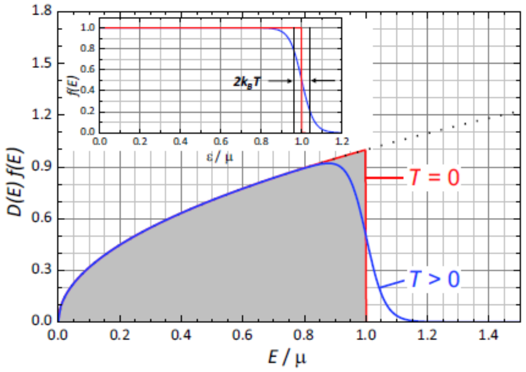
Conductivity – Sommerfeld Model





Source: Gross und Marx, Festkörperphysik

Electron occupation



Drude model: all electrons

Sommerfeld: just the ones at fermi but they have higher velocity

Typical values for metals

$k_F \simeq 10^8$ cm^{-1}

$\lambda_F \simeq$ 1A

$v_F \simeq 10^8$ cm/s

$E_F \simeq$ 4 eV

$T_F \simeq$ 50 000K

Source: Gross und Marx, Festkörperphysik

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Electron waves in metals

From free electron to:

quasi free electron

electron wave in periodic potential of atoms as weak perturbation

quasi bound electron (Tight Binding)

Dispersion and periodicity

$$\mathcal{H}\Psi_{\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\Psi_{\mathbf{k}}(\mathbf{r})$$

Schroedinger equation

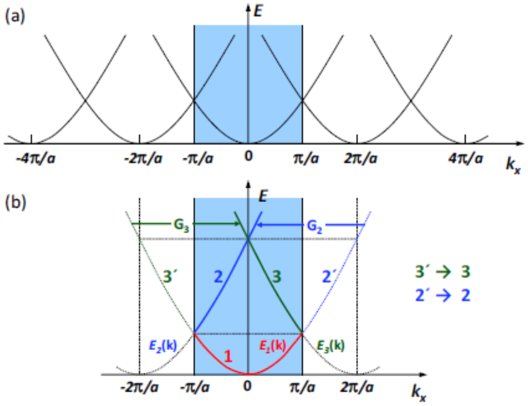
$$\Psi_{\mathbf{k}+\mathbf{G}}(\mathbf{r}) = \Psi_{\mathbf{k}}(\mathbf{r}) .$$

$$E_n(\mathbf{k}) = E_n(\mathbf{k}+\mathbf{G}_n) .$$

G: reciprocal lattice vector

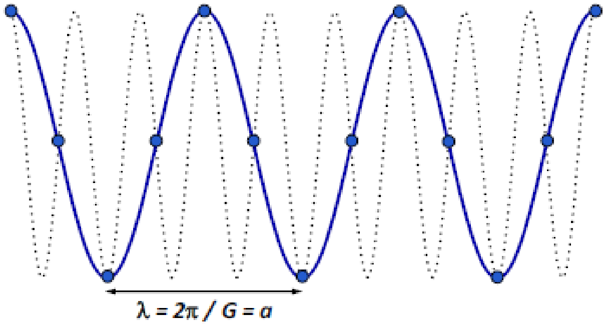
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} .$$

Dispersion



Source: Gross und Marx, Festkörperphysik

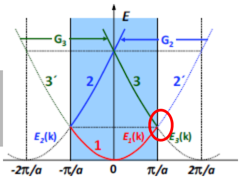
Bloch waves in real space: analog oscillation atoms



Oscillation of lattice atoms with smallest possible wave number (continuous line) and with a larger wave number

Source: Gross und Marx, Festkörperphysik

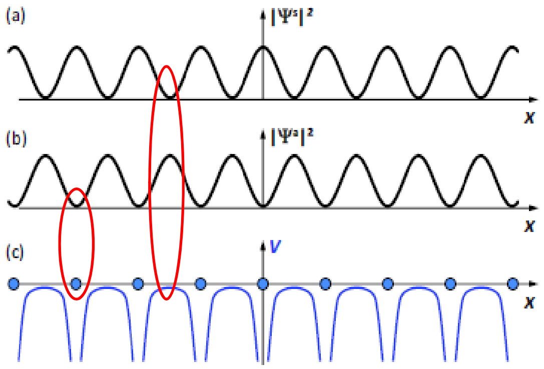
Brillouin zone boarder



degenerated

Bragg reflection condition

standing wave

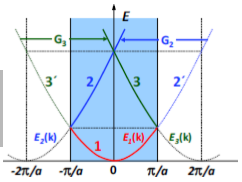


Two different probability densities for standing wave

Different potential energy

Source: Gross und Marx, Festkörperphysik

Brillouin zone boarder



degenerated

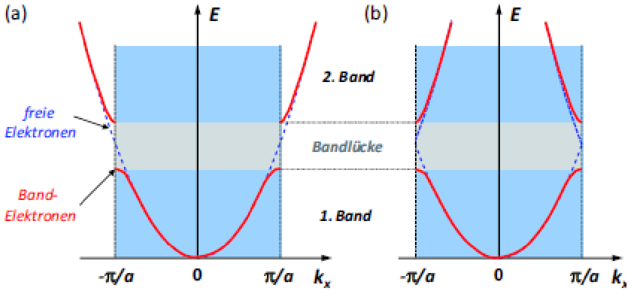
Bragg reflection condition

standing wave

$$\mathbf{v}_{n,\mathbf{k}} = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}} = \frac{\partial \omega_n(\mathbf{k})}{\partial \mathbf{k}} .$$

