Center for Electronic Correlations and Magnetism
University of Augsburg

From infinite dimensions to real materials

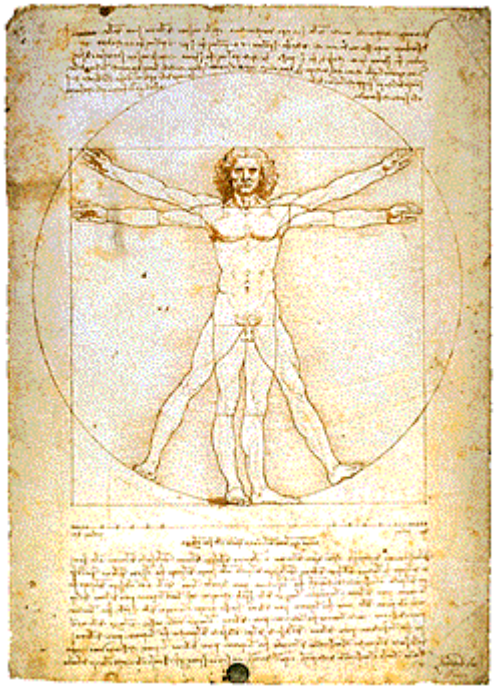
Dieter Vollhardt

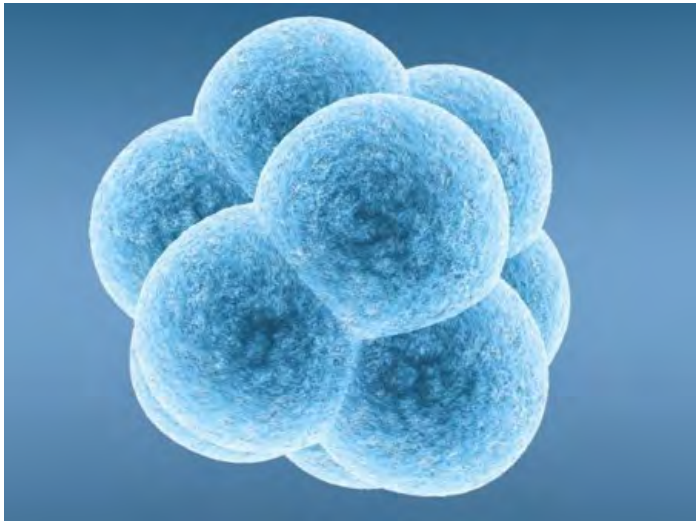
Autumn School on Correlated Electrons:
DMFT – From Infinite Dimensions to Real Materials
Forschungszentrum Jülich; September 17, 2018

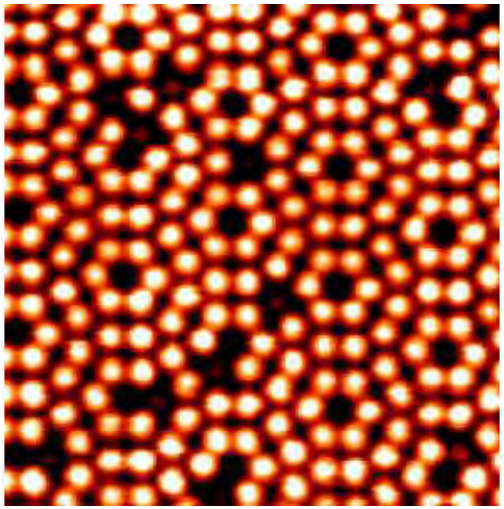
Outline

- Electronic correlations
- From materials to models
- Interacting many-particle systems
  - Mean-field theories
  - Infinite dimensions
  - Hubbard model
- Dynamical mean-field theory (DMFT)
- Application of DMFT: From models back to materials

Correlations







Correlation [lat.] *(with + relation):* mutual relation, interdependence

Temporal/spatial correlations in every-day life

correlated classical
many-body system

Correlations in physics:

$$\langle AB \rangle \neq \langle A \rangle \langle B \rangle$$

e.g., densities:

$$\langle n(\mathbf{r}) n(\mathbf{r}') \rangle \neq \langle n(\mathbf{r}) \rangle \langle n(\mathbf{r}') \rangle = n^2$$

$$\underbrace{\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle}_{\text{quantifies correlations}}$$

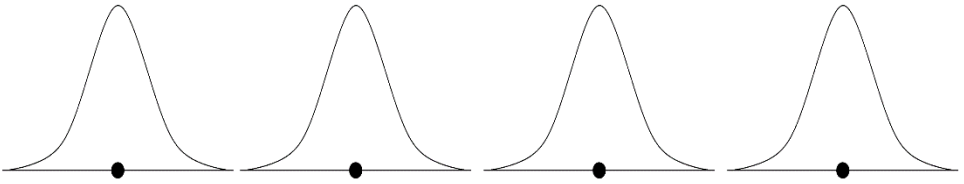
Def. of electronic correlations (I):
Effects beyond a factorization (Hartree-Fock) approximation

The Fermi gas $\psi(1,\ldots,N) = \mathcal{A} \prod_{i=1}^{N} \psi_{\nu_i}(i)$ is "uncorrelated" by definition,

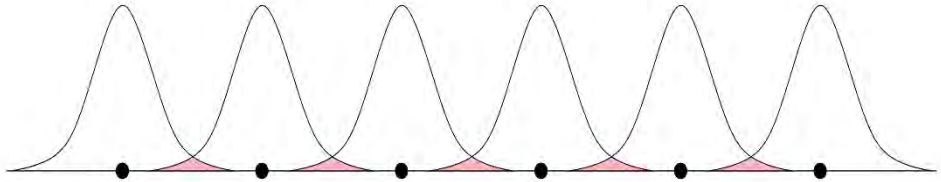
although it is spatially correlated due to Fermi statistics ("exchange hole")

Electronic Correlations in Solids

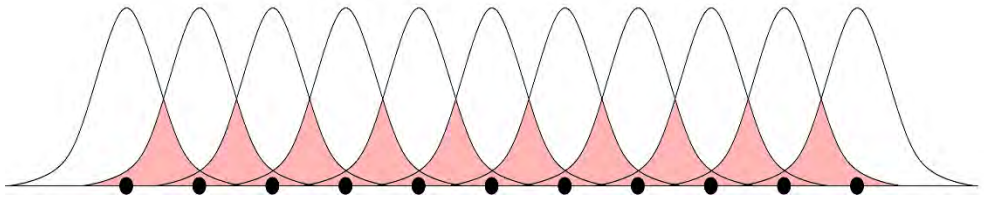
Orbital overlap *vs.* energy bands



No overlap



Weak overlap



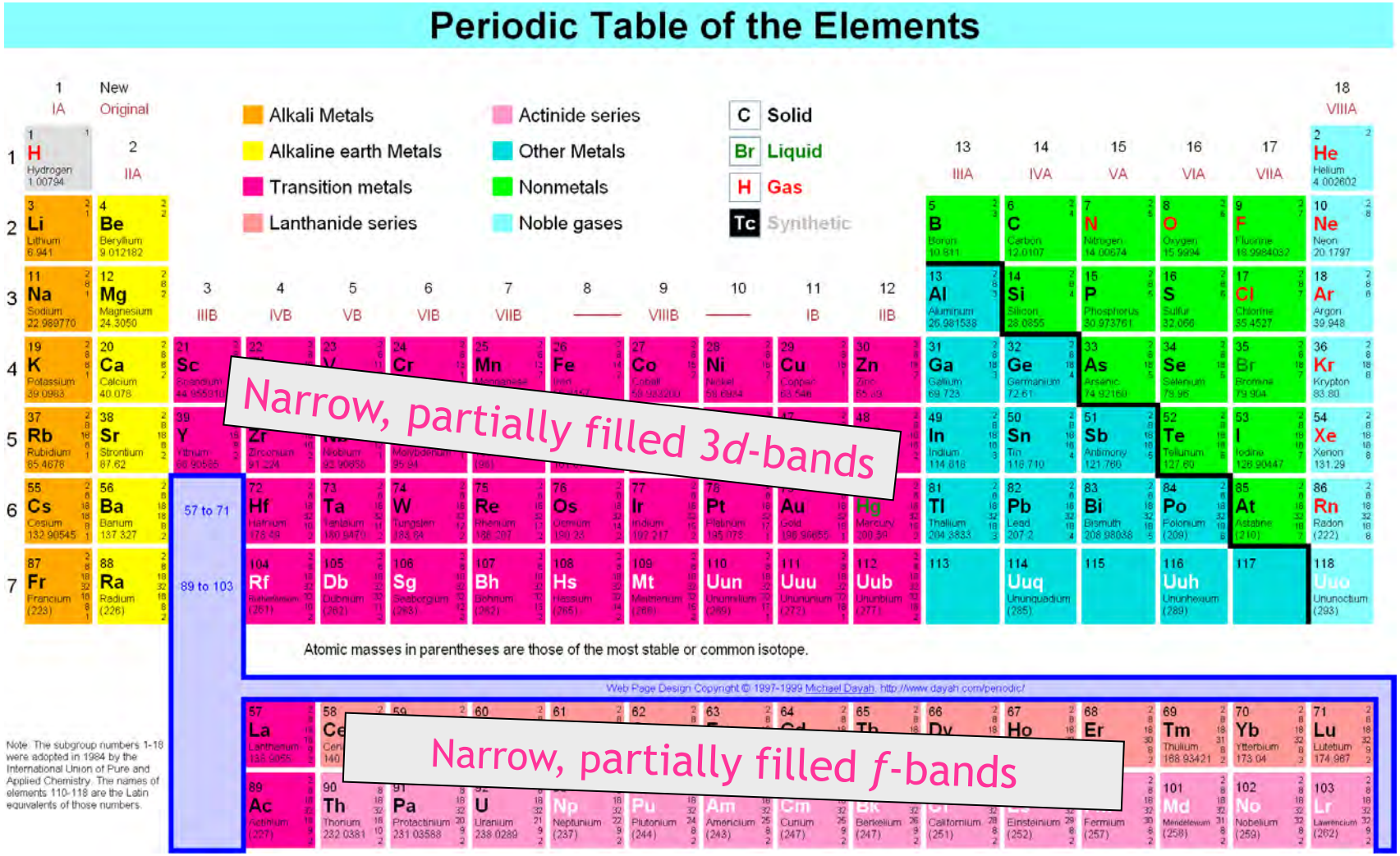
Strong overlap

Energy	Character	Example	Property
Degenerate atomic levels, flat bands	Spatially localized electrons: $n_{i\sigma}$	NaCl, solid H, frustrated/ pyrochlore lattices	(correlated) Insulators
Narrow bands	$n_{i\sigma} \leftrightarrow n_{k\sigma}$	Transition + rare earth elements (Fe, Ce, V_2O_3)	Corre-lated electron systems
Broad bands	Extended waves: $n_{k\sigma}$	Na, Al	Simple metals

Narrow band systems : $|E_{kin}| < E_{\text{int}}$

Interaction + Pauli principle ⟶ correlations + magnetism become important

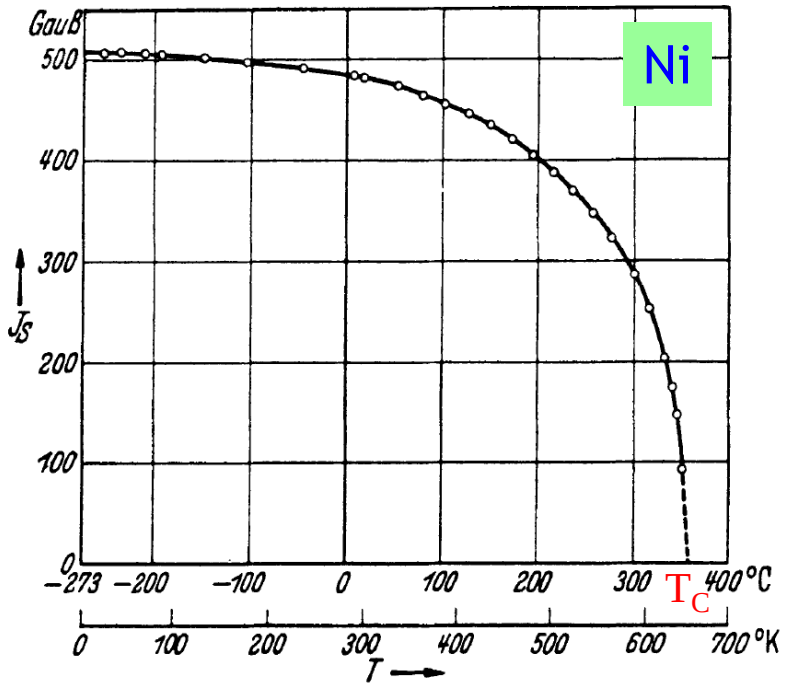
Correlated electron materials



Electronic Correlation Phenomena

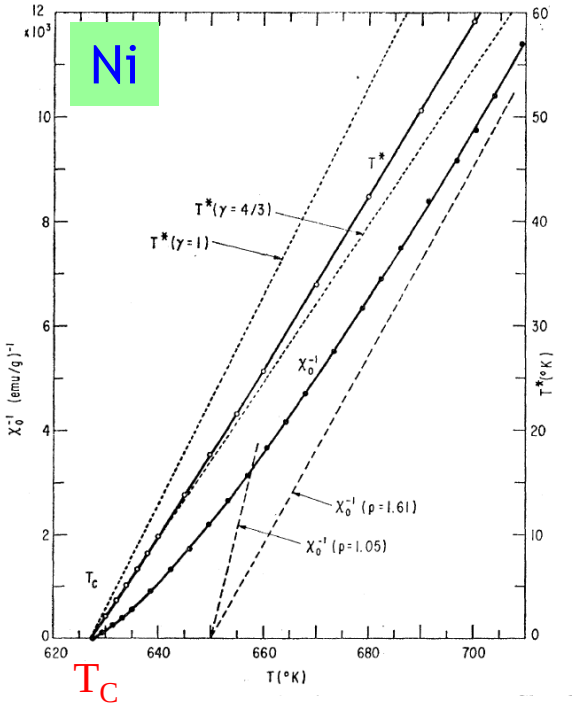
1. Ferromagnetism

Magnetization *vs.* T



Weiss, Forrer (1926)

Inverse susceptibility *vs.* T



Exp.: Weiss, Forrer (1926)
Theory: Kouvel, Fisher (1964)

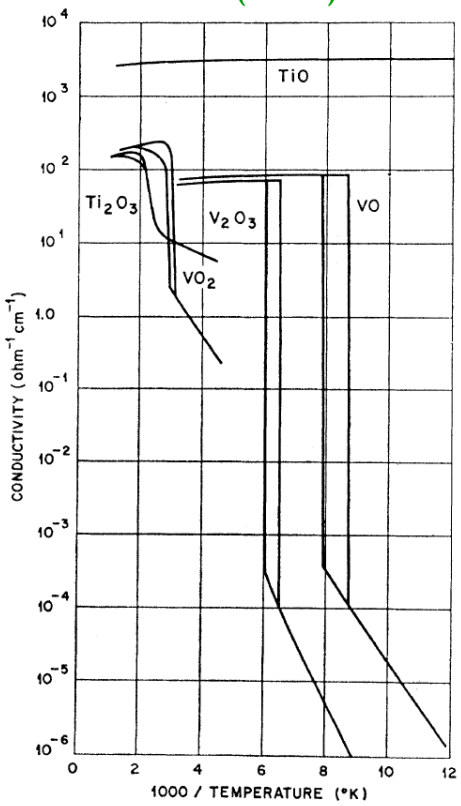
Typical for localized moments — Incompatible? — Curie-Weiss behavior for mobile electrons

Why do mobile electrons order ferromagnetically?

