Center for Electronic Correlations and Magnetism
University of Augsburg

Surprising effects of the interaction between electrons in solids

Dieter Vollhardt

Symposium “Topical aspects of condensed matter physics”
on the occasion of Gernot Güntherodt’s 70th birthday
RWTH Aachen, May 3, 2013

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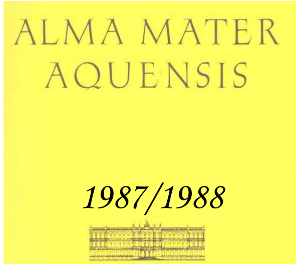
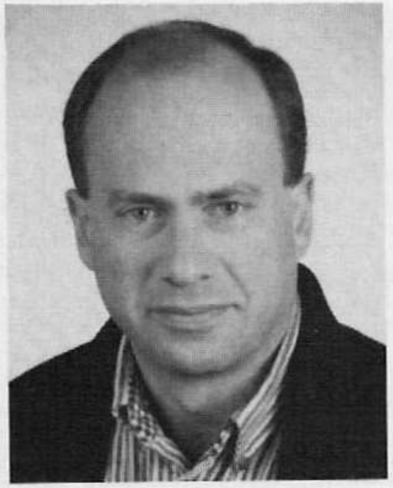


Professor Dr. sc. nat. Gernot ***Güntherodt***

Geboren am 27. April 1943 in Themar, Thüringen. – 1963 Abitur. – 1963–68 Studium der Physik an der ETH Zürich. – 1968–73 Wissenschaftlicher Assistent am Laboratorium für Festkörperphysik der ETH Zürich. – 1973 Promotion. – 1974–75 Postdoctoral Fellow am IBM T. J. Watson Research Center, Yorktown Heights, USA. – 1975–80 Permanenter Wissenschaftlicher Mitarbeiter am Max-Planck-Institut für Festkörperforschung in Stuttgart. – 1979 Ernennung zum C3-Professor am II. Physikalischen Institut der Universität zu Köln. – Seit 1980 Teilprojektleiter im Sonderforschungsbereich 125 (Aachen–Jülich–Köln). – 1981, 1982, 1986 Forschungsaufenthalte in USA (IBM, AT + T Bell Labs.) – 1983–85 Member of the Editorial and Executive Board of „European Journal of Physics". – April 1987 Ernennung zum C4-Professor und Institutsdirektor am 2. Physikalischen Institut (Lehrstuhl II A) der RWTH Aachen.



Professor Dr. rer. nat. Dieter ***Vollhardt***

Geboren am 8. September 1951 in Bad Godesberg. – 1969–71 United World College of the Atlantic, S.-Wales, UK. – 1971 Britischer, amerikanischer, deutscher und internationaler Schulabschluß. – 1971–76 Studium der Physik in Hamburg. – 1976–77 Forschungsaufenthalt an der University of Southern California (USC), Los Angeles, USA. – 1977 Physik-Diplom. – 1978–79 Doktorarbeit an der USC, Los Angeles, USA. – 1979 Promotion zum Dr. rer. nat. an der Universität Hamburg. – 1979–84 Wissenschaftlicher Angestellter am MPI für Physik und Astrophysik, München. – 1983 Forschungsaufenthalt bei den Bell Laboratories, Murray Hill, USA, und dem Institute for Theoretical Physics, Santa Barbara, USA. – 1984–87 Heisenberg-Stipendiat der DFG. – Seit 1. 10. 1987 Inhaber des Lehrstuhls C für Theoretische Physik und Direktor am Institut für Theoretische Physik.

German-Japanese Symposium, Schloss Ringberg (1990)

International Symposium on Competing Physics
in Novel Condensed Matter Systems, Würzburg (1994)

German-Japanese Symposium, Sapporo (2000)

Centro Atomico, Bariloche (2008): Men at work

Bariloche (2008): Men at play

Surprising effects of the interaction between electrons in solids

Outline:

- 1st Surprise: Emergence in quantum many-particle systems
- 2nd Surprise: Dirt with universal properties
- 3rd Surprise: Influence of electronic correlations on the lattice stability of Fe

1. Peculiarities of Interacting Many-Particle Systems

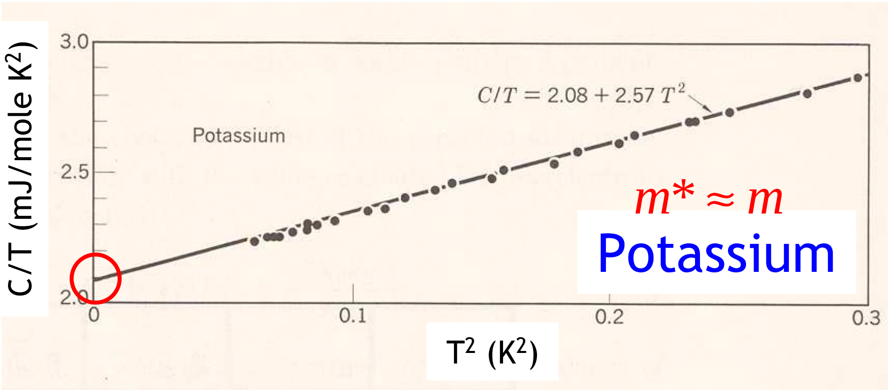
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

$\#$ particles $N \longrightarrow \infty$

Elementary excitations
= new particles
("quasiparticles") + effective interactions