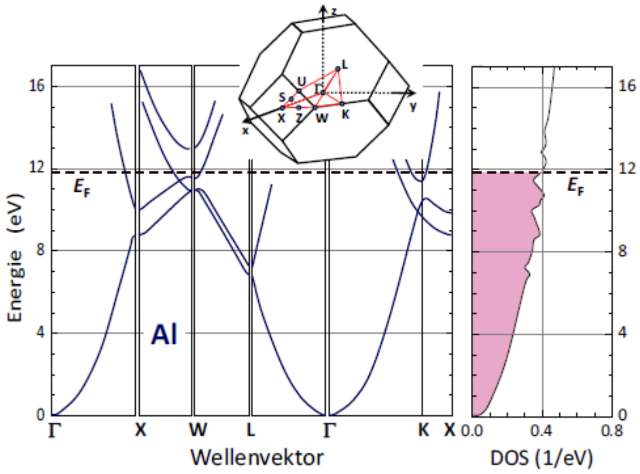
Group velocity

$$\frac{\partial E}{\partial \mathbf{k}} = 0$$



Source: Gross und Marx, Festkörperphysik

Bandstructure simple metal - Aluminum



Electron configuration [Ne] $3s^2 3p^1$

Source: Gross und Marx, Festkörperphysik

Energy scales – metals and oxides

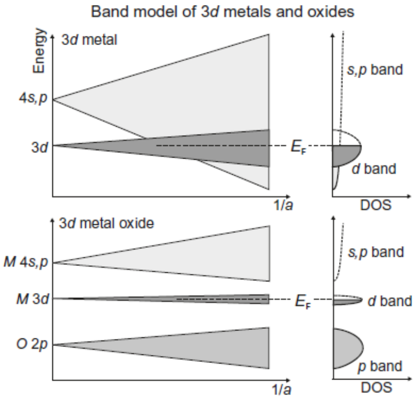
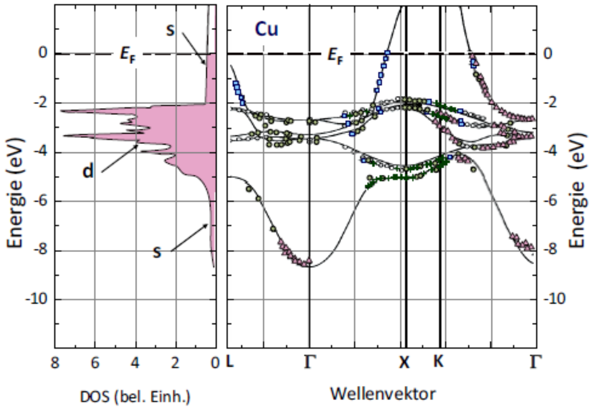


Fig. 7.17. Expected electronic structure for 3*d* transition metals and their oxides in the band model. We have plotted how the atomic valence orbitals, which are located at different binding energies, are expected to split under the influence of bonding interaction between the orbitals. We have assumed the atoms to be separated by a distance a, so that the bonding increases with $1/a$. The lack of direct d-orbital overlap for the oxides leads to a reduced band width and to their correlated nature

Source: Stöhr and Siegmann, Magnetism

Bandstructure of 3d metal



(Elektronenkonfiguration: [Ar]$3d^{10}4s^1$)

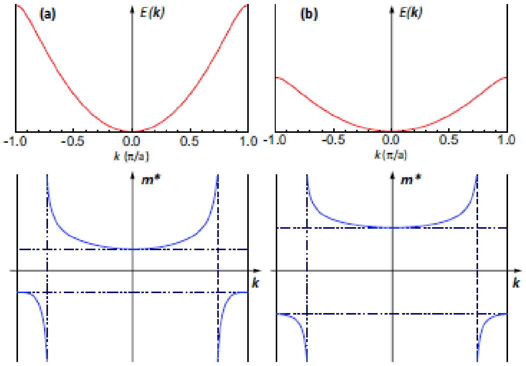
Source: Gross und Marx, Festkörperphysik

Effective mass - dispersion

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}_{n(\mathbf{k})} = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}}$$

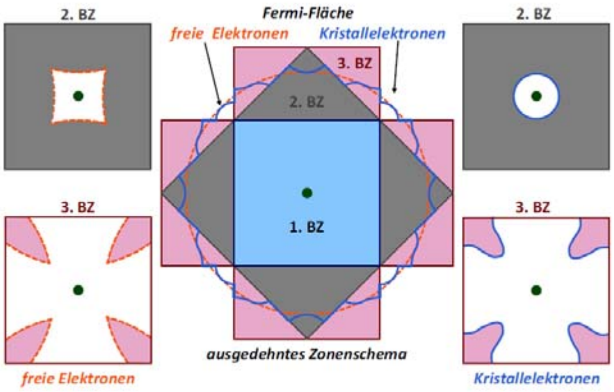
$$\frac{d\mathbf{v}_n(\mathbf{k})}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}}\right) = \frac{1}{\hbar}\sum_{j=1}^{3}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_i \partial k_j}\frac{dk_j}{dt}\,.$$

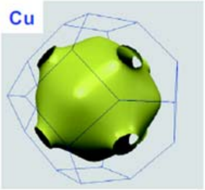
$$\left[(m^*)^{-1}(\mathbf{k})\right]_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_i \partial k_j}$$



Source: Gross und Marx, Festkörperphysik

Fermi surfaces





Aim of the lecture

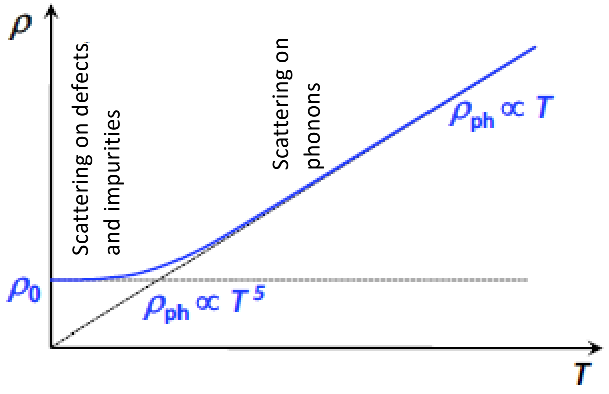
Brief reminder about condensed matter physics – electronic structure as basis for the following lectures

- Resistivity
- Electron bands
- Superconducivity
- Magnetism
- Other example of strongly correlated electron systems

Resistance

Scattering is responsible for resistance

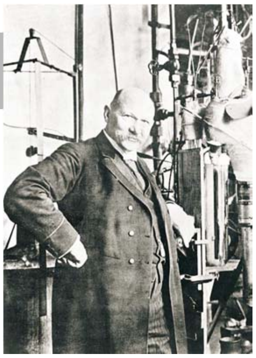
Only deviations from perfect periodicity lead to scattering



$$\rho = \frac{m}{ne^2}\left(\tau_{\mathrm{imp}}^{-1} + \tau_{\mathrm{el-el}}^{-1} + \tau_{\mathrm{el-ph}}^{-1}\right)$$

Matthiessen rule

Discovery of superconductivity

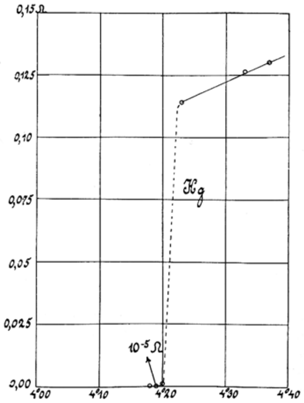


www.scientificamerican.com

Transition Temperatur in Hg: T_C=4.2K (1911)

Resistivity R=0 below T_C; ($R<10^{-23}\ \Omega\cdot$cm)

10^{18} times smaller than for Cu)



H. Kamerlingh Onnes, Commun. Phys. Lab. Univ. Leiden. Suppl. 29 (Nov. 1911).

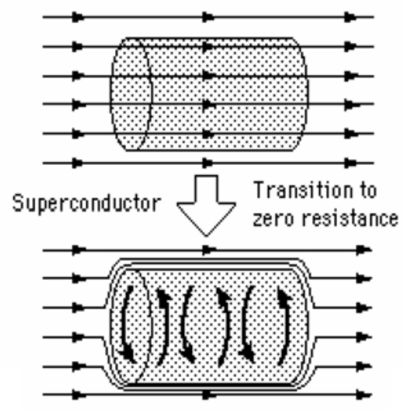
„Mercury has passed into a new state, which on account of its extraordinary electrical properties may be called the superconducting state"

H. Kamerlingh Onnes 1913 (Nobel Prize 1913)

Meissner effect

A superconductor is a perfect diamagnet. Superconducting material expels magnetic flux from the interior.