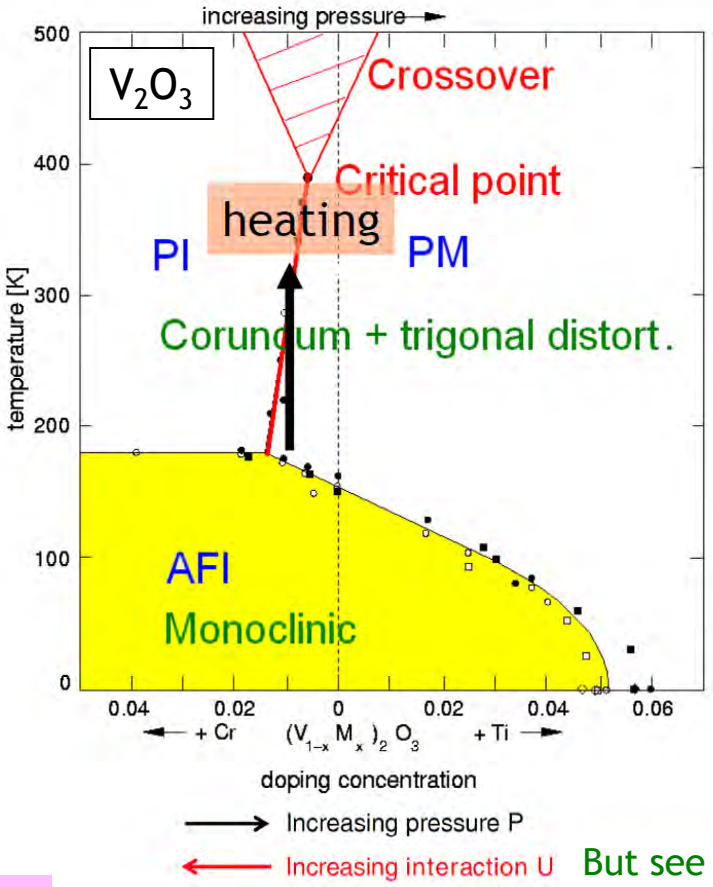
2. Mott metal-insulator transitions

Conductivities of transition metal oxides

Morin (1958)



Rice, McWhan (1970)
McWhan, Menth, Remeika, Brinkman, Rice (1973)

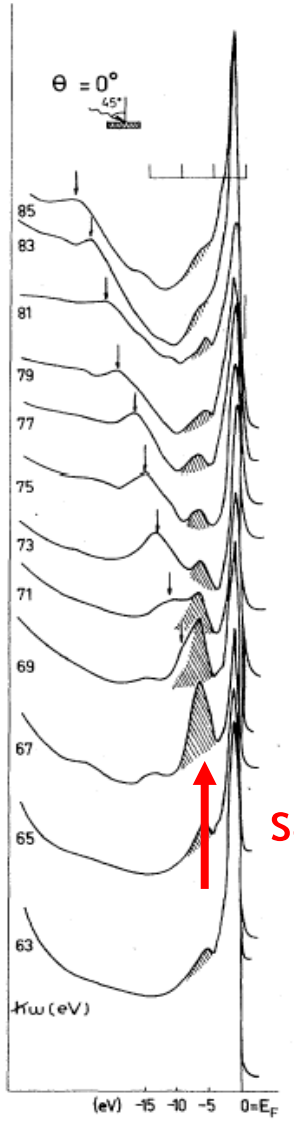


But see Lupi *et al.* (2010)

Why does a metal-insulator transition occur?

PI ⟷ PM: 1. order transition without lattice symmetry change

3. Photoemission spectra of Ni



Guillot *et al.* (1977)

satellite at -6 eV

Why is there spectral weight at -6 eV?

Unusual properties of correlated electron materials

- huge resistivity changes
- gigantic volume anomalies
- colossal magnetoresistance
- high-T_c superconductivity
- correlated metallic behavior at interfaces of insulators, …

With potential for technological applications:

- sensors, switches
- spintronics
- thermoelectrics
- high-T_c superconductor devices
- functional materials: oxide heterostructures, …

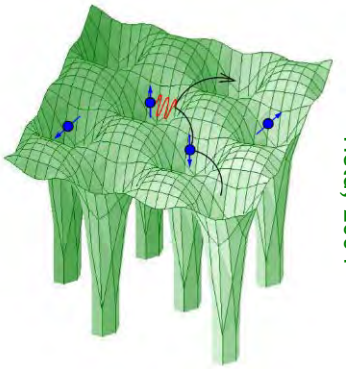
- How to *explain* these properties?
- Theoretical framework needed!

Realistic theoretical investigations of materials

material

simplification needed

$\Rightarrow$



©Held, 2004

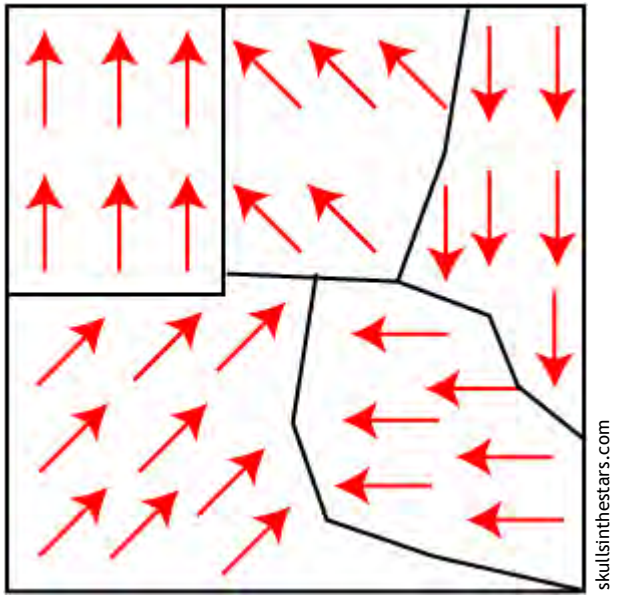
model

The art of modeling:
Reduction (idealization + abstraction)

From materials to models: Ferromagnetism

How to explain ferromagnetism in 3*d* transition metals?

Weiss model of magnetic domains (1906)



Alignment of “elementary magnets” in each domain
due to a “molecular field“
(*Weiss mean field*)

Microscopic origin?

How to explain ferromagnetism in 3*d* transition metals?

Ising model (1925)

Beitrag zur Theorie des Ferromagnetismus [1]).

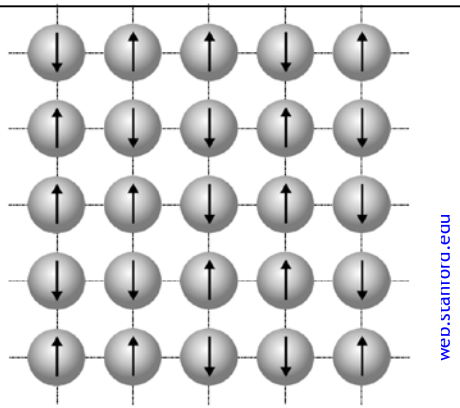
Von **Ernst Ising** in Hamburg.

(Eingegangen am 9. Dezember 1924.)

Es wird im wesentlichen das thermische Verhalten eines linearen, aus Elementarmagneten bestehenden Körpers untersucht, wobei im Gegensatz zur Weisschen Theorie des Ferromagnetismus kein molekulares Feld, sondern nur eine (nicht magnetische) Wechselwirkung benachbarter Elementarmagnete angenommen wird. Es wird gezeigt, daß ein solches Modell noch keine ferromagnetischen Eigenschaften besitzt und diese Aussage auch auf das dreidimensionale Modell ausgedehnt.

Z. Physik **31**, 253 (1925)

$$\mathcal{H} = -J \sum_{<i,j>} s_i s_j \quad , s_i = \pm 1$$



Exact solution in d=1: no order (also in d=3?!)

But: Magnetism is a quantum effect Bohr (1911), van Leeuwen (1919)

How to explain ferromagnetism in 3*d* transition metals?

Heisenberg model (1928)

Zur Theorie des Ferromagnetismus.

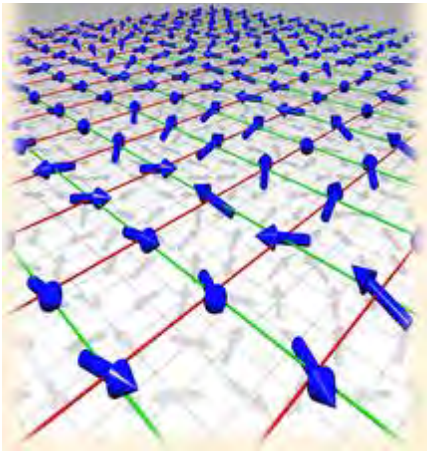
Von **W. Heisenberg** in Leipzig.

Mit 1 Abbildung. (Eingegangen am 20. Mai 1928.)

Die Weissschen Molekularkräfte werden zurückgeführt auf ein quantenmechanisches Austauschphänomen; und zwar handelt es sich um diejenigen Austauschvorgänge, die in letzter Zeit von Heitler und London mit Erfolg zur Deutung der homöopolaren Valenzkräfte herangezogen worden sind.

Z. Physik **49**, 619 (1928)

$$H_{\text{Heis}} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$
$$= -J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right)$$



complexity-coventry.org

Quantum-mechanical exchange processes
→ Weiss molecular field

But: Electrons are mobile Bloch (1929)

→ need to include their kinetic energy + Coulomb interaction

1929

Next step: Hubbard model ??

Not for another 34 years!

Investigation of many-particle problems required development of

1) mathematical techniques
- field-theoretic/ diagrammatic methods
- Green functions, etc.

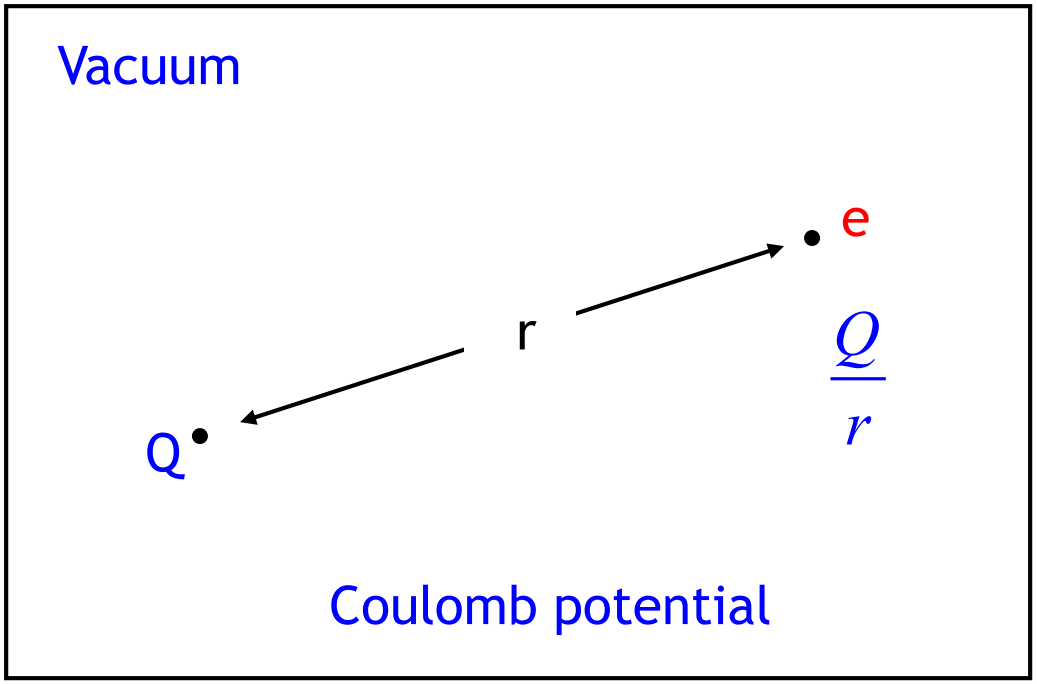
2) physical concepts
- multiple scattering
- screening of the long-range Coulomb interaction
- quasiparticles and Fermi liquid theory
- electron-phonon coupling
- superconductivity
- metal-insulator transitions
- disorder
- super-exchange, etc.

Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

↓ # particles $N \to \infty$

effective ("quasi") particles + effective interactions



Interacting many-particle systems

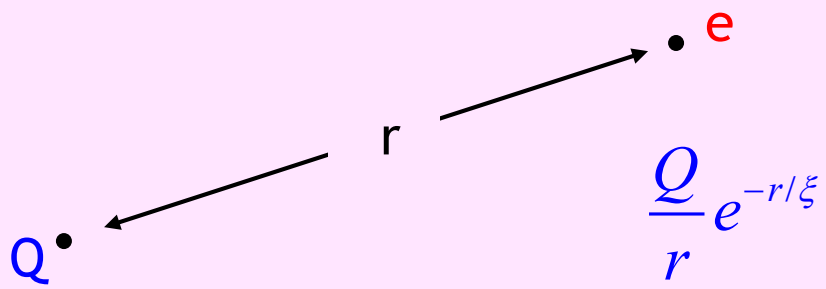
Elementary ("bare") particles + fundamental interactions

↓ # particles $N \to \infty$

effective ("quasi") particles + effective interactions

Electron gas: Screening

Simplest approximation: Thomas-Fermi



Effective Yukawa potential

Interacting many-particle systems

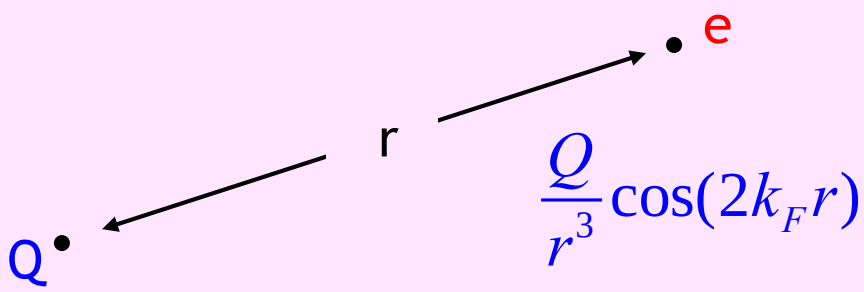
Elementary ("bare") particles + fundamental interactions

↓ # particles $N \to \infty$

effective ("quasi") particles + effective interactions

Electron gas: Screening

Better approximation: Lindhard



Friedel oscillations

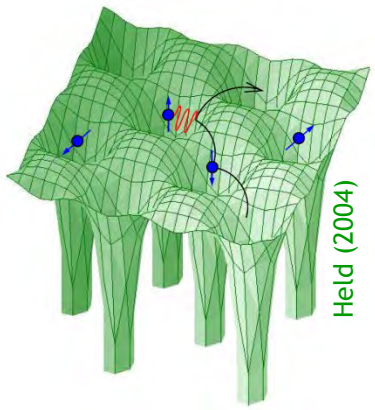
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