Simple metals

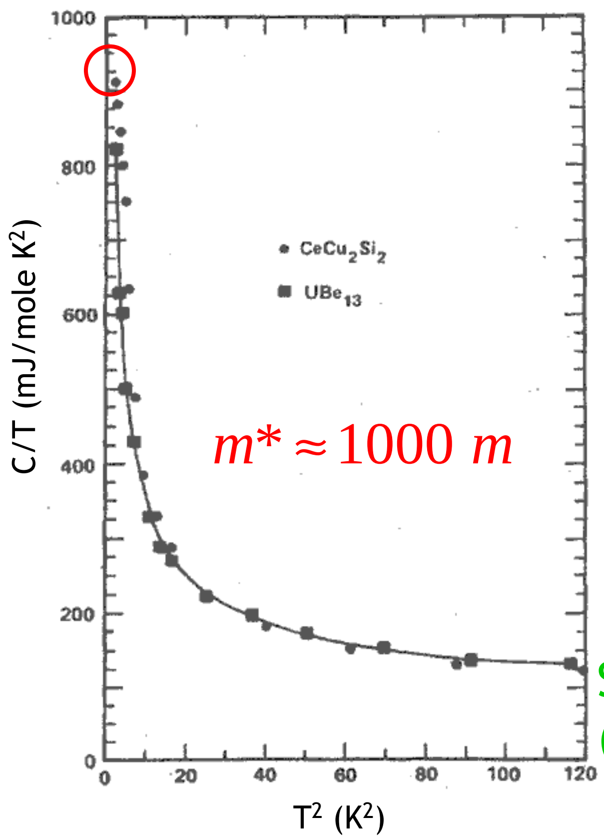


$$\lim_{T\to 0}\frac{c_V}{T} = \gamma \propto \frac{m^*}{m}$$

Result of
elementary excitations
(quasiparticles)

"Heavy Fermions"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

$CeCu_2Si_2$, UBe_{13}:
very heavy quasiparticles

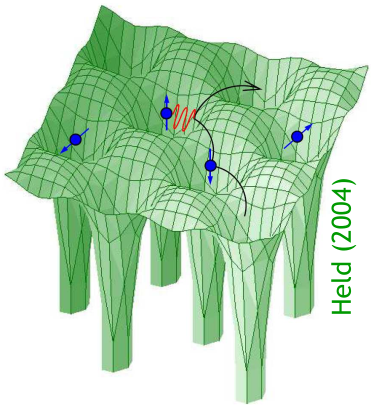
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

$\downarrow$ $\boxed{\#\ \text{particles}\ N \longrightarrow \infty}$

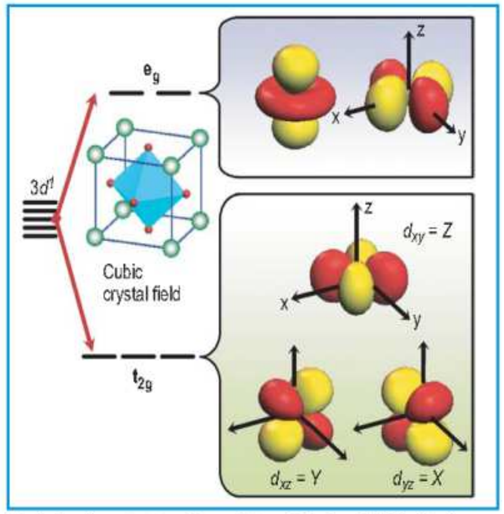
Elementary excitations
= new particles
("quasiparticles") + $\boxed{\text{effective interactions}}$

Electrons in real solids



Complicated modification of the bare Coulomb interaction

Q • ← r → • e



Strong effective interaction of electrons in narrow orbitals

Interacting many-particle systems

$\downarrow$ # particles $N \to \infty$

Entirely new phenomena, e.g., phase transitions

$\downarrow$

Unpredicted behavior "emerges"

Examples:

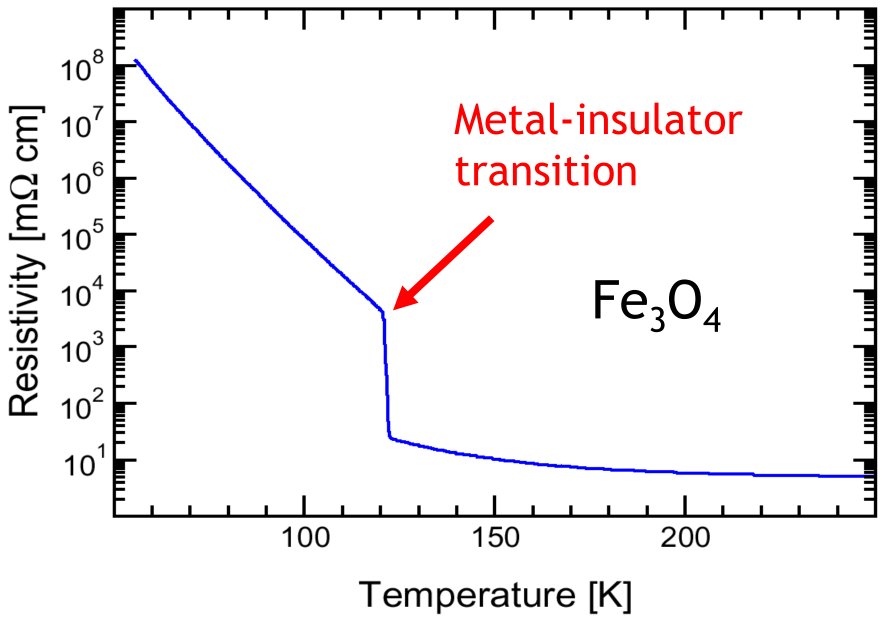
Superconductivity	Traffic
Magnetism	Weather
Metal-insulator transition	Stock market

Interacting many-particle systems

$\downarrow$ # particles $N \to \infty$

Entirely new phenomena, e.g., phase transitions

$\downarrow$

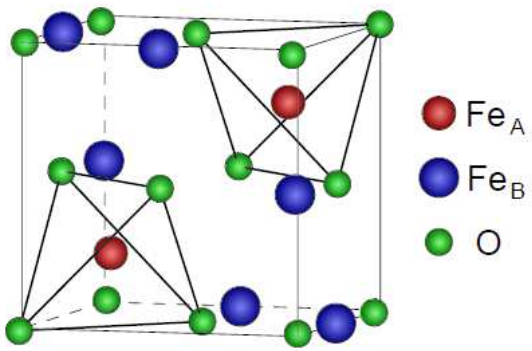


Why?