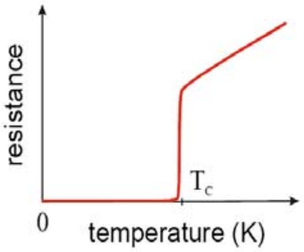
W. Meissner, R. Ochsenfeld (1933)



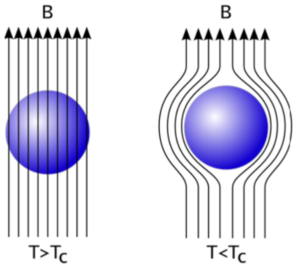
On the surface of a superconductor ($T<T_C$) superconducting current will be induced. This creates a magnetic field compensating the outside one.

Screening (shielding) currents

Main Characteristics:



Kamerlingh Onnes

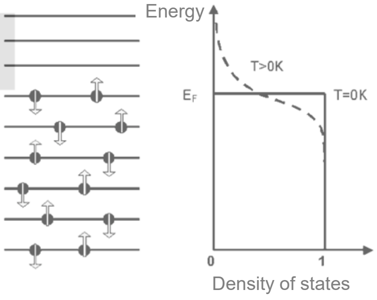


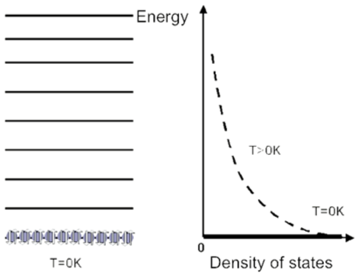
Meissner and Ochsenfeld

Is a superconductor “just” an ideal conductor?

See lecture on Friday, Alex Amato

Fermi / Bose statistics

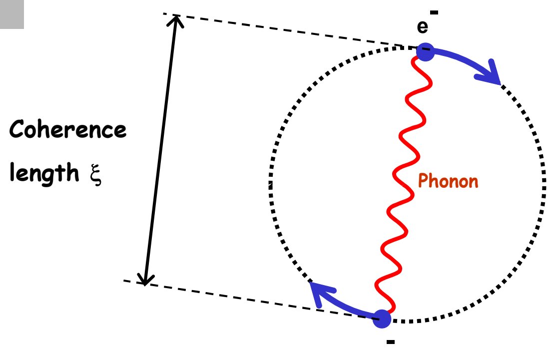




- Fermions- elemental particles with half integer spin (e.g. electrons, protons, neutrons..)
- Pauli-Principle –every energy level can be occupied with maximum two electrons with opposite spins.

- Bosons – elemental particles with integer spin.
- A state can be populated by many particles

Electrons form pairs: Cooper pairs



Cooper pair model

Microscopic Theory of Superconductivity*

J. Bardeen, L. N. Cooper, and J. R. Schrieffer

Department of Physics, University of Illinois, Urbana, Illinois

(Received February 18, 1957)

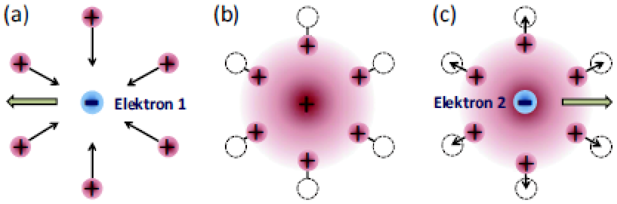
Microscopic theory of conventional superconductivity:

BCS theory

Cooper pairs can undergo Bose condensation

Interaction that form Cooper pairs

BCS theory: An electron on the way through the lattice interacts with lattice sites. The electron produces a charged lattice deformation.



During one phonon oscillation an electron can cover a distance of ~10^4Å. The second electron will be attracted without experiencing the repulsing electrostatic force .

The lattice deformation creates a region of relative positive charge which can attract another electron.

1957 John Bardeen, Leon Cooper, and John Robert Schrieffer

Discovery of "high-T_c" superconductivity

1911-1986: "Low temperature superconductors" highest T_C=23K for Nb_3Ge

1986 (January): High Temperature Superconductivity $(LaBa)_2\,CuO_4$ T_C=35K

K.A. Müller und G. Bednorz (IBM Rüschlikon) (Nobel 1987)

1987 (January): $YBa_2Cu_3O_{7-x}$ T_C=93K

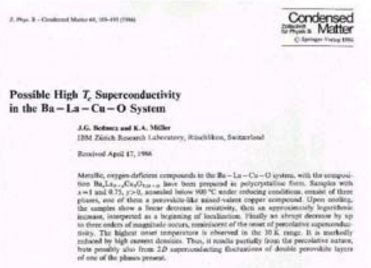
1987 (December): Bi-Sr-Ca-Cu-O T_C=110K

1988 (January): Tl-Ba-Ca-Cu-O T_C=125K

1993: Hg-Ba-Ca-Cu-O T_C=133K

$\}$ Cuprates


Professor Dr. Dr. h. c. mult. Karl Alex Müller (links) und Dr. Johannes Georg Bednorz


Z. Phys. B – Condensed Matter 64, 189–193 (1986)

Condensed Matter
Zeitschrift für Physik B
© Springer-Verlag 1986

Possible High T_c Superconductivity in the Ba – La – Cu – O System

J.G. Bednorz and K.A. Müller
IBM Zürich Research Laboratory, Rüschlikon, Switzerland

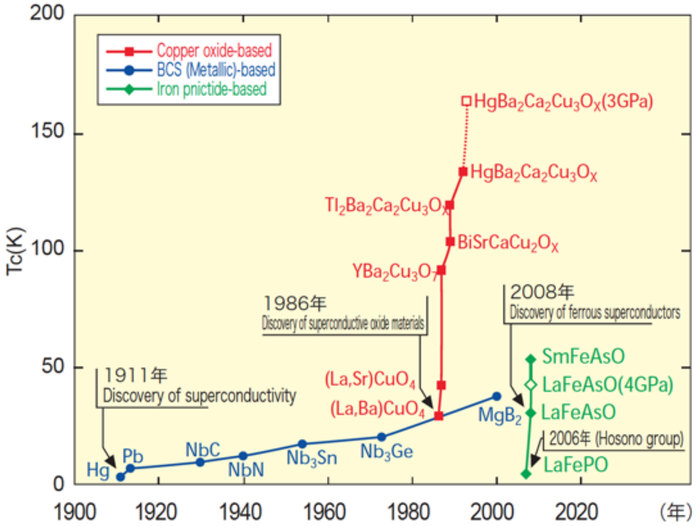
Received April 17, 1986

Metallic, oxygen-deficient compounds in the Ba – La – Cu – O system, with the composition $Ba_xLa_{5-x}Cu_5O_{5(3-y)}$ have been prepared in polycrystalline form. Samples with x=1 and 0.75, y>0, annealed below 900 °C under reducing conditions, consist of three phases, one of them a perovskite-like mixed-valent copper compound. Upon cooling, the samples show a linear decrease in resistivity, then an approximately logarithmic increase, interpreted as a beginning of localization. Finally an abrupt decrease by up to three orders of magnitude occurs, reminiscent of the onset of percolative superconductivity. The highest onset temperature is observed in the 30 K range. It is markedly reduced by high current densities. Thus, it results partially from the percolative nature, bute possibly also from 2D superconducting fluctuations of double perovskite layers of one of the phases present.