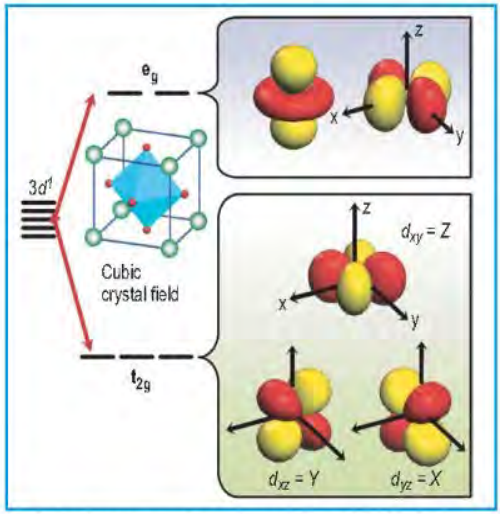
↓ # particles $N \to \infty$

effective ("quasi") particles + effective interactions

Electrons in real solids



Q • Complicated modification of the bare Coulomb interaction r • e



(strong) effective interaction between electrons

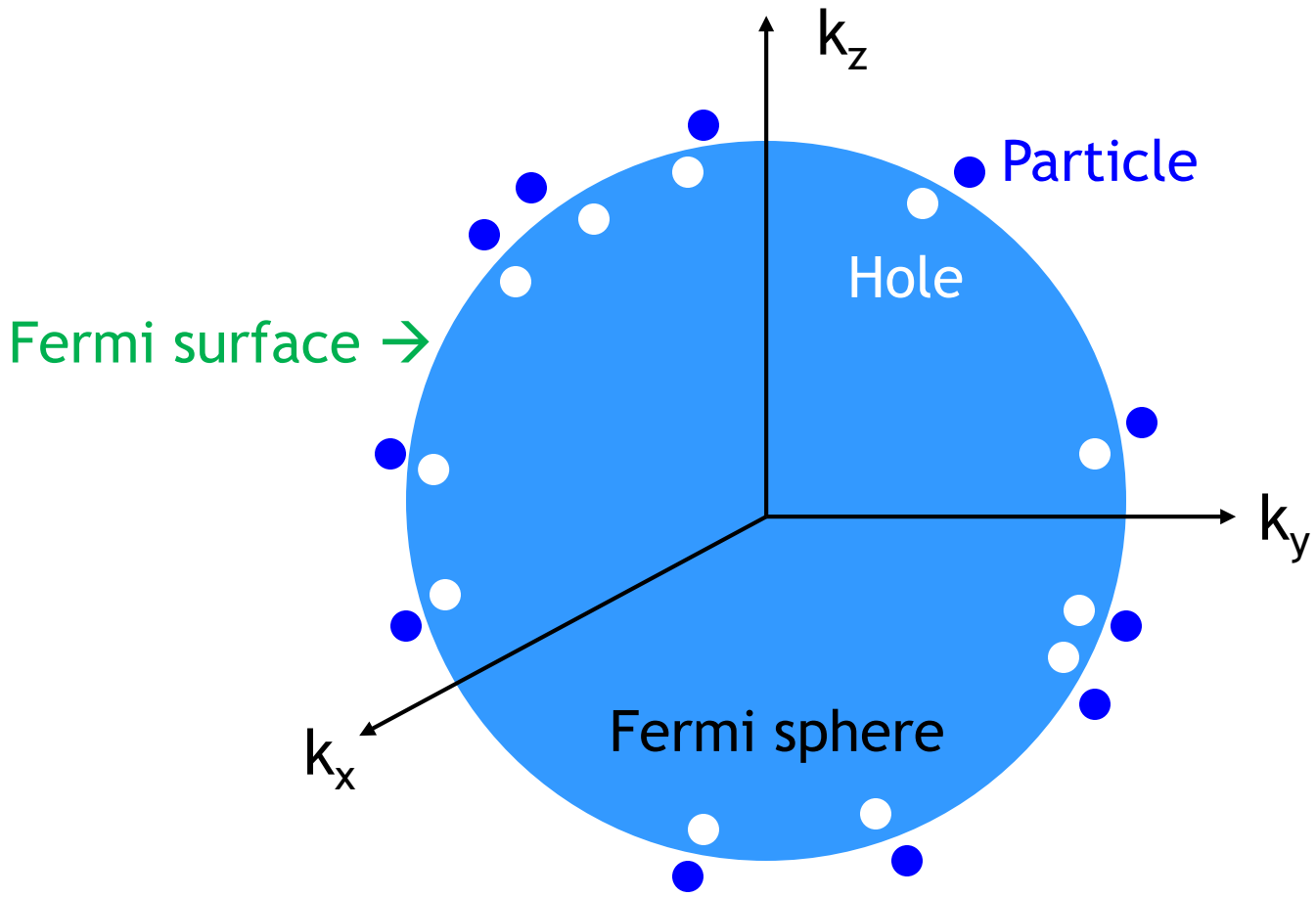
→ Lecture by F. Aryasetiawan

Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

effective ("quasi") particles + effective interactions

Fermi gas: **Excited state**



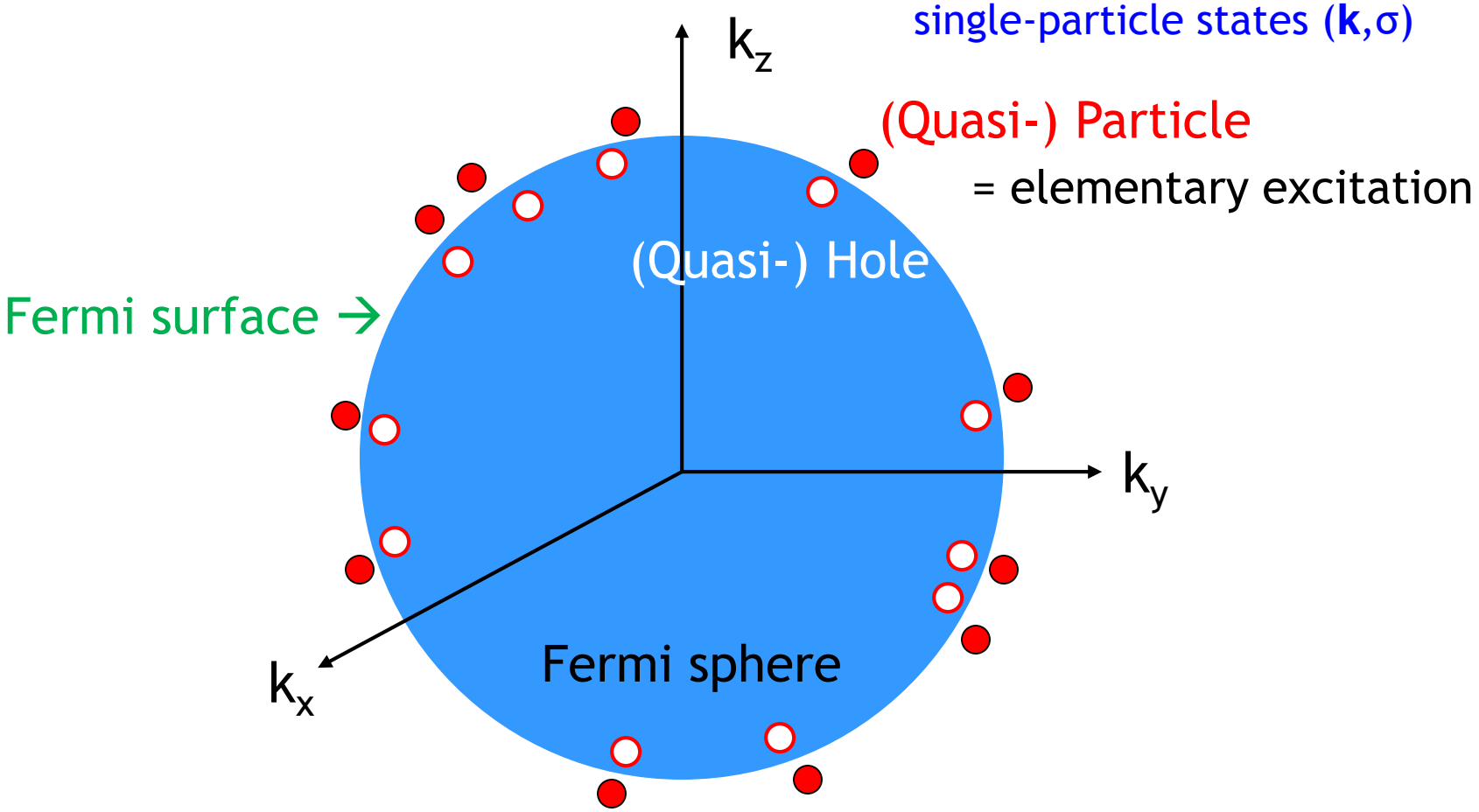
k-eigenstates: infinite life time

Switch on repulsive interaction → unsolvable many-body problem

Fermi liquid

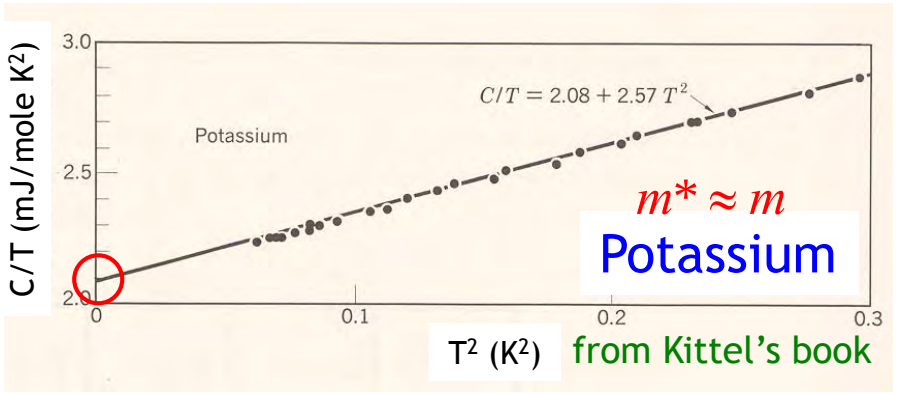
Landau (1956/58)

1-1 correspondence between
single-particle states (**k**,σ)



"Standard model of condensed matter physics"

Simple metals



$m^* \approx m$

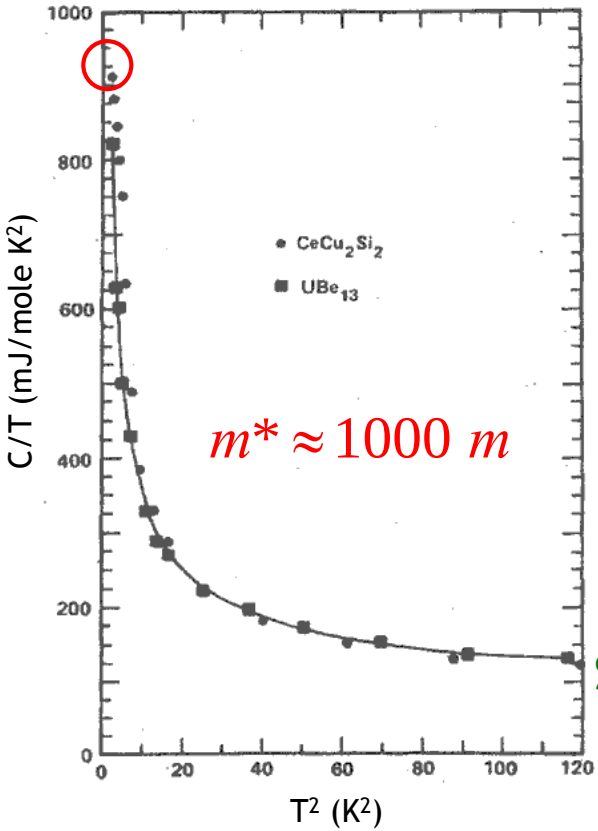
Potassium

from Kittel's book

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

"Heavy Fermion systems"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

$CeCu_2Si_2$, UBe_{13}

Result of elementary excitations (quasiparticles)

Beginning of the 1960s

1) Two major unsolved intermediate coupling problems in solid state physics:

- Ferromagnetism in *3d* transition metals
- Mott metal-insulator transition

No many-body models for extended systems available

2) Independent, parallel development:

Localized magnetic states in metals

Exp.: Matthias *et al.* (1960)
Theory: Anderson (1961)
Kondo (1964)

Hubbard model 1963 to explain ferromagnetism in transition metals

VOLUME 10, NUMBER 5 PHYSICAL REVIEW LETTERS 1 MARCH 1963

EFFECT OF CORRELATION ON THE FERROMAGNETISM OF TRANSITION METALS

Martin C. Gutzwiller
Research Laboratory Zurich, International Business Machines Corporation, Rüschlikon ZH, Switzerland
(Received 27 September 1962)

Source: *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. 276, No. 1365 (Nov. 26, 1963), pp. 238-257

Electron correlations in narrow energy bands

BY J. HUBBARD
Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(*Communicated by B. H. Flowers, F.R.S.—Received* 23 *April* 1963)

Progress of Theoretical Physics, Vol. 30, No. 3, September 1963

Electron Correlation and Ferromagnetism of Transition Metals

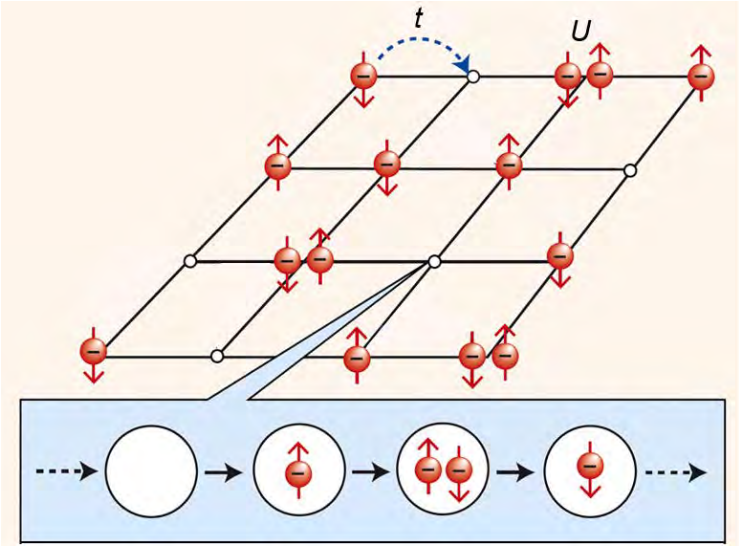
Junjiro KANAMORI

Department of Physics
Osaka University, Osaka

(Received May 14, 1963)

Hubbard model

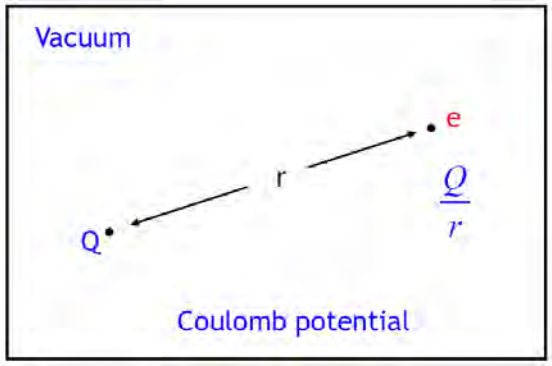
- tight binding
- strong screening:
  local interaction
- no classical analogue



Gutzwiller (1963)
Hubbard (1963)
Kanamori (1963)

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

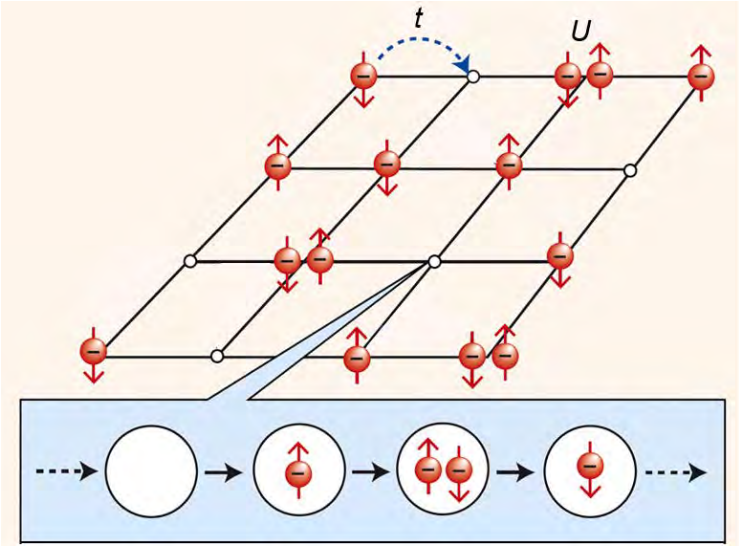
1929



Hubbard model: Far from obvious!