Example: Magnetite (Fe_3O_4)

Macroscopic view

Microscopic view



Electrons in Fe are correlated

→ quantum many-particle problem

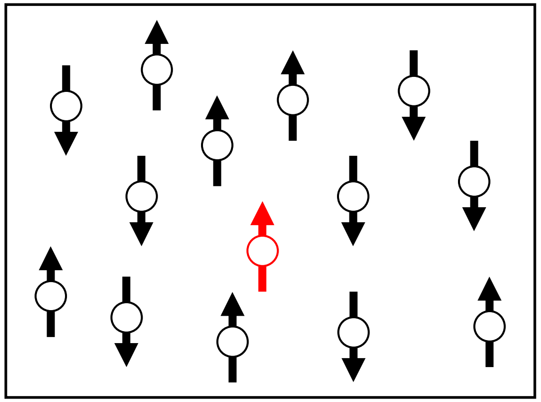
2. Universality of Dirt

Fe_3O_4

- *"Die Festkörperphysik ist eine Schmutzphysik"* (Pauli)
- *"One shouldn't wallow in dirt"* (Pauli to Peierls)

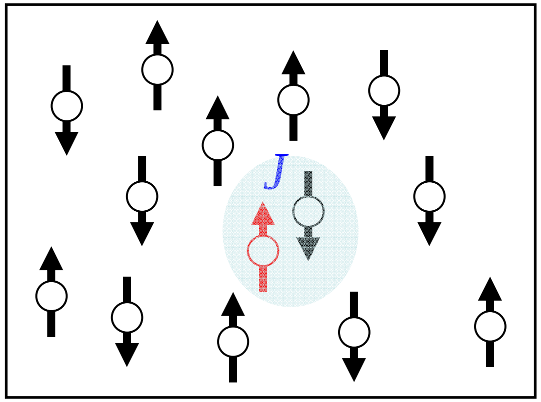
… but "dirt physics" can be fundamental and universal

Magnetic impurity in a host of non-interacting (itinerant) electrons



$T>T_K$ (high energies)

Asymptotically free local moment



$T<T_K$ (low energies)

Screening of moment (confinement)

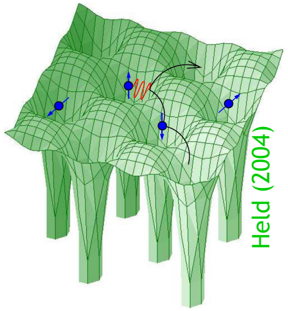
"Kondo effect"

$$\boxed{T_K \sim E_F e^{-1/|J(\Lambda)|N(E_F)}}$$

Prototypical correlation problem with "running coupling constant" $J(\Lambda)$

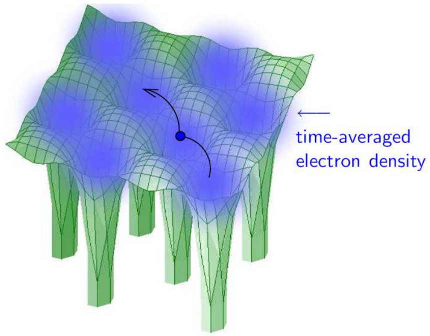
→ QED, QCD

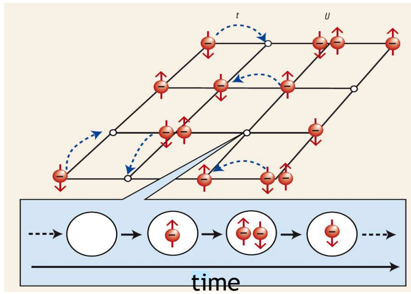
Theory of Correlated Electron Materials



Comprehensive, non-perturbative approximation scheme needed

DFT/LDA		Model Hamiltonians	
+	material specific: "ab initio"	−	input parameters unknown: unrealistic
−	fails for strong correlations	+	systematic many-body approach

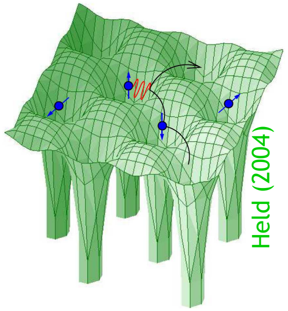




Materials-specific
Density functional theory
(LDA/GGA) or GW

?

Correlations-specific
Many-body theory



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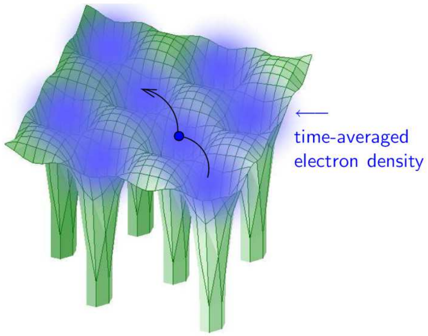
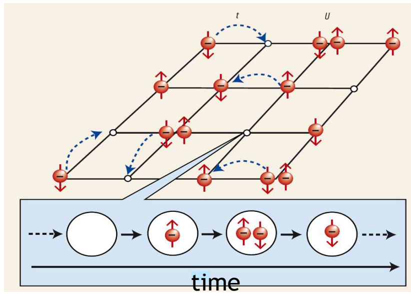