2001 MgB_2 T_C=39K

2008 $La(O_{1-x}F_x)FeAs$: T_C=26K; $SmFeAsO_{1-\delta}$: T_C=55K

Comparison of superconductors



Japan Science and Technology Agency Breakthrough Report, Vol 13

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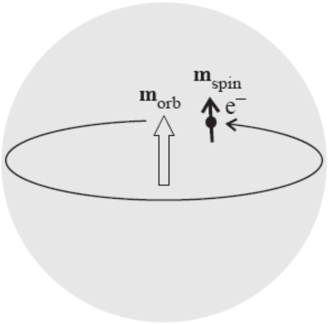
Source of magnetism (atomic)



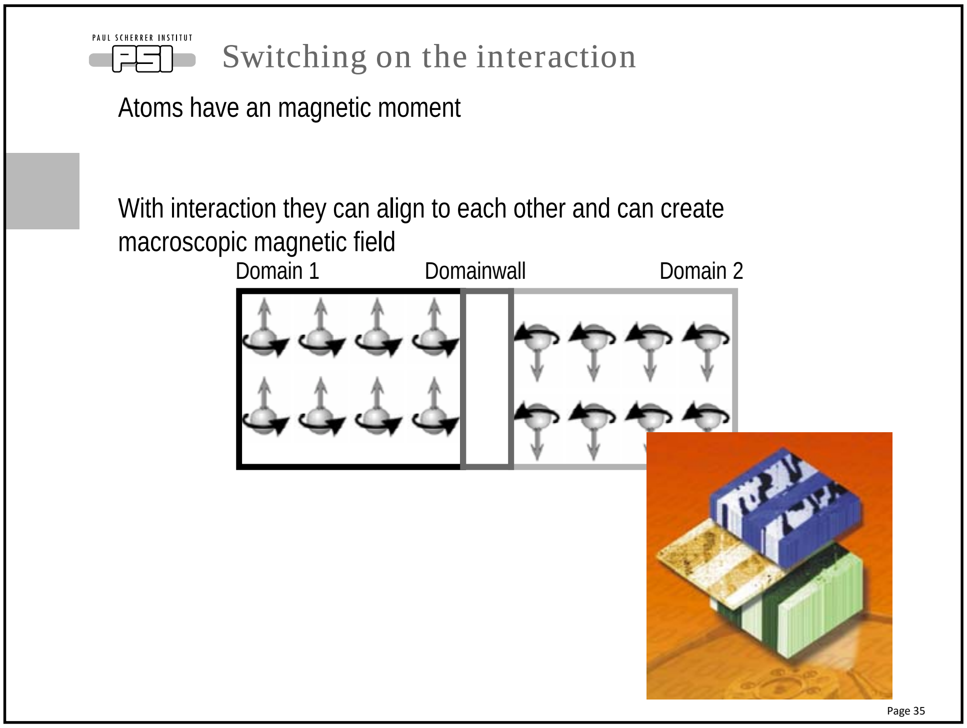
Spin moment	~ 1.5 μ_B / atom	isotropic
Orbital moment	~ 0.1 μ_B / atom	isotropic/anisotropic

They interact via the spin-orbit coupling L · S

Switching on the interaction

- Atoms have an magnetic moment

Without interaction (and no applied magnetic field) they point in random directions and no macroscopic magnetic field is created