Hubbard model

- tight binding
- strong screening:
  local interaction
- no classical analogue



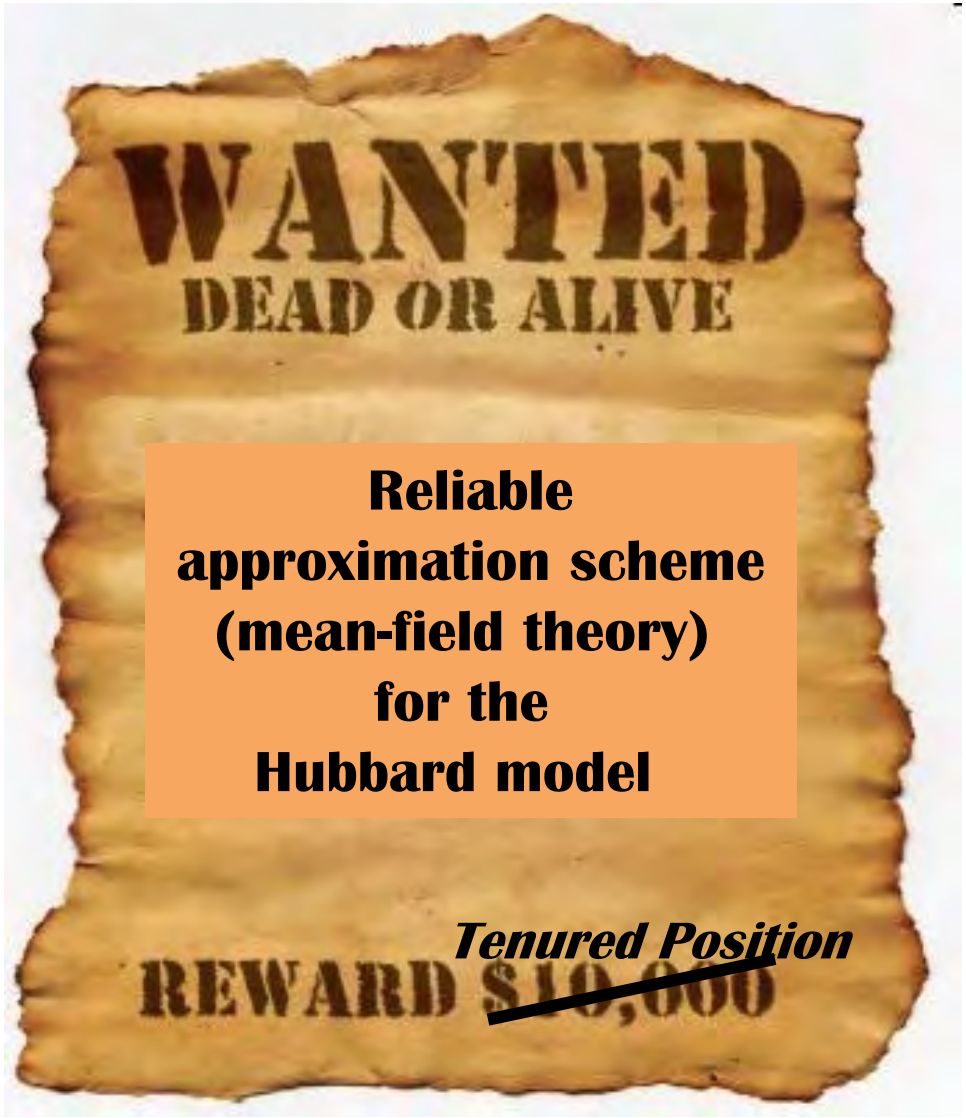
Gutzwiller (1963)
Hubbard (1963)
Kanamori (1963)

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Diagonal in momentum space (waves)

Diagonal in position space (particles)

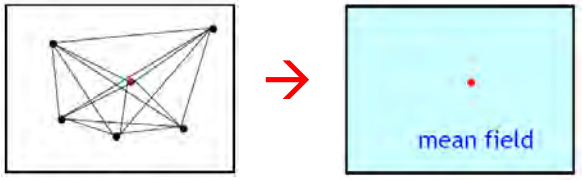
- How to solve?
- At least: find good approximation
- Does it describe ferromagnetism?


WANTED
DEAD OR ALIVE
Reliable
approximation scheme
(mean-field theory)
for the
Hubbard model
Tenured Position
REWARD $10,000

How to construct a mean-field theory?

Mean-Field Theory (MFT)

1. Construction by factorization

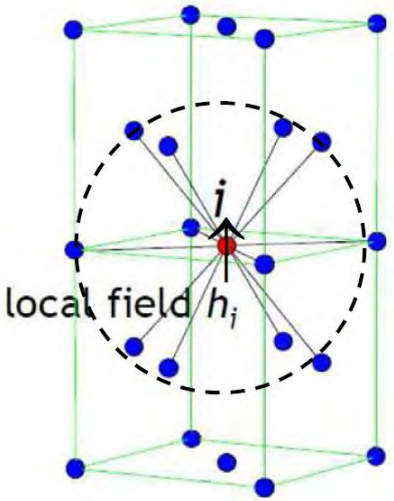


Ising model

$$H = -\frac{1}{2} J \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} S_i S_j = \sum_{\boldsymbol{R}_i} h_i S_i$$

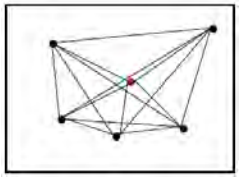
$$h_i = -J \sum_{\boldsymbol{R}_j}^{(i)} S_j$$

local (fluctuating) field

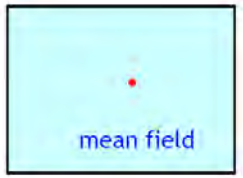


Mean-Field Theory (MFT)

1. Construction by factorization



→



Ising model

$$H = -\frac{1}{2} J \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} S_i S_j = \sum_{\boldsymbol{R}_i} h_i S_i$$

$$h_i = -J \sum_{\boldsymbol{R}_j}^{(i)} S_j$$

local (fluctuating) field

$\langle h_i \rangle$: Global ("molecular") static field

$$h_{\mathrm{MF}} = \langle h_i \rangle \equiv -JZ \langle S_i \rangle$$

Factorization → Weiss MFT

$$H^{\mathrm{MF}} = h_{\mathrm{MF}} \sum_{\boldsymbol{R}_i} S_i + E_{\mathrm{shift}}$$

Effective single-site problem

Mean-Field Theory

2. Construction by exaggeration

Spin S

Degeneracy N

Range of interaction, density — Brout (1960)

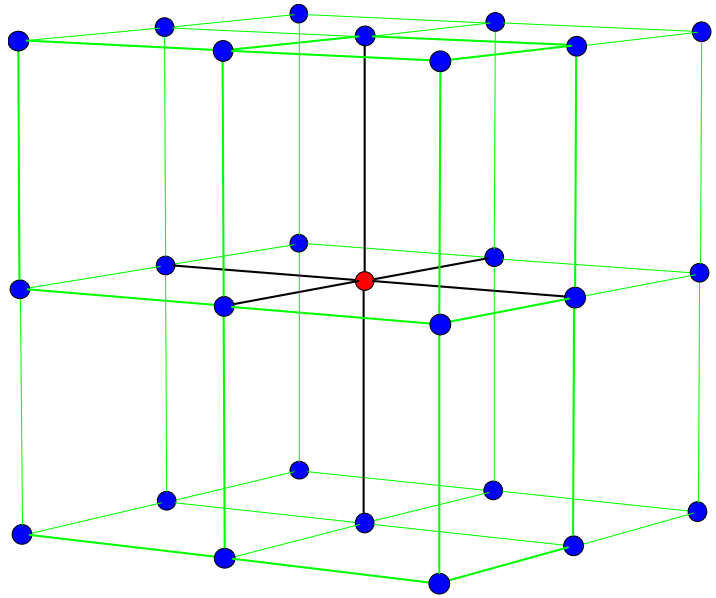
Spatial dimension d or coordination number Z — Fisher, Gaunt (1964)

$\left.\begin{array}{l}\\\\\\\end{array}\right\} \rightarrow \infty$

Mean-Field Theory

Hypercubic lattices: Coordination number Z=2d

Dimension d=3

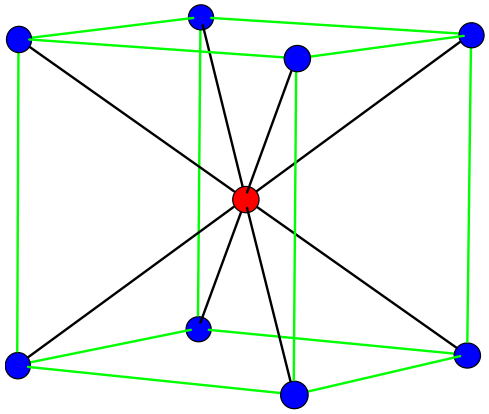


Z=6

Mean-Field Theory

Body-centered cubic lattice

Dimension d=3

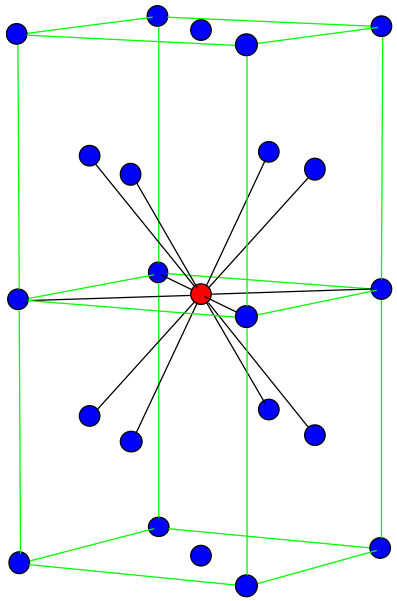


Z=8

Mean-Field Theory

Face-centered cubic lattice

Dimension d=3

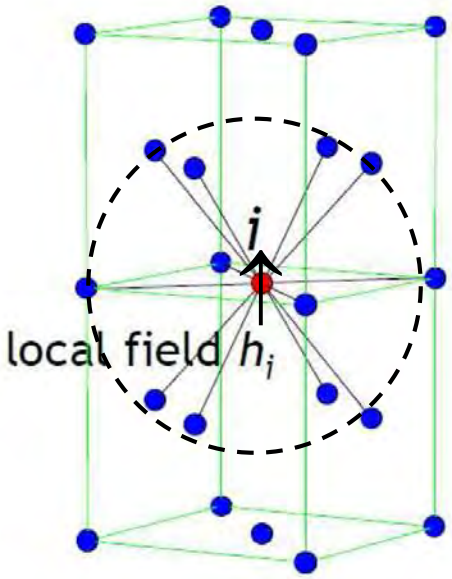


Z=12

$d, Z \to \infty$ ⟶ simplifications ?

Mean-Field Theory

Spin model (Ising)



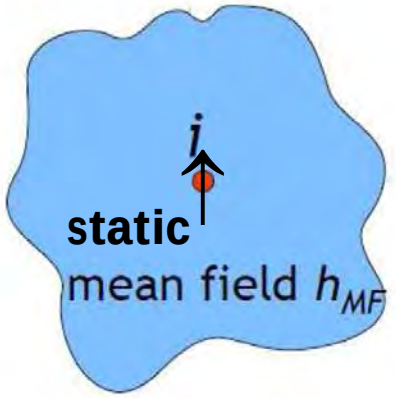
fcc-lattice (d=3): Z=12

$$Z \text{ or } d \to \infty$$

fluctuations in h_i irrelevant

$$h_i S_i \to \underbrace{\langle h_i \rangle}_{h_{MF}} S_i \quad \text{exact}$$

$$h_{MF} = -\underbrace{JZ}_{J^*} \langle S_i \rangle$$



Weiss MFT

$$J \to \frac{J^*}{Z}, \quad J^* = \text{const}$$ "Classical scaling"

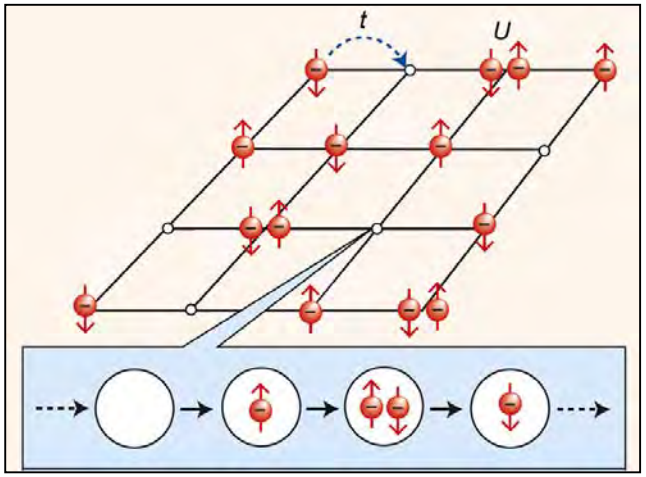
Effective static single-site (single-spin) problem

Mean-Field Theory

Electronic model (Hubbard)

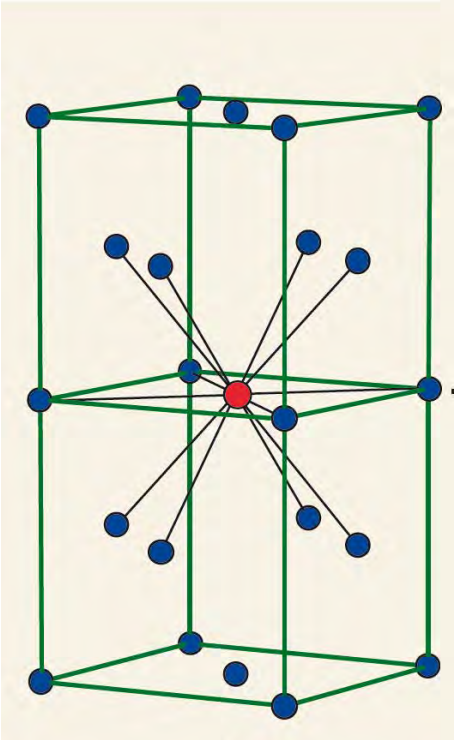
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Purely local interaction:
independent of d, Z



$$\left\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle \neq \left\langle n_{\mathbf{i}\uparrow} \right\rangle \left\langle n_{\mathbf{i}\downarrow} \right\rangle$$

Static (Hartree-Fock-type) mean-field theories do not become exact in $d \rightarrow \infty$



Z=12

$$\xrightarrow{d, Z \rightarrow \infty}$$

- MFT ?
- what simplifications ?