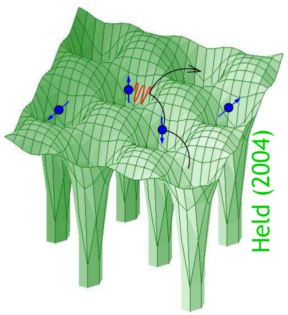
Materials-specific
Density functional theory
(LDA/GGA) or GW

+

Correlations-specific
Many-body theory
(DMFT)

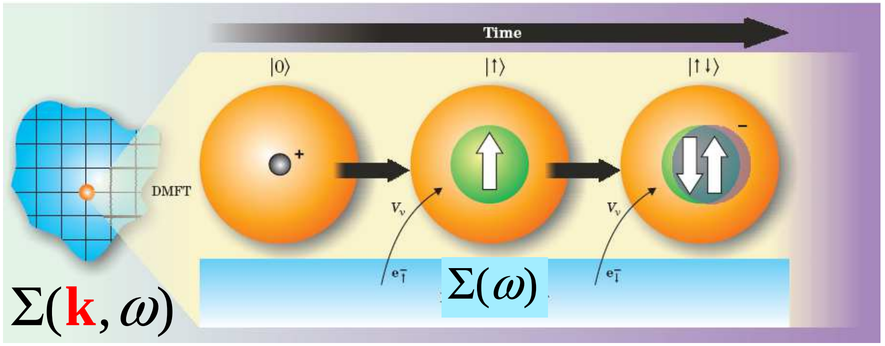
⇓

LDA+DMFT



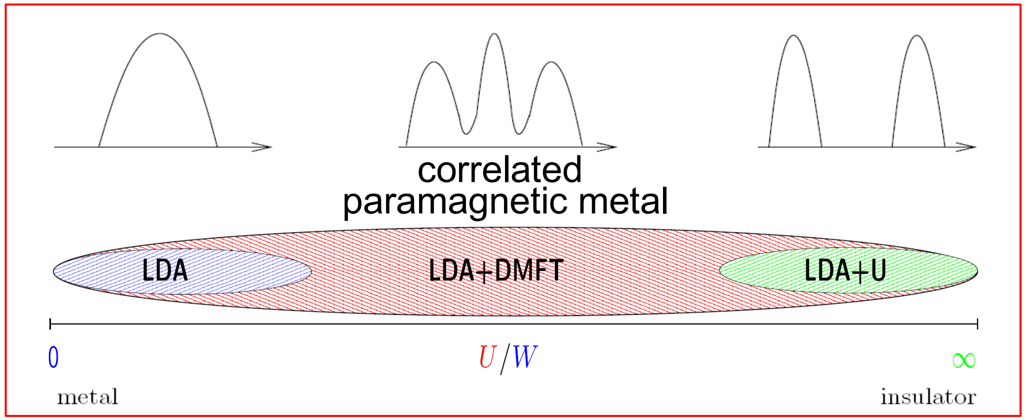
Comprehensive, non-perturbative approximation scheme needed

DMFT



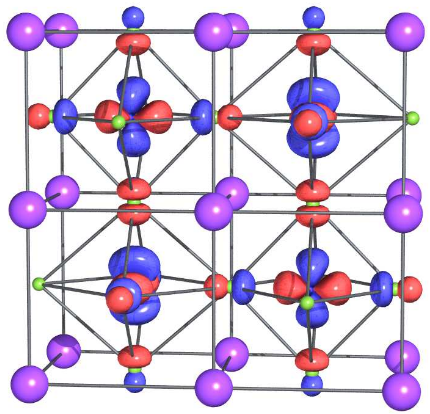
Self-consistent Anderson impurity problem

LDA+DMFT



Until recently: Investigation of electronic correlation effects
for a given lattice structure

→ Influence of electrons on lattice structure ignored



- How do electrons + ions influence each other ?
- Can electronic correlations (de)stabilize the lattice structure ?

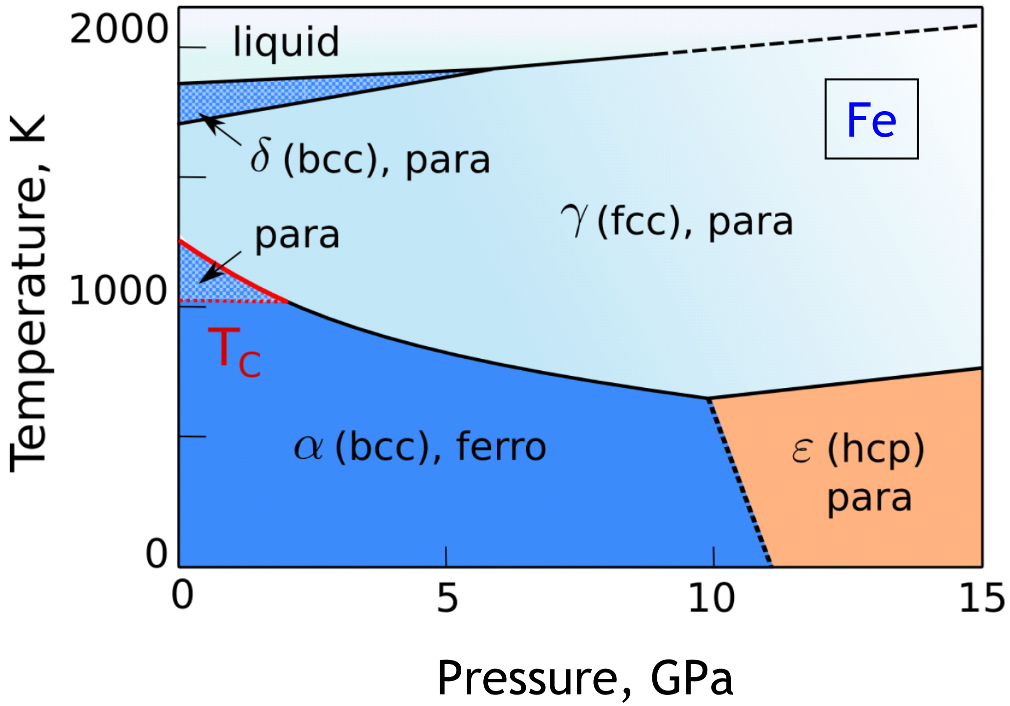
3. Correlation-induced lattice transformations