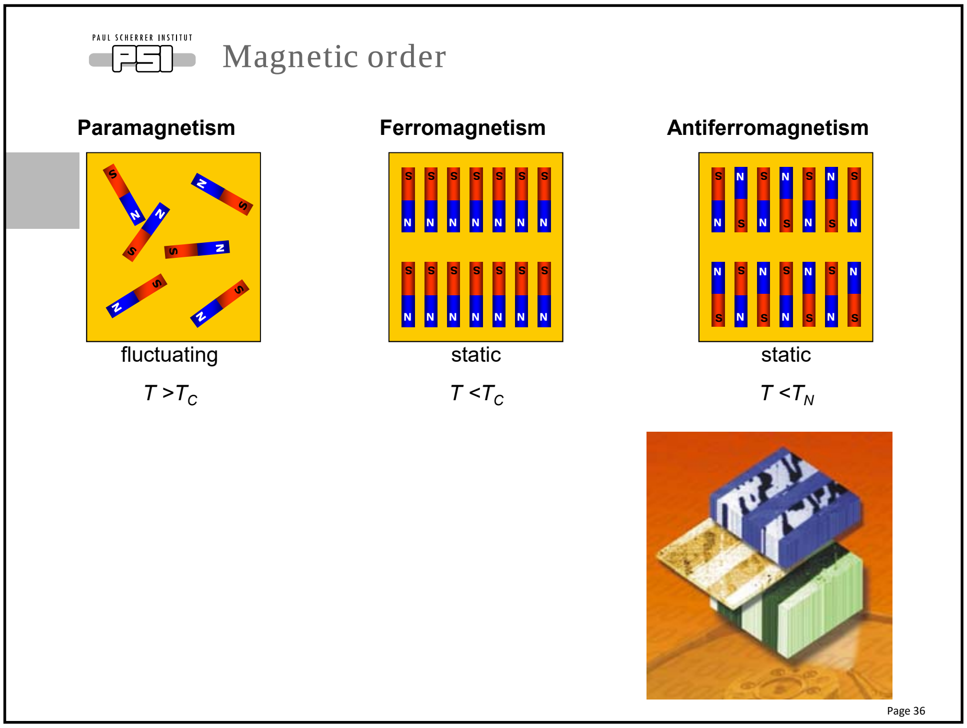


Switching on the interaction

Atoms have an magnetic moment

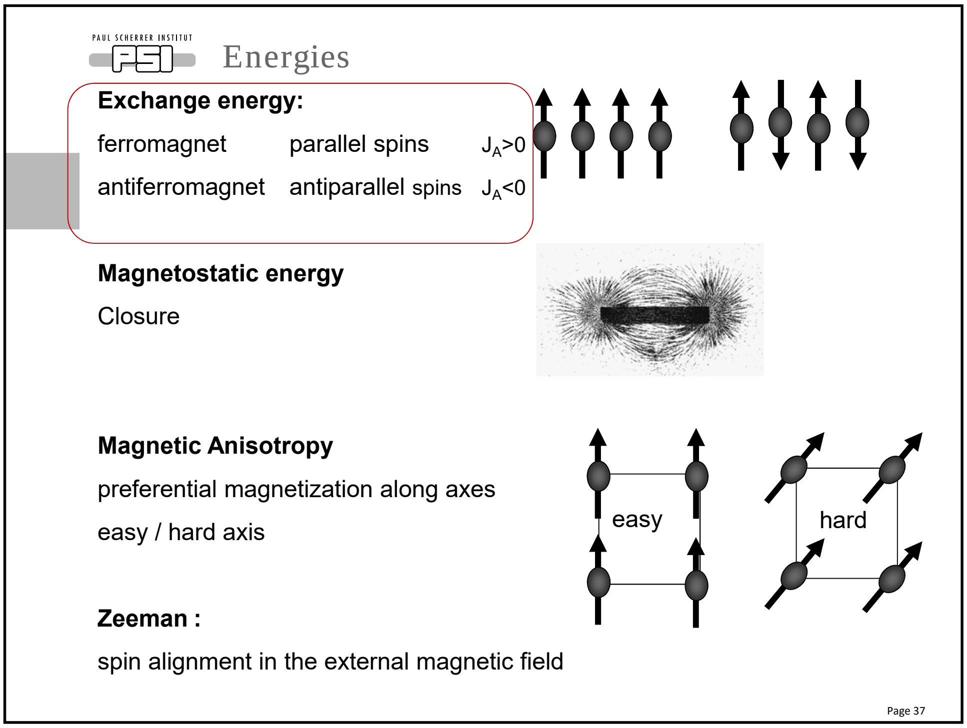
With interaction they can align to each other and can create macroscopic magnetic field

Domain 1 Domainwall Domain 2



Magnetic order

Paramagnetism	**Ferromagnetism**	**Antiferromagnetism**
fluctuating	static	static
$T > T_C$	$T < T_C$	$T < T_N$



Energies

Exchange energy:

ferromagnet	parallel spins	$J_A>0$
antiferromagnet	antiparallel spins	$J_A<0$

Magnetostatic energy

Closure

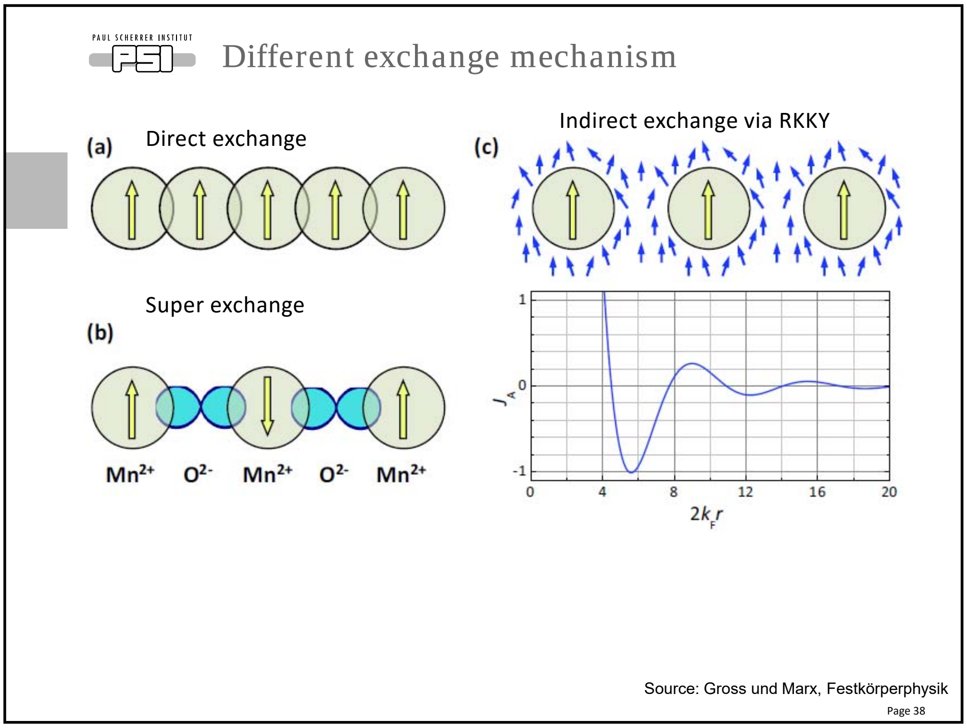
Magnetic Anisotropy

preferential magnetization along axes

easy / hard axis

Zeeman :

spin alignment in the external magnetic field

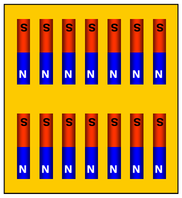


Different exchange mechanism

Source: Gross und Marx, Festkörperphysik

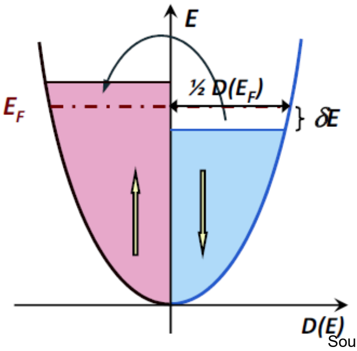
Exchange: delocalized electrons

Ferromagnetism



static

$T < T_C$



Source: Gross und Marx, Festkörperphysik

Two electrons with same spin not at same position.

Exchange hole leads to reduced screening of coulomb interaction between atom (+) and electron (-) which lower the coulomb energy

but

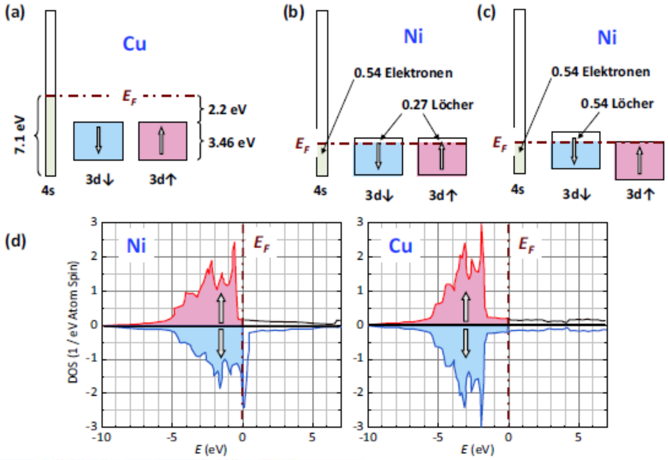
Stoner criterion

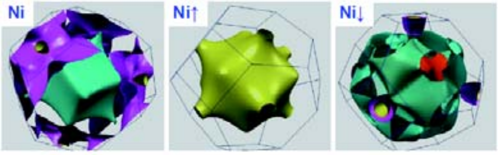
Increase of kinetic energy

$$\Delta E_{\text{kin}} \sim \delta p^2/2m^* \propto k_{\text{F}}^2/m^*$$

$$\tfrac{1}{2} U D(E_{\text{F}}) > 1$$

Density of states at the fermi energy

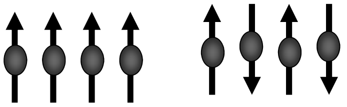




Source: Gross und Marx, Festkörperphysik

Energies

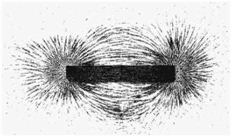
Exchange energy:



ferromagnet	parallel spins	$J_A>0$
antiferromagnet	antiparallel spins	$J_A<0$

Magnetostatic energy

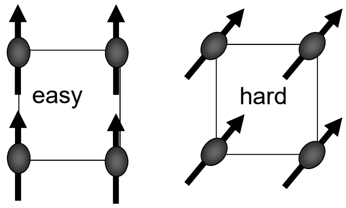
Closure



Magnetic Anisotropy

preferential magnetization along axes

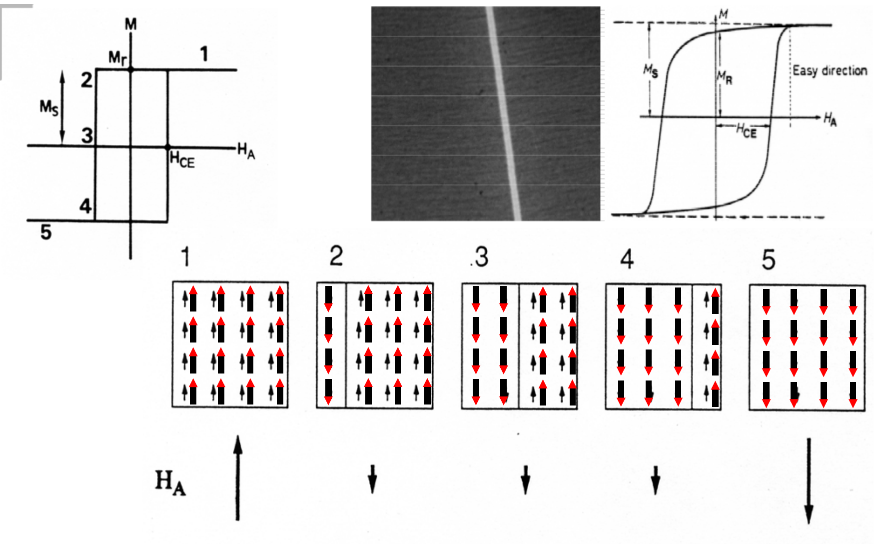
easy / hard axis

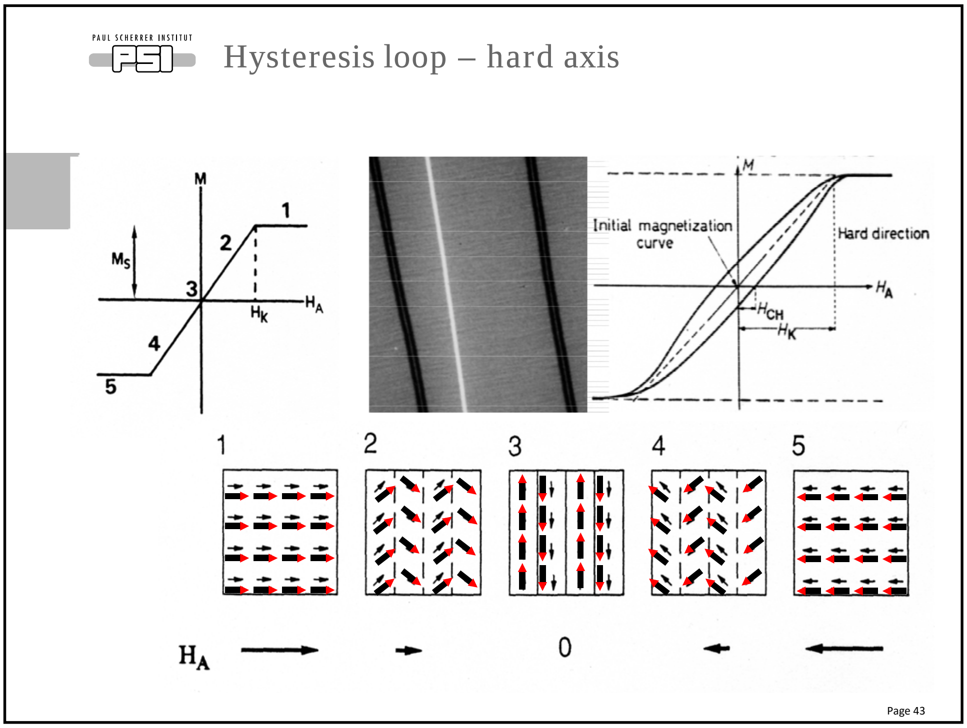


Zeeman :

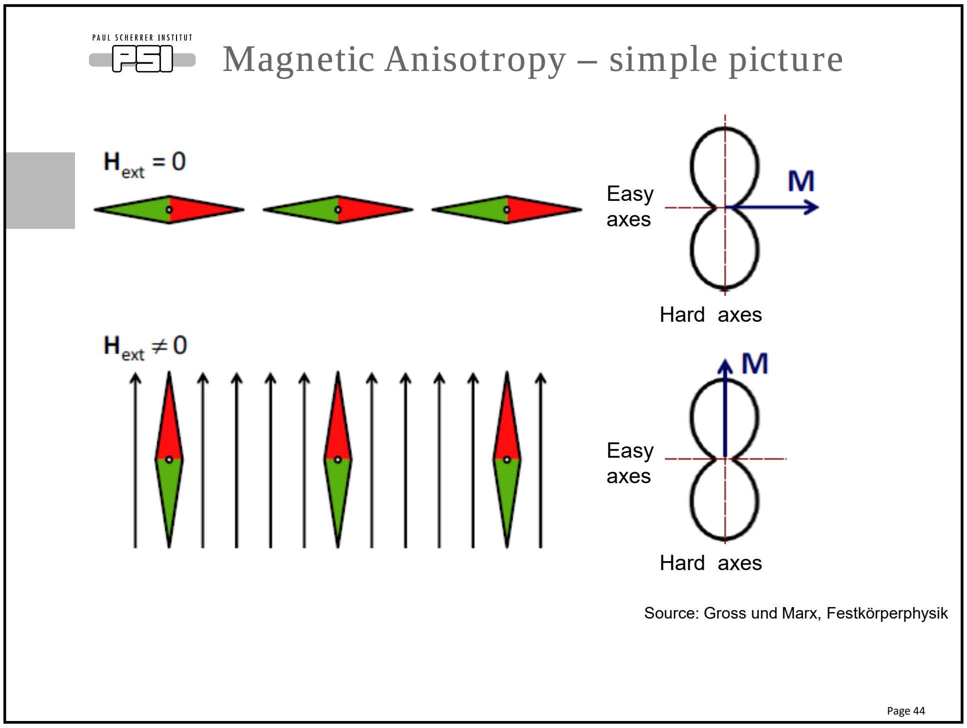
spin alignment in the external magnetic field