MFT will be very different from Weiss/Hartree

Hubbard model: Simplifications in d,Z $\rightarrow \infty$

Metzner, DV (1989)

$$\langle H_{kin} \rangle = -t \sum_{\mathbf{i},\sigma} \sum_{\mathbf{j}(NN\ \mathbf{i})} \underbrace{\langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle}_{\propto \frac{1}{\sqrt{Z}}}$$

$d, Z \rightarrow \infty$

$\propto \frac{1}{\sqrt{Z}}$ $\quad$ $\underbrace{\quad}_{Z}$

Quantum scaling $\quad t = \frac{t^*}{\sqrt{Z}}$

$$g_{ij,\sigma} = \lim_{t \rightarrow 0-} G_{ij,\sigma}(t) \sim \mathcal{O}\left(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\right)$$

$g_{ij,\sigma}$: Amplitude for hopping $j \rightarrow$ NN i

$$\left|\text{Amplitude for hopping } j \rightarrow \text{NN } i\right|^2 \propto \text{Probability for hopping from } j \rightarrow \text{NN } i = \frac{1}{Z}$$

Actual history:

- Discussion of the Gutzwiller variational approach — DV (1984)
- Exact, analytic calculation of expectation values in d=1 — Metzner, DV (1987)
- Great simplifications observed numerically in d $\rightarrow \infty$ — Metzner, DV (1988)
  $\rightarrow$ Diagrammatic derivation of the Gutzwiller approximation in d $\rightarrow \infty$

Hubbard model: Simplifications in d,Z $\to \infty$

Metzner, DV (1989)

$$\langle H_{kin} \rangle = -t \sum_{\mathbf{i},\sigma} \sum_{\mathbf{j}(NN\ \mathbf{i})} \langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle$$

$d, Z \to \infty$

$-t \propto \frac{1}{\sqrt{Z}}$

$\sum_{\mathbf{j}(NN\ \mathbf{i})}$: Z terms

$\langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle \propto \frac{1}{\sqrt{Z}}$

Quantum scaling $t = \frac{t^*}{\sqrt{Z}}$

$$g_{\bar{i}j,\sigma} = \lim_{t \to 0-} G_{\bar{i}j,\sigma}(t) \sim \mathcal{O}\left(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\right)$$

Alternative derivation of the scaling of t in $\boldsymbol{k}$-space

→ Dispersion for a hypercubic lattice (Z=2d)

→ Lecture by M. Kollar

Hubbard model: Simplifications in d,Z $\to \infty$

Metzner, DV (1989)

$$\langle H_{kin} \rangle = \underbrace{-t}_{\propto \frac{1}{\sqrt{Z}}} \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\langle c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \rangle}_{\propto \frac{1}{\sqrt{Z}}}$$

$d, Z \to \infty$

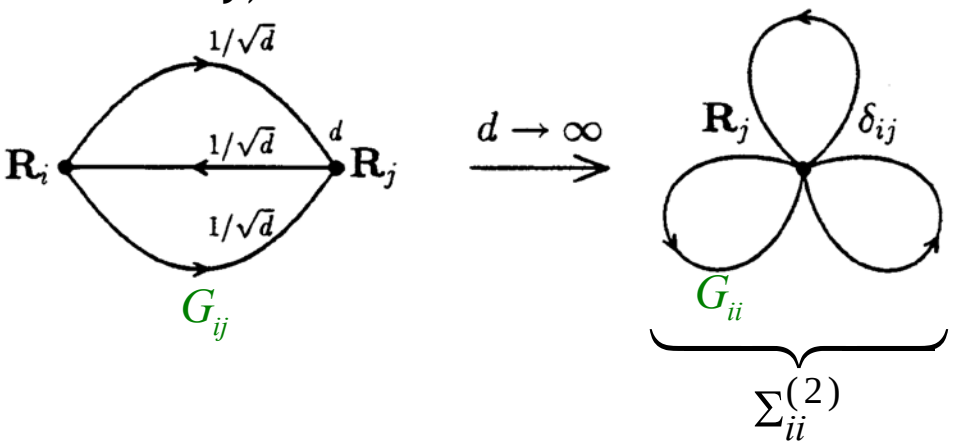
Quantum scaling $t = \frac{t^*}{\sqrt{Z}}$

$$g_{\bar{i}j,\sigma} = \lim_{t \to 0-} G_{\bar{i}j,\sigma}(t) \sim \mathcal{O}\left(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\right)$$

Z or $d \to \infty$ ⟶ Collapse of irreducible diagrams in position space

Example (2. order perturbation theory):

Self-energy $\Sigma^{(2)}_{ij} =$



→ great simplifications in diagrammatic perturbation theory

→ diagrams can be summed to infinite order

Hubbard model: Simplifications in d,Z $\to \infty$

Müller-Hartmann (1989), Janiš (1991)

Most important quantities (local): $G_{ii}(\omega) \equiv G(\omega), \quad \Sigma_{ii}(\omega) \equiv \Sigma(\omega)$

Dynamical, but mean-field in position space

Local lattice Green function =

$$G_\sigma(\omega) \equiv G_{ii,\sigma}(\omega) = \overbrace{\frac{1}{V_B}\sum_{\boldsymbol{k}} \frac{1}{\omega + E_F - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(\omega)}}^{G_k(\omega)} \underbrace{e^{i\mathbf{k}(\mathbf{R_i}-\mathbf{R_i})}}_{1}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{N^0(\varepsilon)}{\omega + E_F - \epsilon - \Sigma_\sigma(\omega)}$$

$$= G^0_\sigma(\omega - \Sigma_\sigma(\omega))$$

free electrons in a dynamic potential Σ(ω) (mean field)

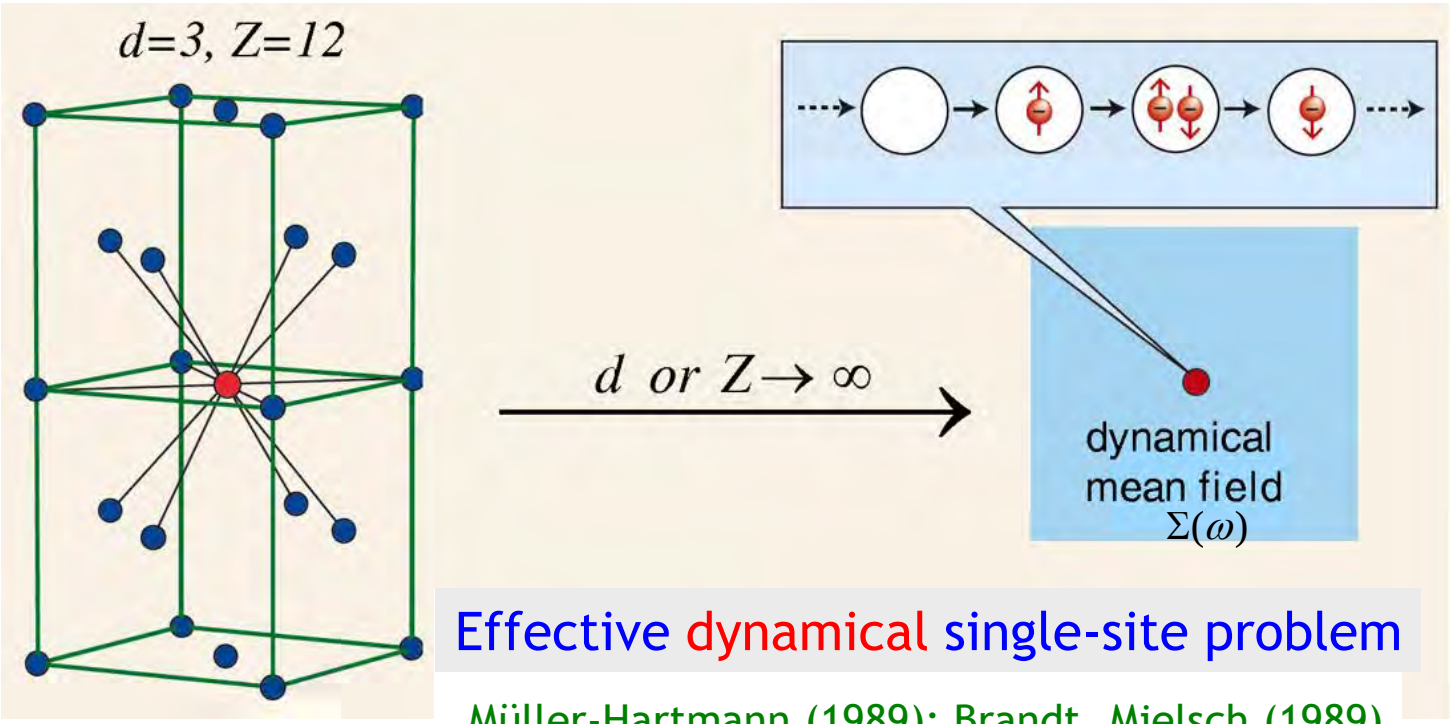
Dynamical Mean-Field Theory (DMFT) for Correlated Electrons

Hubbard model: Simplifications in d,Z $\rightarrow \infty$

Metzner, DV (1989)

$$H = -\frac{t^*}{\sqrt{Z}} \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Quantum scaling $\quad t = \frac{t^*}{\sqrt{Z}}$



Effective dynamical single-site problem

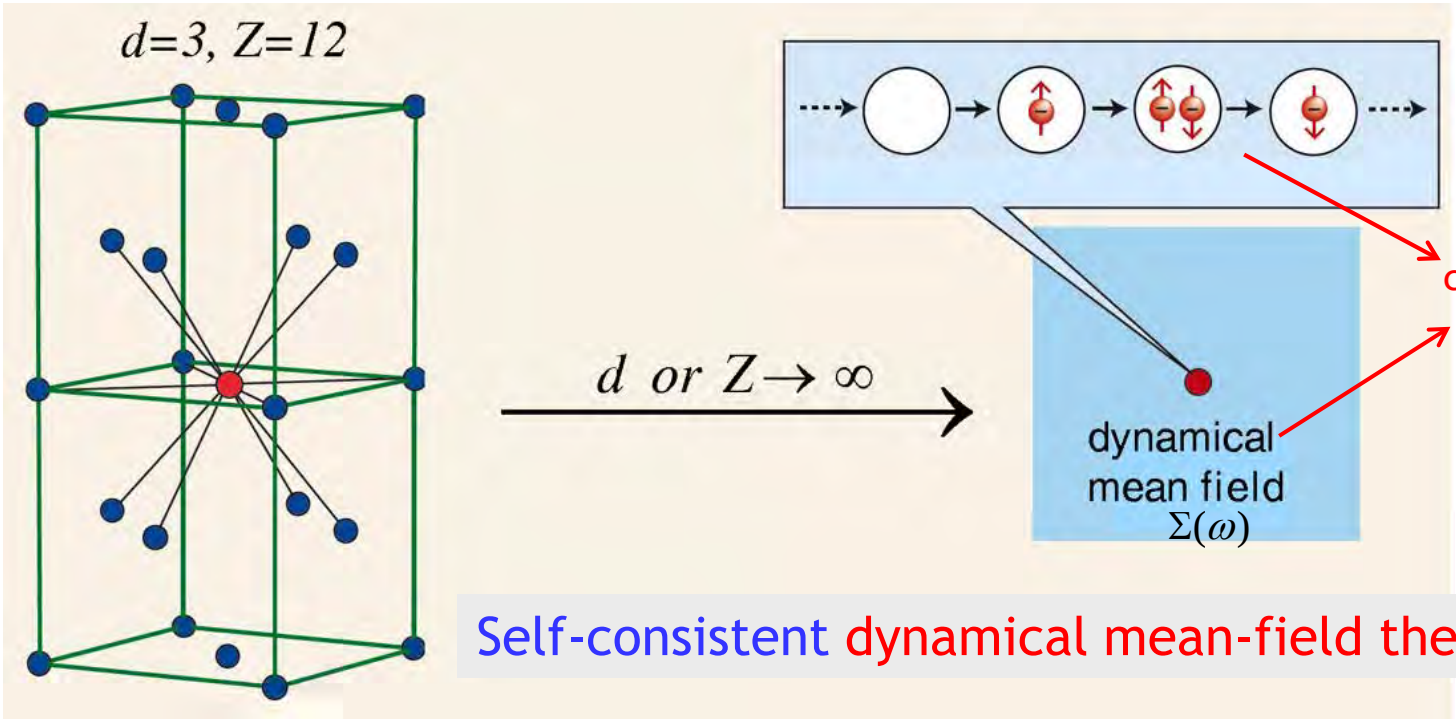
Müller-Hartmann (1989); Brandt, Mielsch (1989)

Hubbard model: Simplifications in d,Z → ∞

Metzner, DV (1989)

$$H = -\frac{t^*}{\sqrt{Z}} \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Quantum scaling $t = \frac{t^*}{\sqrt{Z}}$



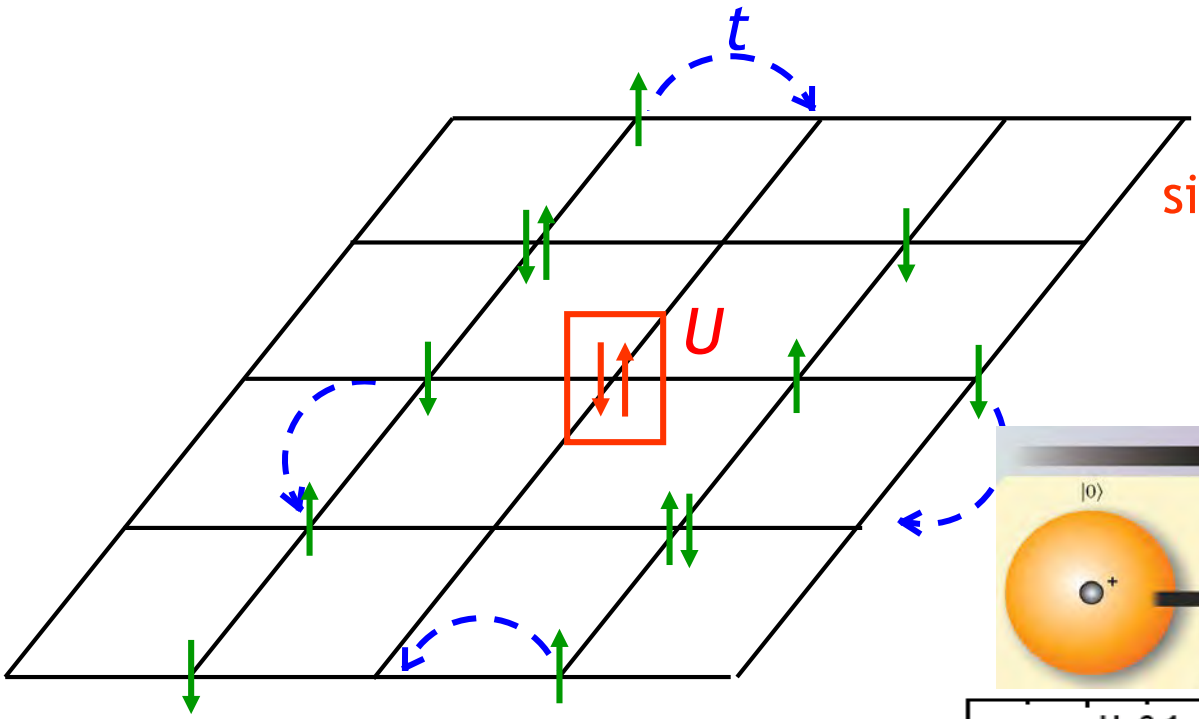
Self-consistent dynamical mean-field theory

Janiš (1991): Generalization of *coherent potential approximation*

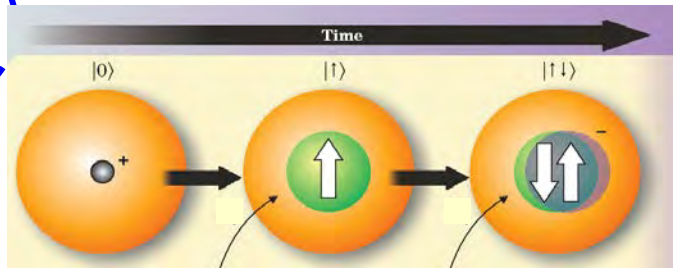
Georges, Kotliar (1992), Jarrell (1992):
Self-consistent *single-impurity Anderson model*