Application of LDA+DMFT

α-γ structural phase transition in paramagnetic Fe

Leonov, Poteryaev, Anisimov, DV; PRL **106**, 106405 (2011)

Electronic correlations at the α-γ structural phase transition in paramagnetic Fe

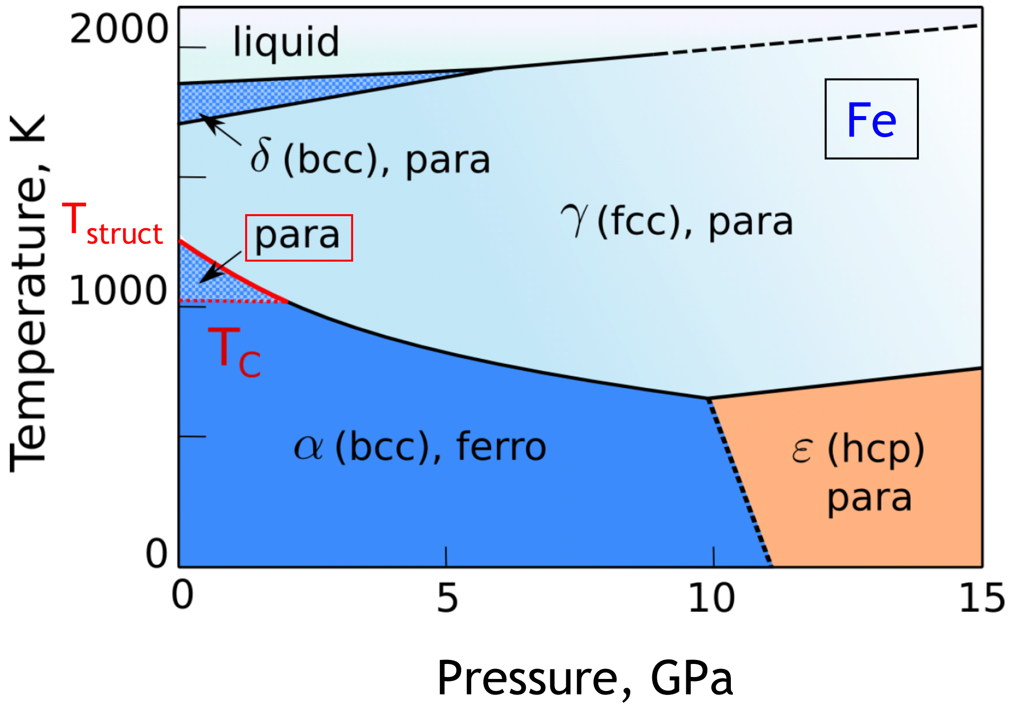


bcc structure at T→0: exceptional (covalency, magnetism, ...)

In general:

- Cohesion prefers close packed structure (*fcc*, *hcp*) for T→0
- *bcc* at higher T (lattice vibrations)

Electronic correlations at the α-γ structural phase transition in paramagnetic Fe



→ Separation of magnetism and structure: Difficult theoretical problem

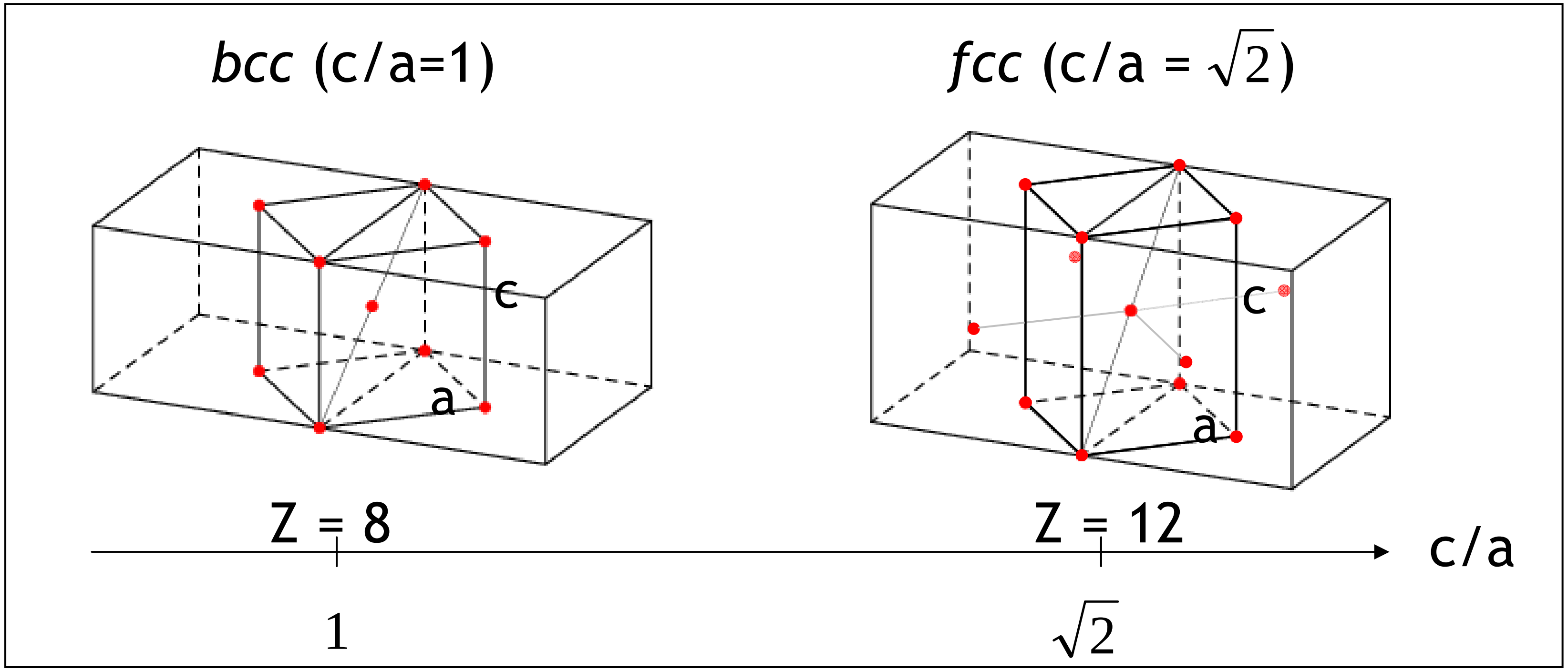
DFT(GGA): finds paramagnetic ***bcc*** structure to be unstable