Hysteresis loop – soft axis





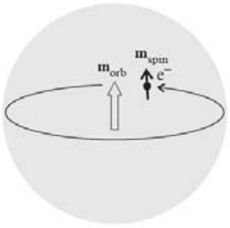
Hysteresis loop – hard axis

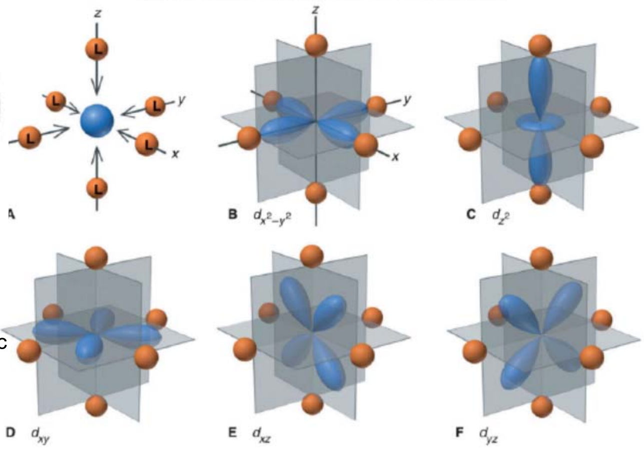


Magnetic Anisotropy – simple picture

Source: Gross und Marx, Festkörperphysik

Anisotropy: magneto crystalline

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Spin: isotropic

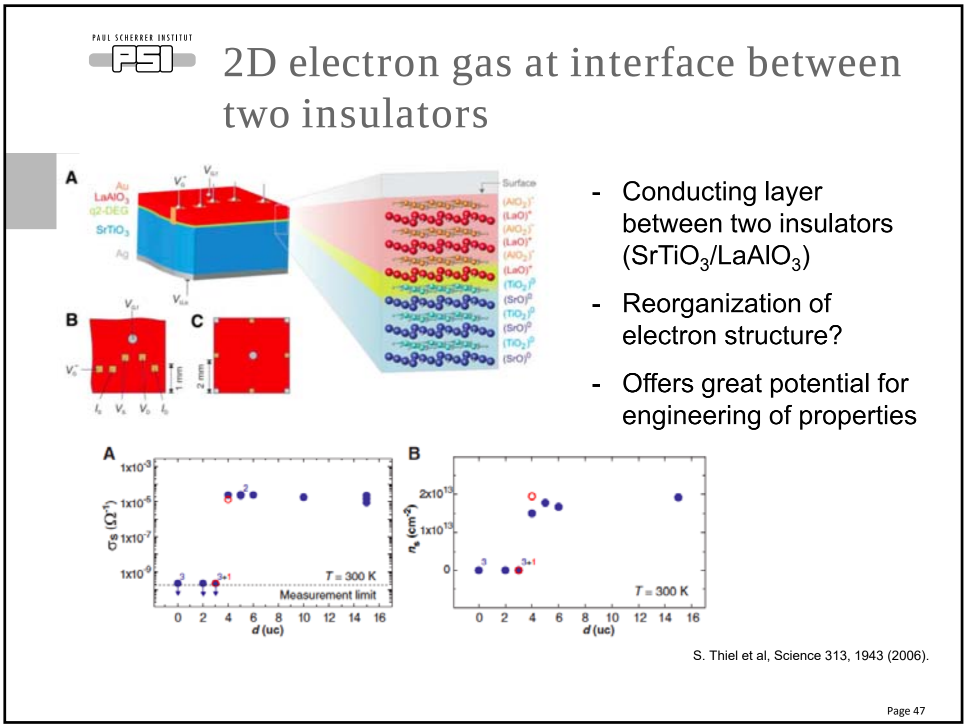
Orbit: can be anisotropic

They interact via the spin-orbit coupling $L \cdot S$

Aim of the lecture

Brief reminder about condensed matter physics – electronic structure as basis for the following lectures

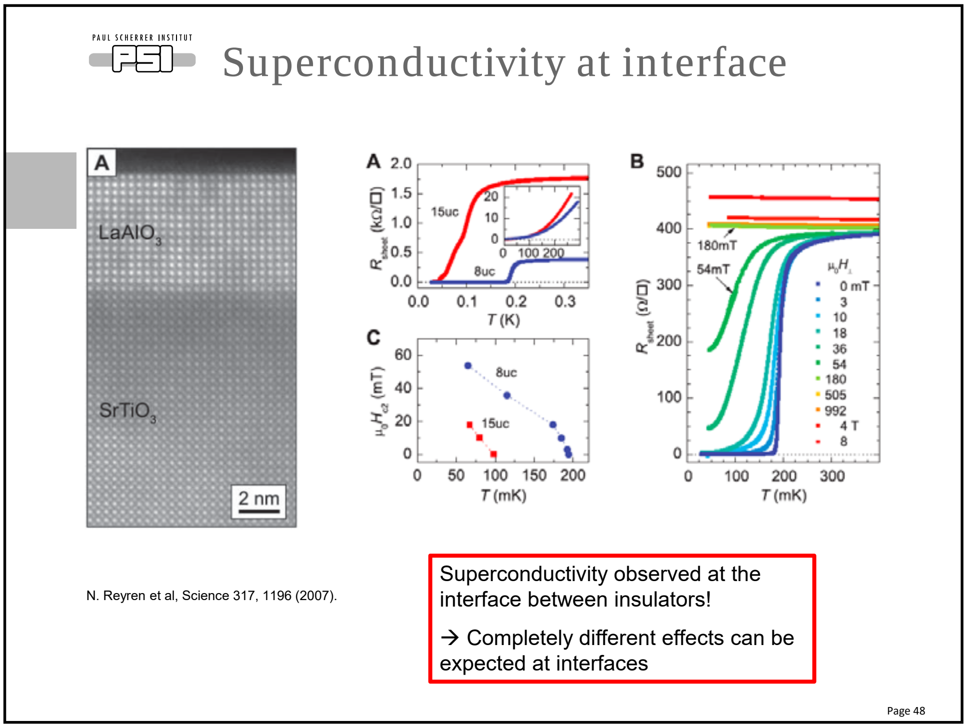
- Resistivity
- Electron bands
- Superconducivity
- Magnetism
- Other example of strongly correlated electron systems



2D electron gas at interface between two insulators

- Conducting layer between two insulators ($SrTiO_3/LaAlO_3$)
- Reorganization of electron structure?
- Offers great potential for engineering of properties

S. Thiel et al, Science 313, 1943 (2006).



Superconductivity at interface

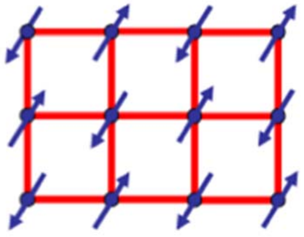
N. Reyren et al, Science 317, 1196 (2007).

Superconductivity observed at the interface between insulators!