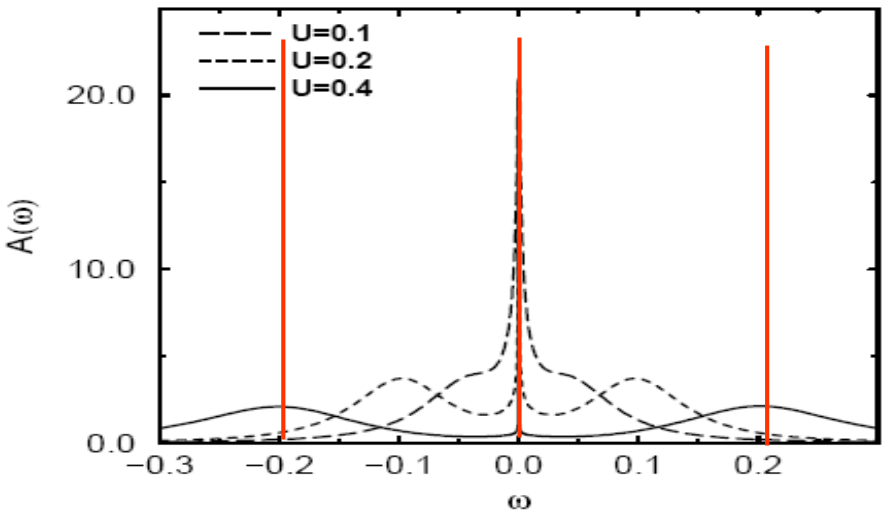
→ Lecture by M. Kollar

Excursion: Single-impurity Anderson model



Non-interacting
conduction (*s*-) electrons
+
single *d*-orbital ("impurity")
(with interaction *U*)
+
s,*d*-hybridization V

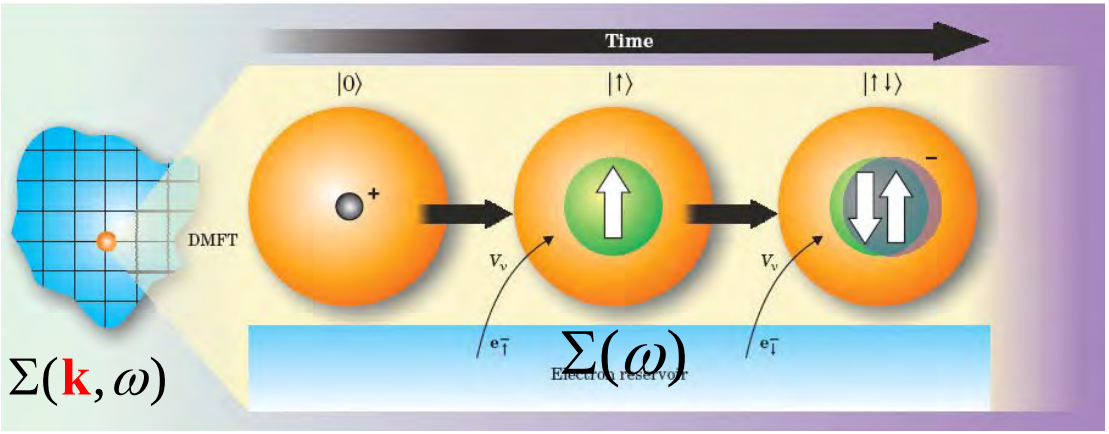




- Characteristic 3-peak structure
- *non-perturbative* energy scale ("Kondo physics")

Useful physical *interpretation*:

Hubbard model $\xrightarrow{d\to\infty}$ single-impurity Anderson model
+ self-consistency condition



Kotliar, DV (2004)

Fully dynamical,
but mean-field
in position space

"Dynamical Mean-Field Theory (DMFT)"

DMFT self-consistency equations

T>0

In Matsubara frequencies

self-energy $\Sigma_{\sigma n} \equiv \Sigma_\sigma(i\omega_n)$

Green function $G_{\sigma n} \equiv G_\sigma(i\omega_n)$

$$G_{\sigma n} = -\langle \psi_{\sigma n} \psi^*_{\sigma n} \rangle_{\mathcal{A}}$$

$$G_{\sigma n} = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, \frac{N^0(\varepsilon)}{i\omega_n + \mu - \Sigma_{\sigma n} - \varepsilon}$$

Self-consistency condition

Impurity Green Function = Local lattice Green function

→ information about lattice structure

Coherent-state path-integral formulation

Fermionic operator $\hat{c}$ → Grassmann variable ψ

Thermal average

$$\langle \hat{C} \rangle_{\mathcal{A}} = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi] \, \mathcal{D}[\psi^*] \, C[\psi, \psi^*] \, \mathrm{e}^{\mathcal{A}[\psi, \psi^*, \mathcal{G}]}$$

Partition function

$$\mathcal{Z} = \int \mathcal{D}[\psi] \, \mathcal{D}[\psi^*] \, \mathrm{e}^{\mathcal{A}[\psi, \psi^*, \mathcal{G}]}$$

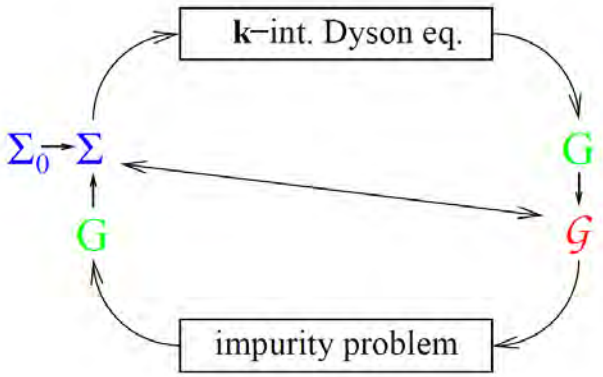
Single-site ("impurity") action

$$\mathcal{A}[\psi, \psi^*, \mathcal{G}] = \sum_{\sigma, n} \psi^*_{\sigma n} \mathcal{G}^{-1}_{\sigma n} \psi_{\sigma n} - \frac{U}{2} \sum_{\sigma\sigma'} \int_0^\beta \mathrm{d}\tau \, \psi^*_\sigma(\tau) \psi_\sigma(\tau) \psi^*_{\sigma'}(\tau) \psi_{\sigma'}(\tau)$$

$$\mathcal{G}^{-1}_{\sigma n} = G^{-1}_{\sigma n} + \Sigma_{\sigma n}$$

$\mathcal{G}_{\sigma n}$: *effective local propagator/ bath Green function* ("Weiss mean field")

DMFT self-consistency cycle



Blümer (2003)

→ Lecture by M. Kollar

Impurity solver

Semi-analytical approximations:

IPT
NCA
Hubbard I

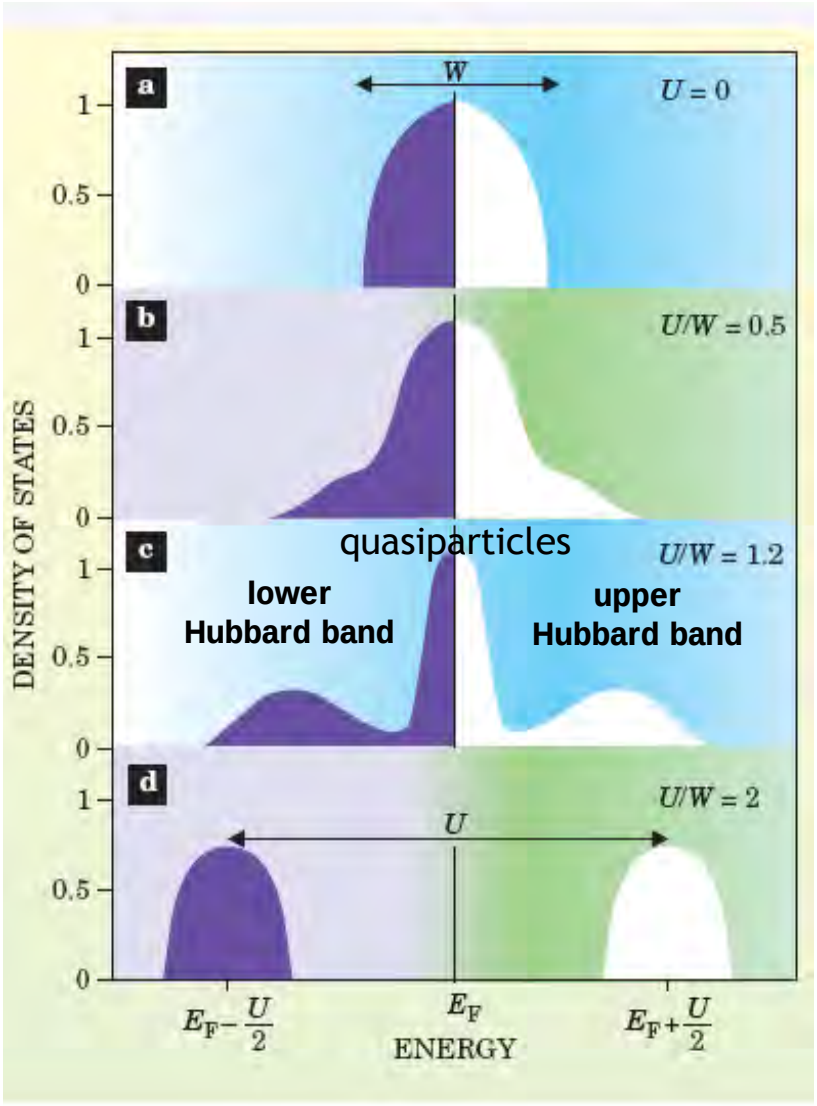
Numerical:

CT-QMC
ED
Lanczos
NRG
DMRG

→ Lectures by F. Assaad, E. Koch, H. G. Evertz

Application of DMFT:
1. Mott-Hubbard metal-insulator transition

Mott-Hubbard metal-insulator transition

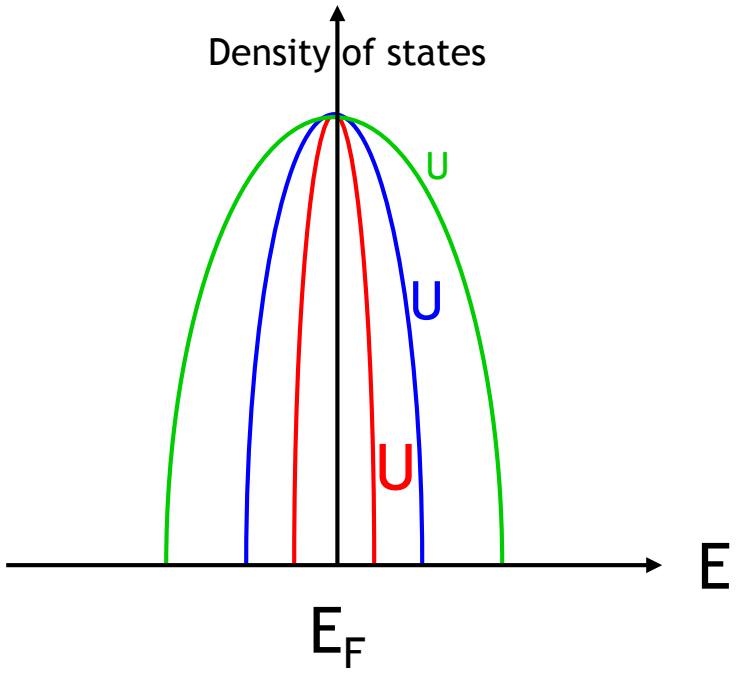


Intermediate-coupling problem

metal

insulator

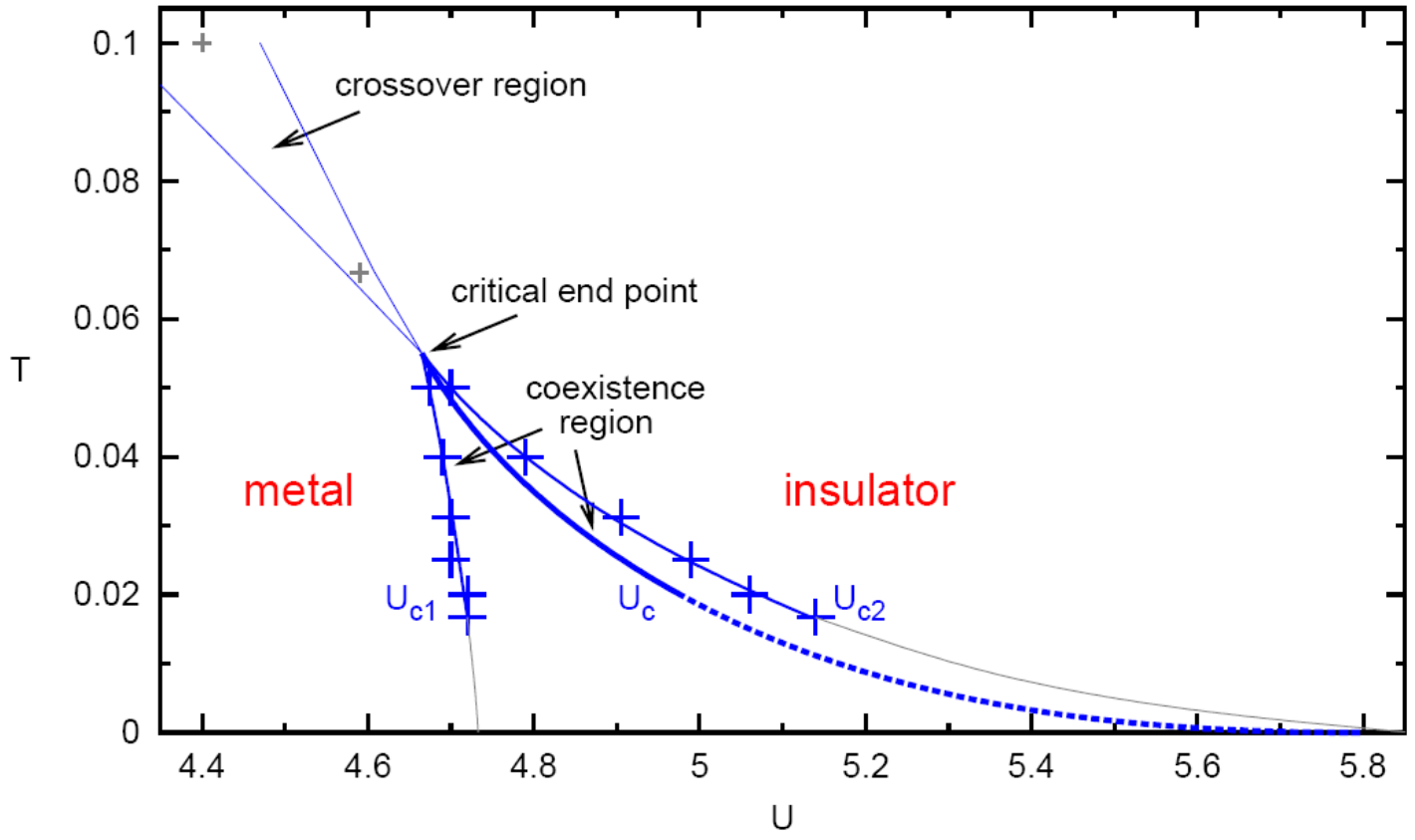
Hubbard model, n=1



Quasiparticle renormalization , $Z^{-1} = \frac{m^*}{m} \to \infty$

DMFT: Metal-insulator transition in the one-band Hubbard model

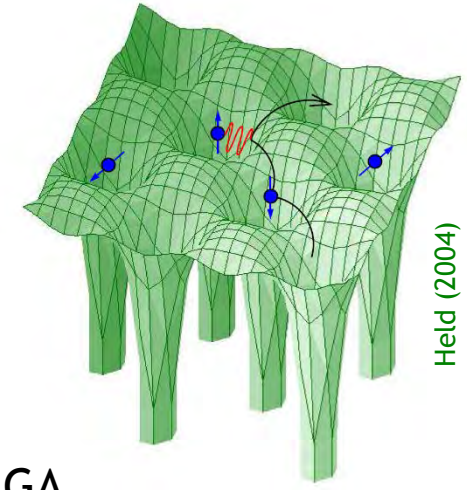
Paramagnetic solution



Blümer (2002)