bcc-fcc structural phase transition in paramagnetic Fe

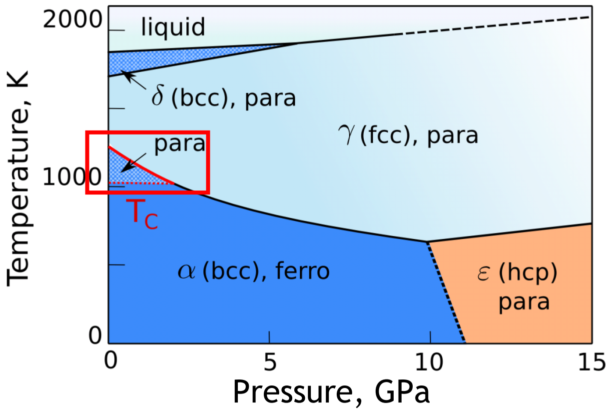
Total energies calculated along *bcc-fcc* Bain transformation path:

Bain and Dunkirk (1924)

Continuous transformation path to account for *bcc-fcc* transition in Fe



bcc-fcc structural phase transition in paramagnetic Fe



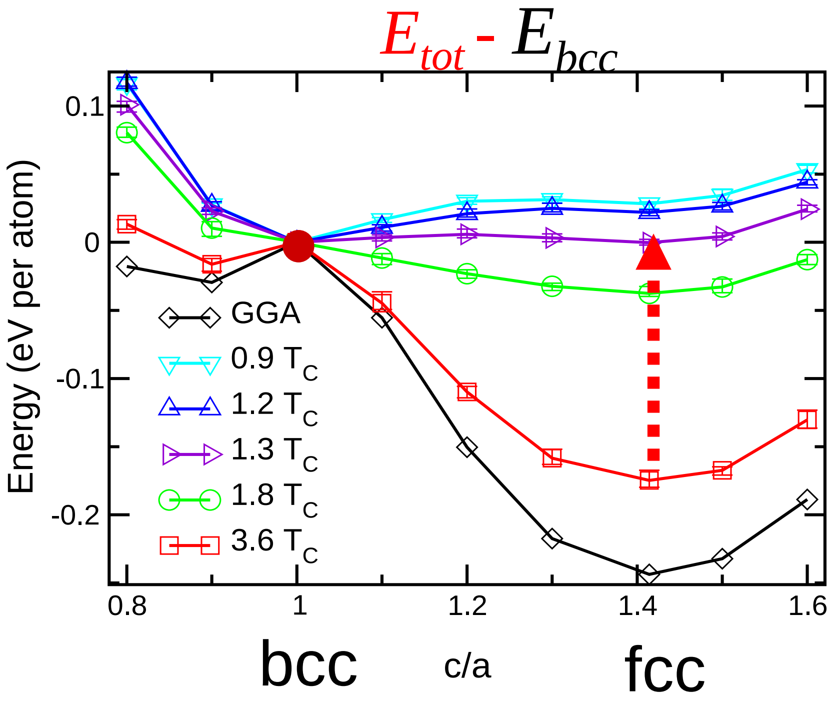
Why is the low-T paramagnetic *bcc* phase stable ?

GGA:
paramagnetic ***fcc*** structure stable

GGA+DMFT:

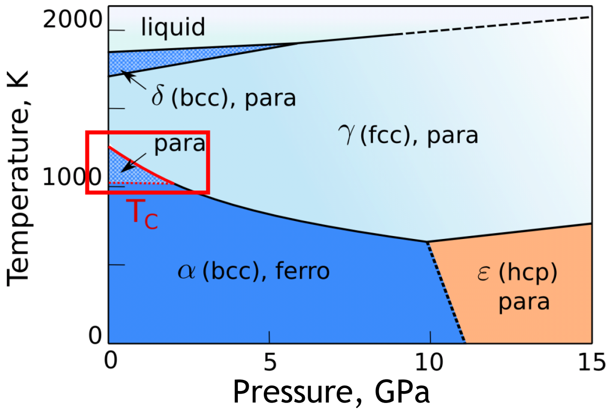
- *bcc-fcc* structural phase transition at $T_{struct} \approx 1.2\ T_C > T_C$
- LDA+DMFT and GGA+DMFT: qualitatively similar results

GGA+DMFT total energy



What determines the temperature and *c/a* dependence of the total energy?

bcc-fcc structural phase transition in paramagnetic Fe



Why is the low-T paramagnetic *bcc* phase stable ?