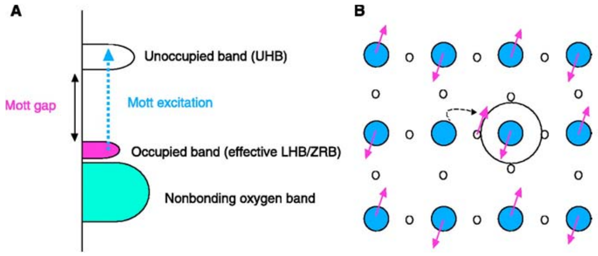
→ Completely different effects can be expected at interfaces

Magnetic order in a Mott insulator

One electron per site on a square lattice with strong Coulomb repulsion: electrons are localized, but their spins interact → Neel order at low T

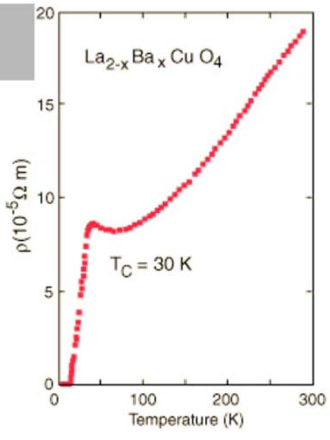


Neel state



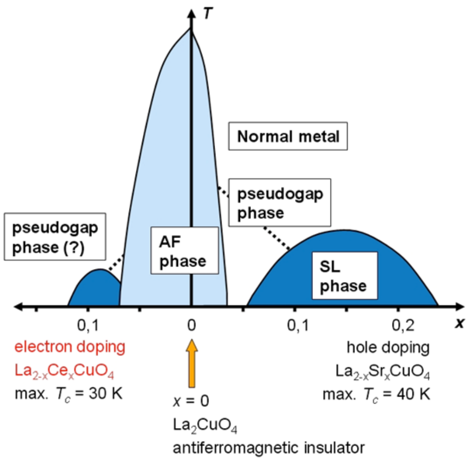
M.Z. Hasan et al, Science **288**, 1811 (2000)

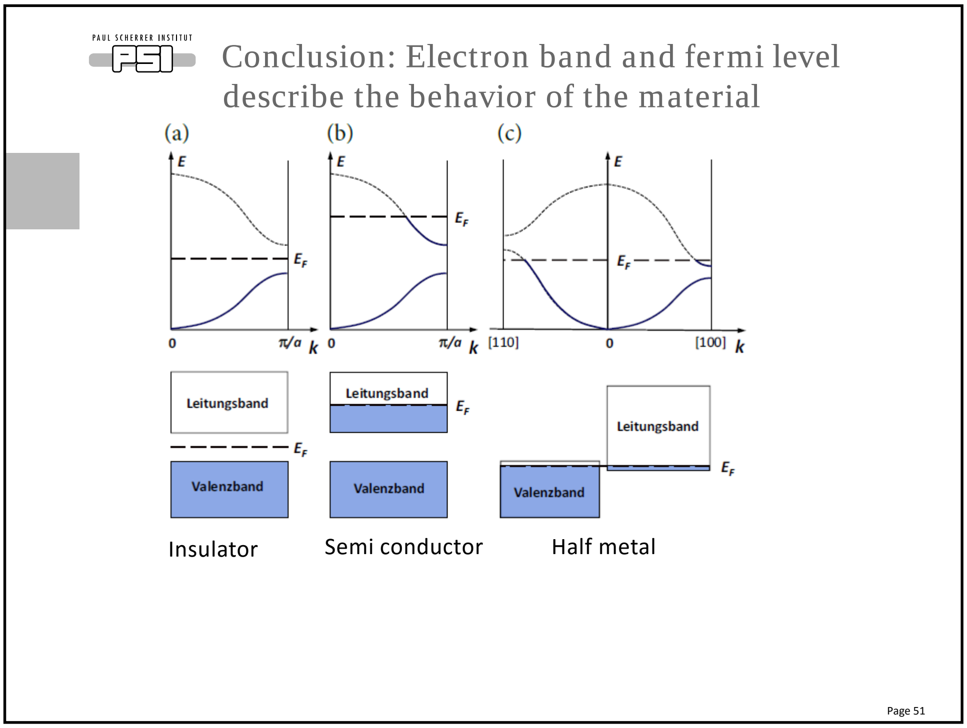
Doping of Mott insulator leads to superconductivity



Bednorz and Muller, Z. Physik B **64**, 189 (1986)

x(T) phase diagram of the cuprates





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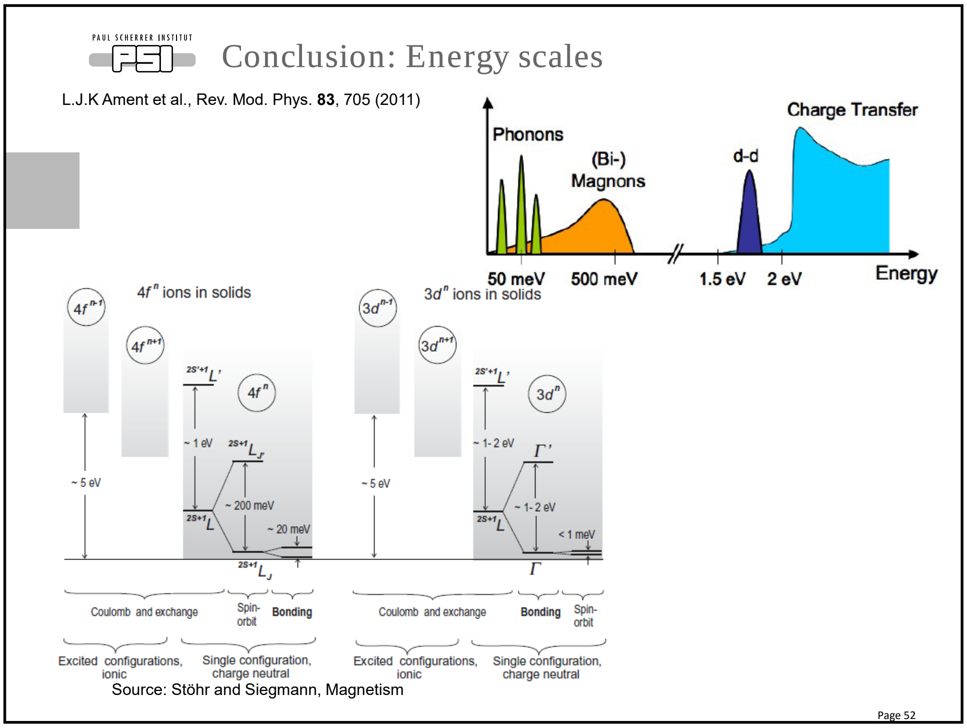
Conclusion: Electron band and fermi level describe the behavior of the material

Insulator

Semi conductor

Half metal



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Conclusion: Energy scales

L.J.K Ament et al., Rev. Mod. Phys. **83**, 705 (2011)

Source: Stöhr and Siegmann, Magnetism