Application of DMFT:
2. From models back to materials

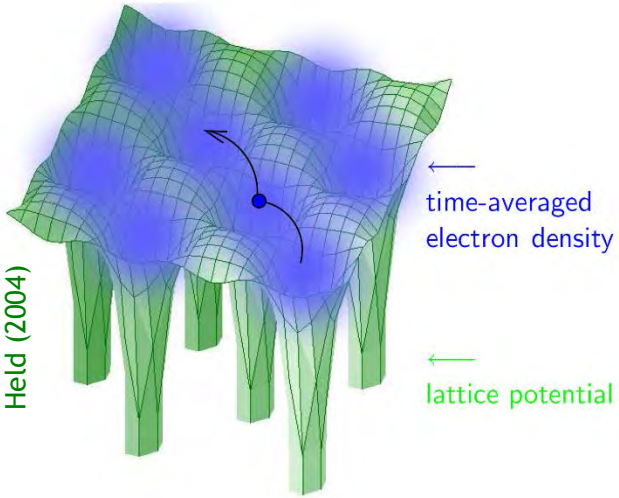
Non-perturbative approximation schemes for real materials



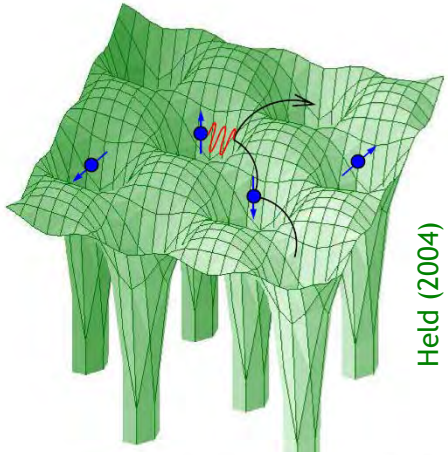
DFT/LDA, GGA

+	material specific
+	fast code packages
−	fails for strong correlations

→ Lecture by O. K. Andersen

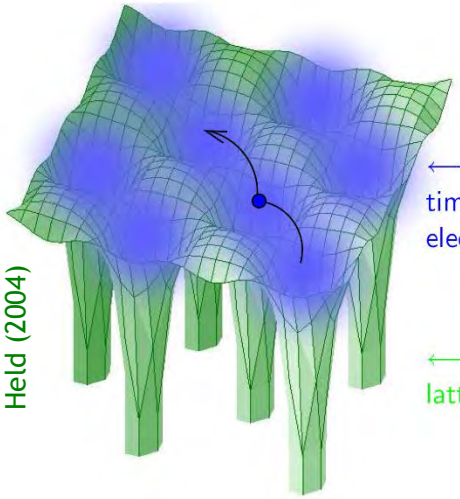


Non-perturbative approximation schemes for real materials



Held (2004)

DFT/LDA, **GGA**		Model Hamiltonians	
+	material specific	−	input parameters unknown
+	fast code packages	−	computationally expensive
−	fails for strong correlations	+	systematic many-body approach

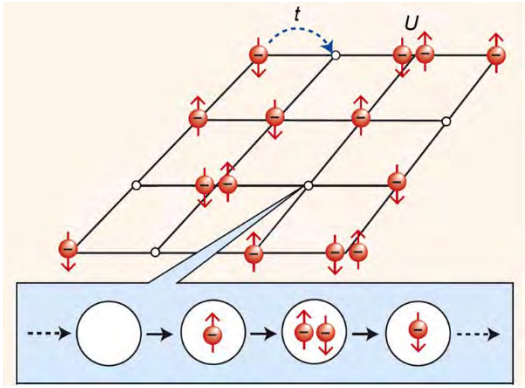


Held (2004)

time-averaged electron density

lattice potential

How to combine?



Computational scheme for correlated electron materials:

Material specific electronic structure
(Density functional theory: **LDA, GGA, ...**) or **GW**

+

Local electronic correlations
(Many-body theory: **DMFT**)

=

LDA+DMFT

→ Lecture by E. Pavarini

Anisimov, Poteryaev, Korotin, Anokhin, Kotliar (1997)
Lichtenstein, Katsnelson (1998)
Nekrasov, Held, Blümer, Poteryaev, Anisimov, DV (2000)

Computational scheme for correlated electron materials:

Material specific electronic structure
(Density functional theory: **LDA, GGA, ...**) or **GW**

+

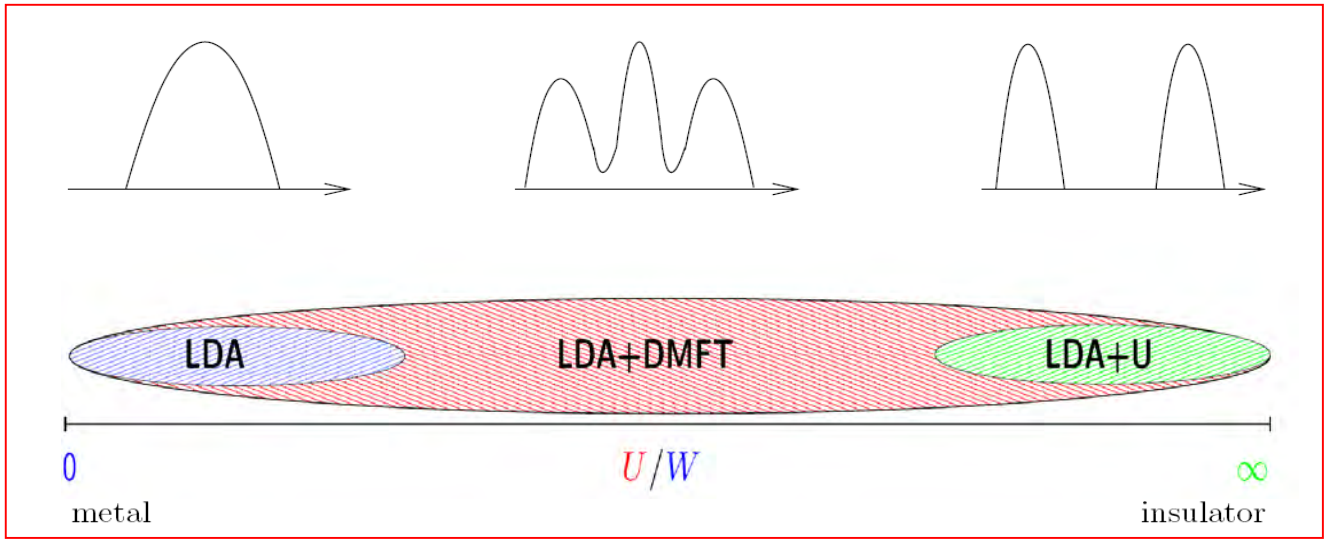
Local electronic correlations
(Many-body theory: **DMFT**)

=

X+DMFT X= DFT (LDA, GGA); GW, ...

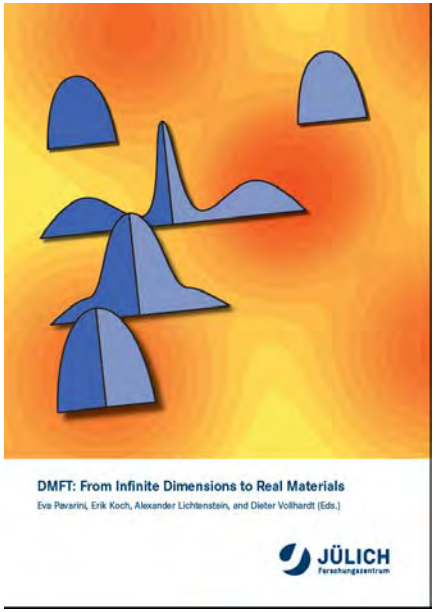
Solve self-consistently with an impurity solver

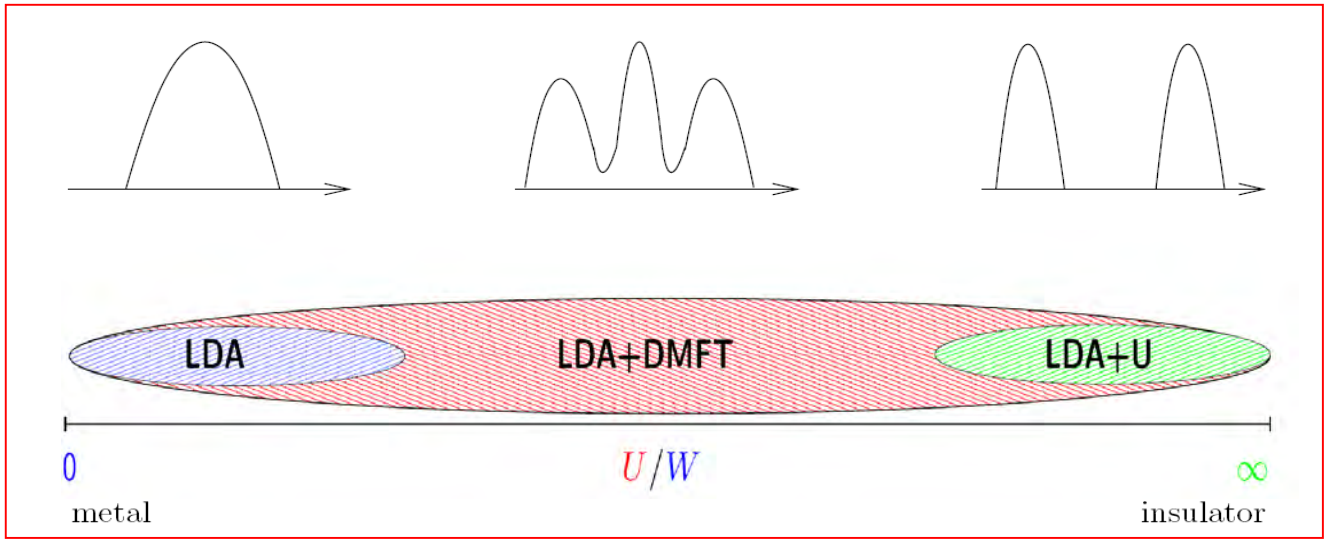
Charge self-consistency → Lecture by F. Lechermann



Held, Nekrasov, Keller, Eyert, Blümer, McMahan, Scalettar, Pruschke, Anisimov, DV (Psi-k, 2003)

LDA+U: No correlations, but often good results for long-range ordered states



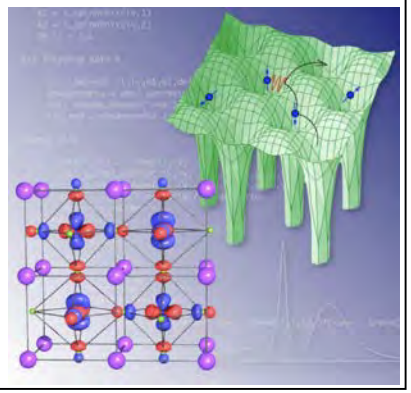


Held, Nekrasov, Keller, Eyert, Blümer, McMahan, Scalettar, Pruschke, Anisimov, DV (Psi-k, 2003)

LDA+U: No correlations, but often good results for long-range ordered states

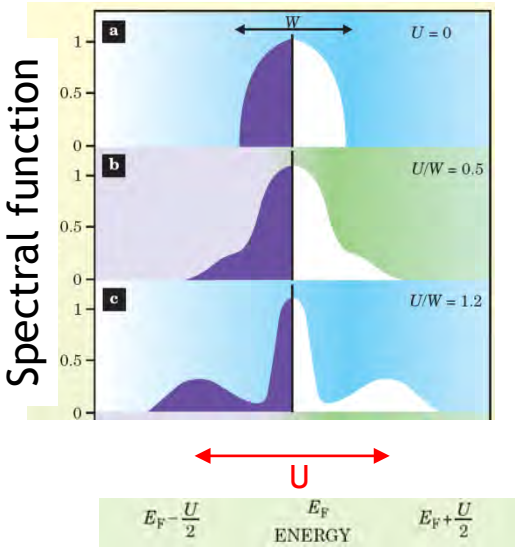
Goal: Dynamical mean-field approach with predictive power for strongly correlated materials

DFG Research Unit FOR 1346
(2010-2017)



http://www.physik.uni-augsburg.de/for1346/

Dynamical mean-field theory



Definition of electronic correlations (II):

- transfer of spectral weight - due to $\mathrm{Re}\,\Sigma(\omega)$
- finite lifetime of excitations - due to $\mathrm{Im}\,\Sigma(\omega)$

Experimentally testable
(PES, ARPES, …)

→ Lecture by H. Tjeng

Contact with experiment via

Spectral function in DMFT

k-integrated spectral function
→ PES

$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathbf{G}(\omega)$$

k-resolved spectral function
→ ARPES

$$\mathbf{G}(\mathbf{k},\omega) = [\omega - \boldsymbol{\Sigma}(\omega) - \mathbf{H}^{0}_{LDA}(\mathbf{k})]^{-1}$$

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,Tr\,\mathbf{G}(\mathbf{k},\omega)$$