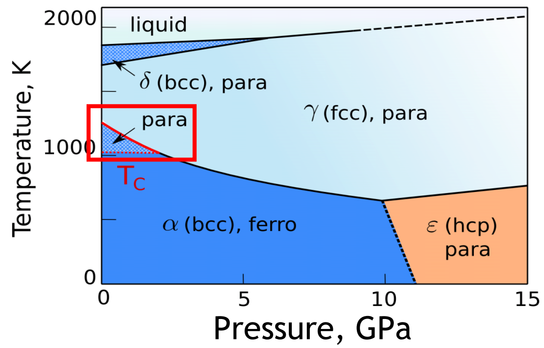
Magnetic correlation energy of the electrons ($\sim -\langle \hat{m}_z^2 \rangle$) stabilizes *bcc* structure → $T_{struct} > T_C$

Application of LDA+DMFT

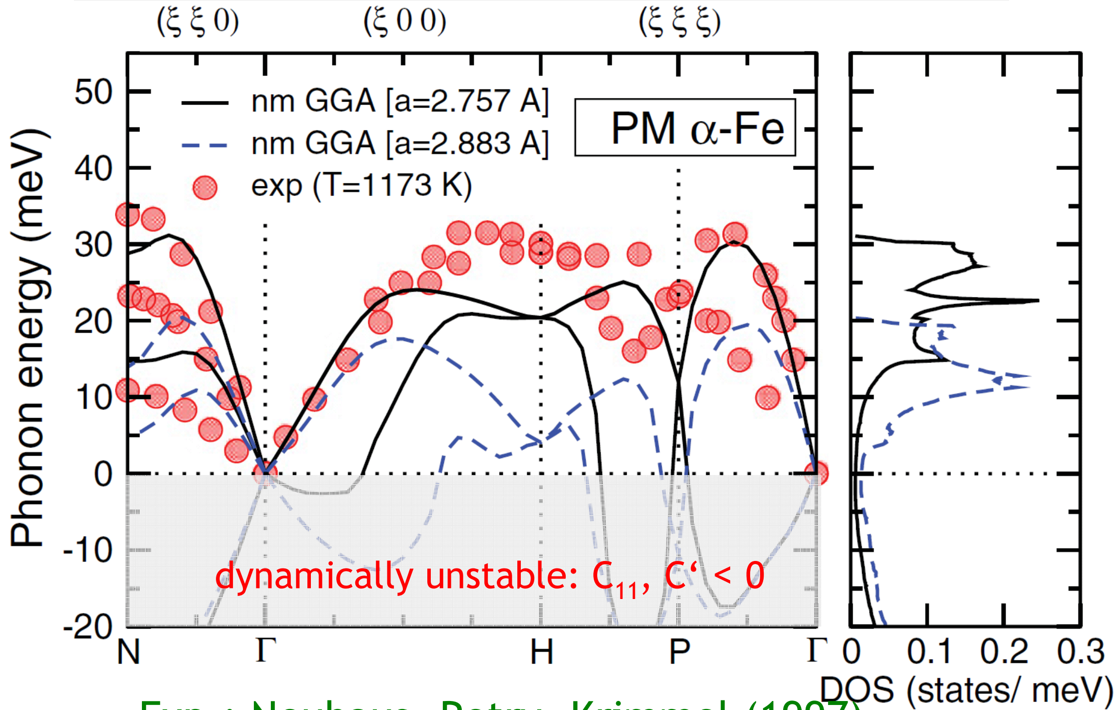
Lattice dynamics and phonon spectra of Fe

Leonov, Poteryaev, Anisimov, DV; PRB **85**, 020401(R) (2012)

Lattice dynamics of paramagnetic *bcc* iron

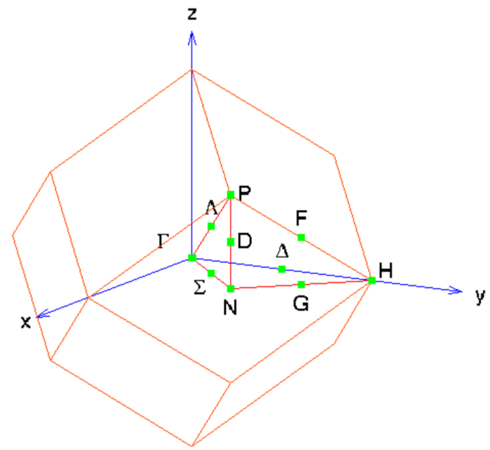


Non-magnetic GGA phonon dispersion



Exp.: Neuhaus, Petry, Krimmel (1997)

1. Brillouin zone



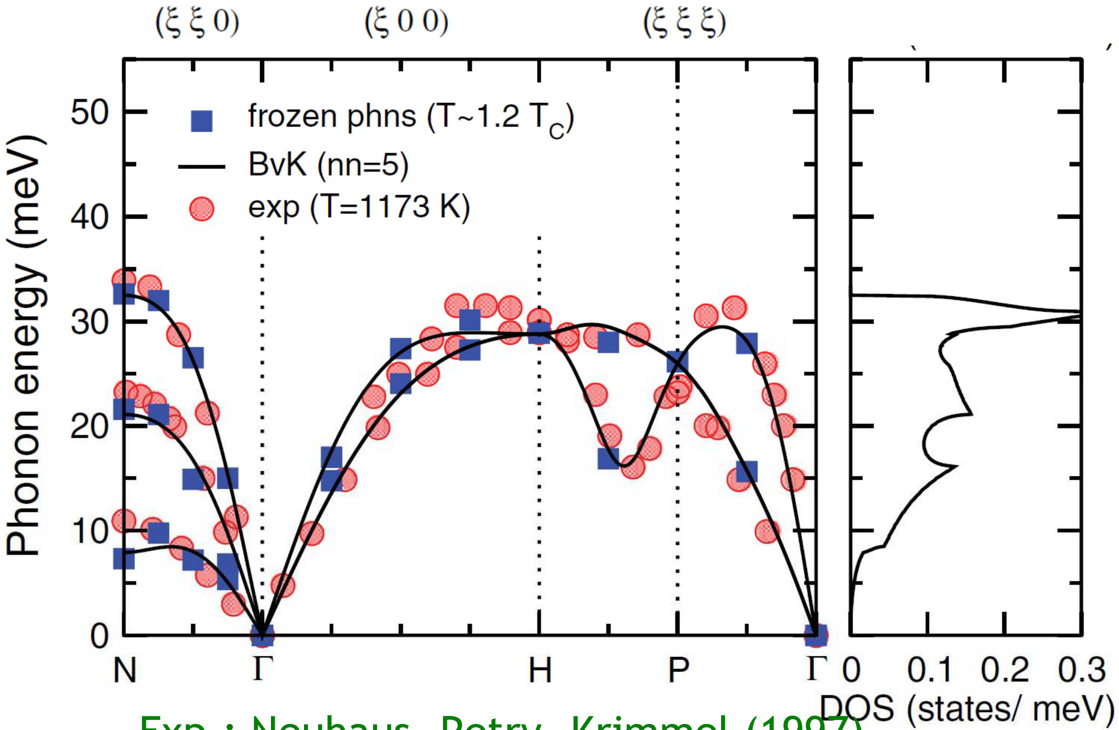
Leonov, Poteryaev, Anisimov, DV (2012)

Lattice dynamics of paramagnetic *bcc* iron

- phonon frequencies calculated with frozen-phonon method
- harmonic approximation

Stokes, Hatch, Campbell (2007)

GGA+DMFT phonon dispersion at 1.2 T_C



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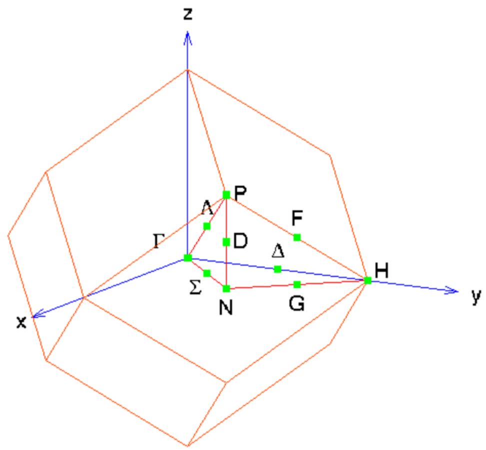

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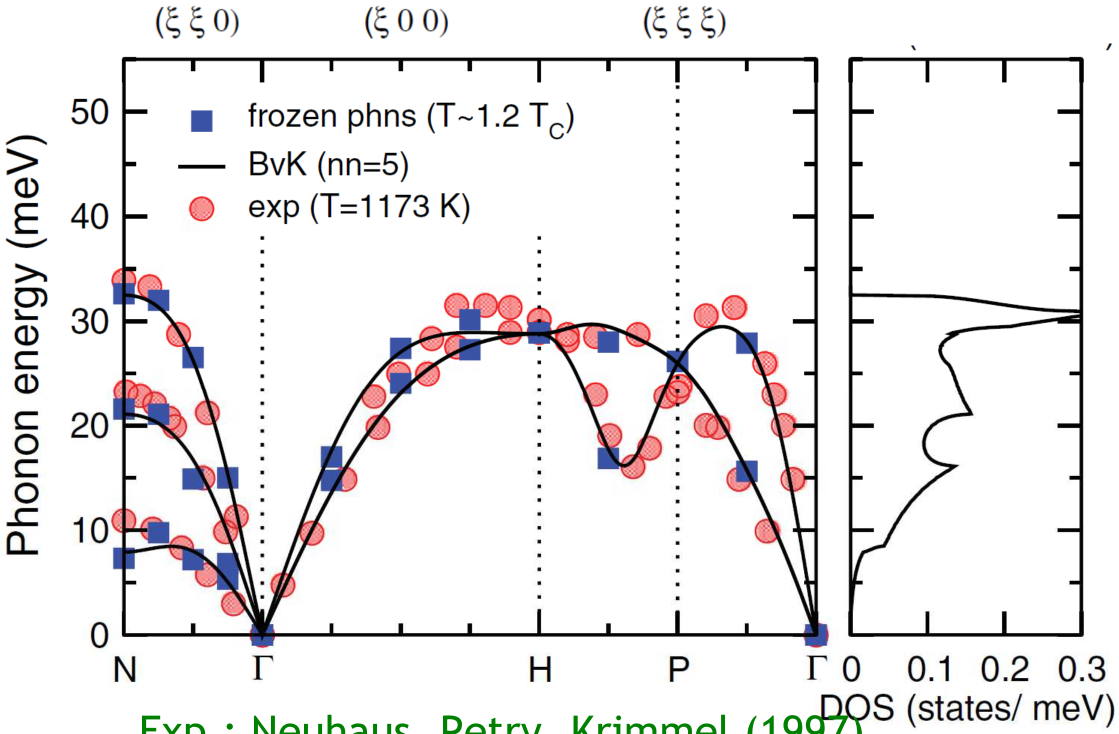

Exp.: Neuhaus, Petry, Krimmel (1997)

Electronic correlations strongly influence lattice-dynamical properties

Leonov, Poteryaev, Anisimov, DV (2012)

Herzlichen Glückwunsch, Gernot!