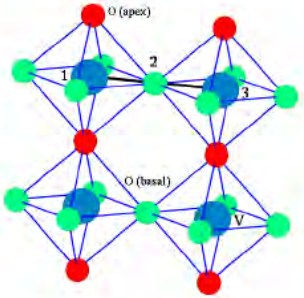
1. Application of DFT+DMFT

$(Sr,Ca)VO_3$: 3d1 system

Electronic structure

Crystal structure

$SrVO_3$: $\angle V - O - V = 180°$

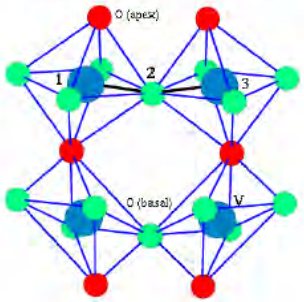


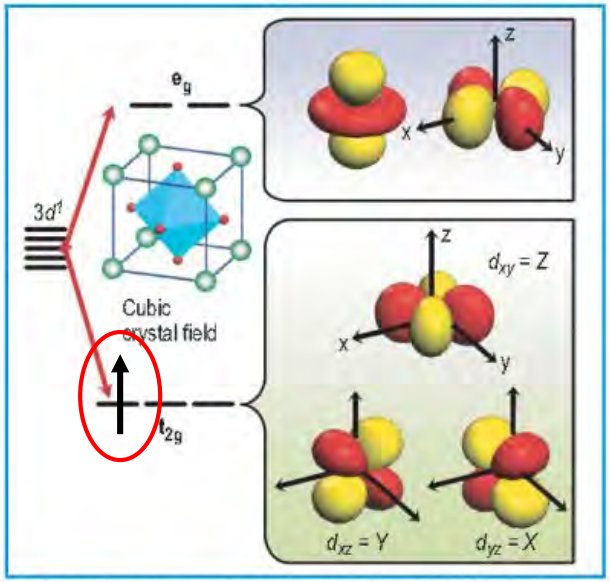
⇓

orthorhombic distortion

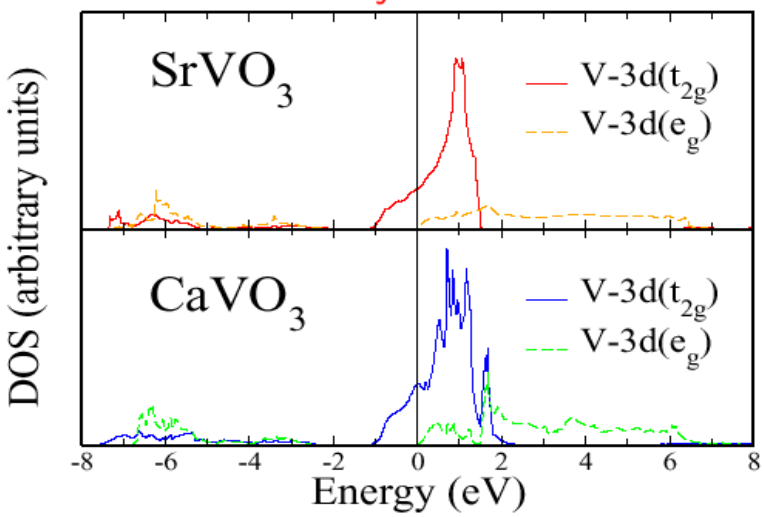
⇓

$CaVO_3$: $\angle V - O - V \approx 162°$





LDA density of states



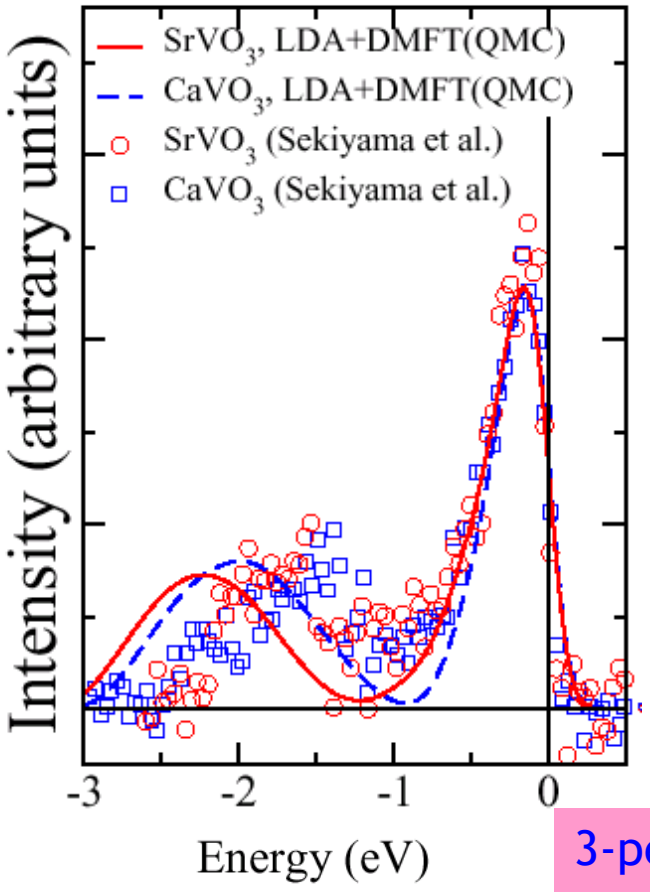
No correlation effects/spectral transfer

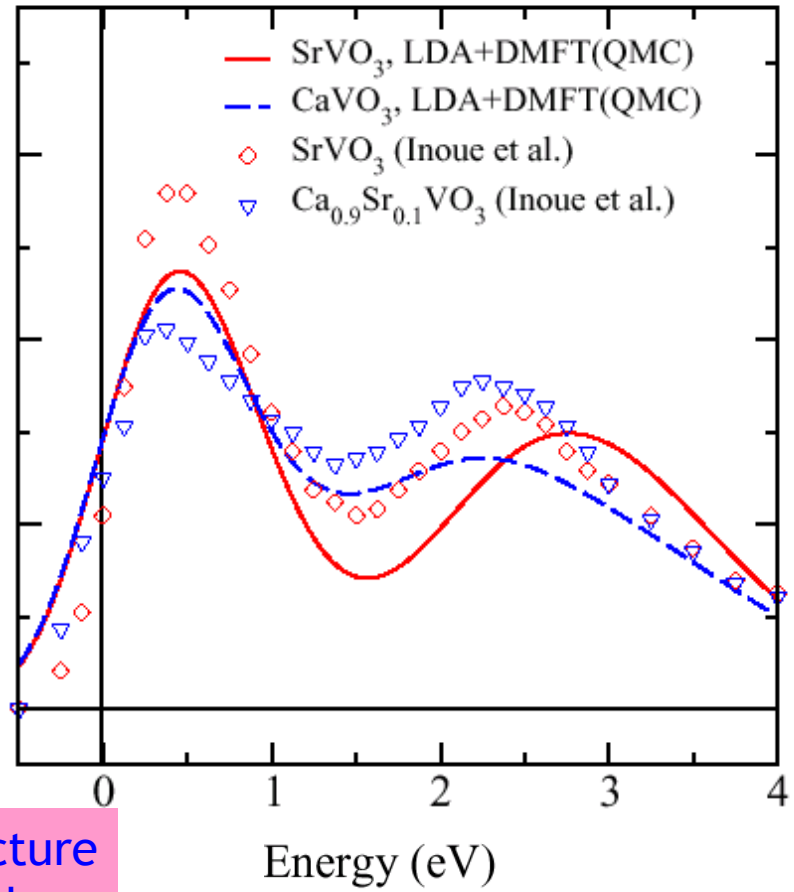
LDA+DMFT for $(Sr,Ca)VO_3$: Comparison with experiment

Osaka – Augsburg – Ekaterinburg collaboration (2004, 2005)

(i) bulk-sensitive high-resolution photoemission spectra (PES) → occupied states

(ii) $1s$ x-ray absorption spectra (XAS) → unoccupied states

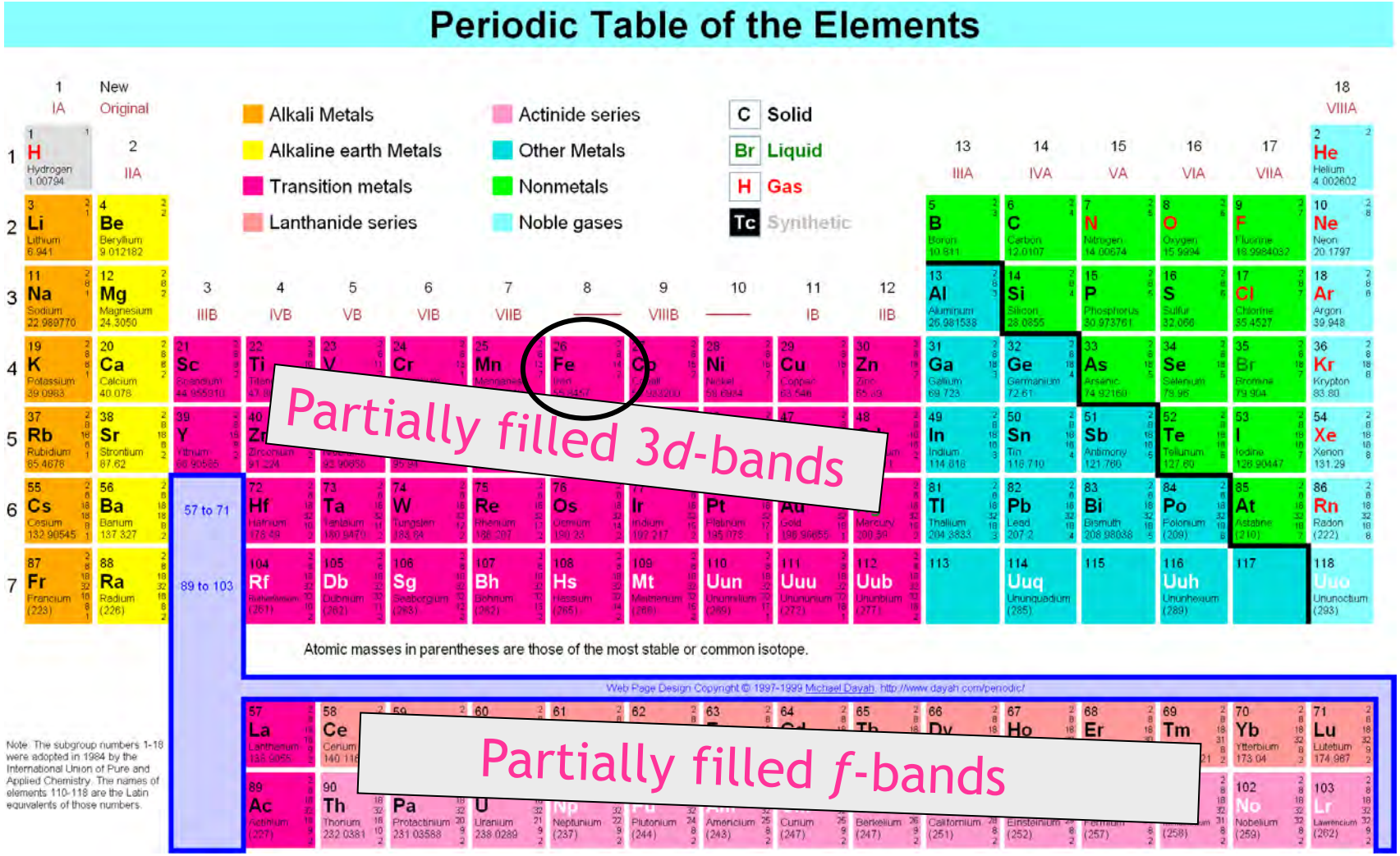




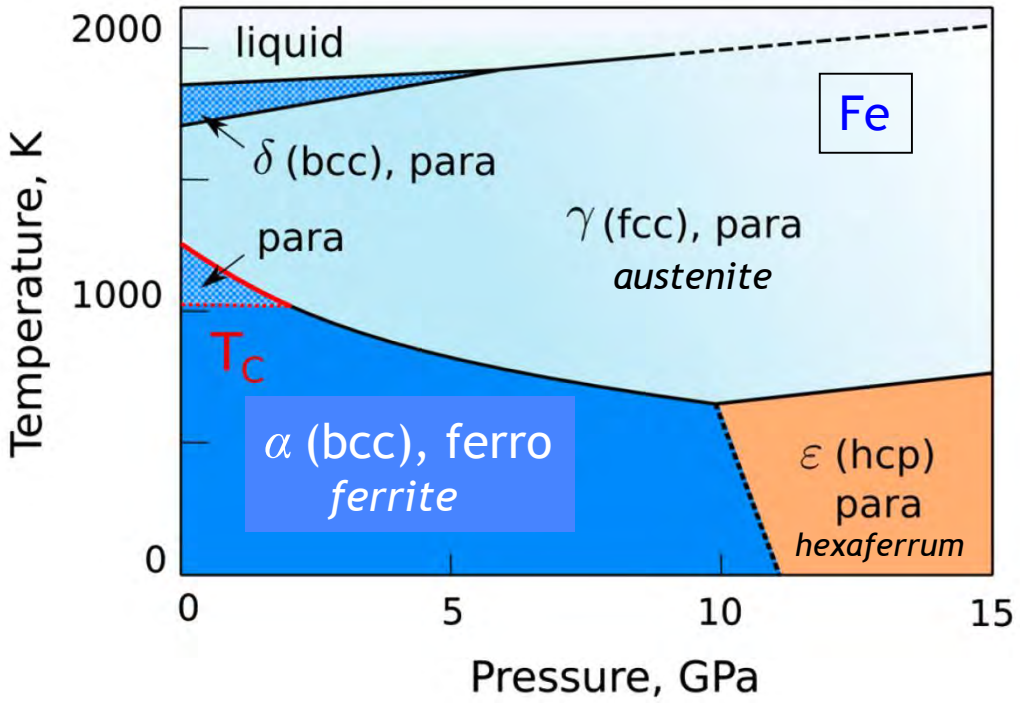
3-peak structure detected

2. Application of DFT+DMFT

Elemental Fe



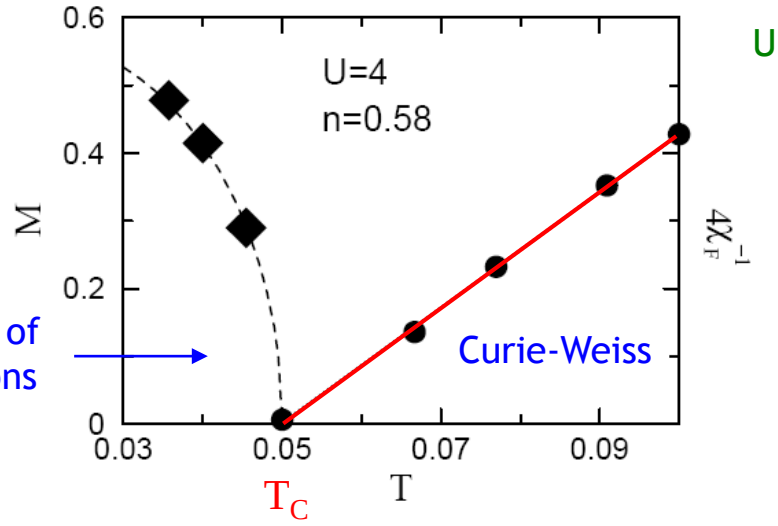
Narrow *d*,*f*-bands → electronic correlations



Origin of metallic ferromagnetism?

DMFT: Ferromagnetism in the one-band Hubbard model

Generalized fcc lattice ($Z \to \infty$)



Ulmke (1998)

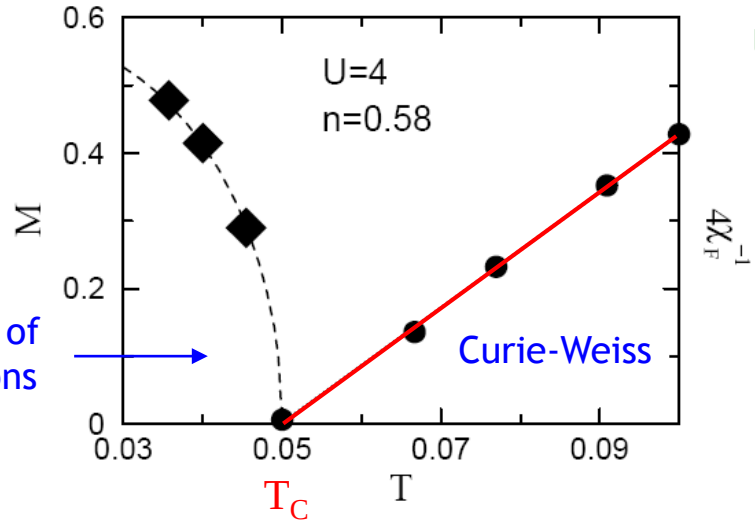
Ferromagnetism of itinerant electrons

Paradox "spins *vs.* electrons" reconciled

Intermediate-coupling problem

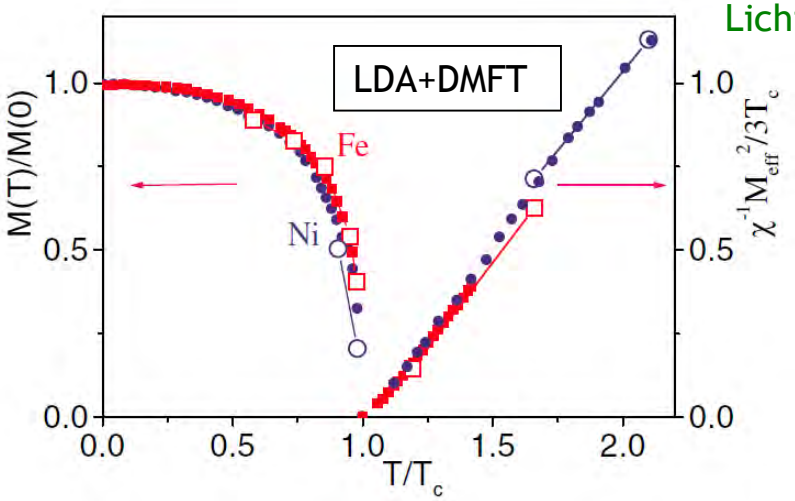
DMFT: Ferromagnetism in the one-band Hubbard model

Generalized fcc lattice ($Z \to \infty$)



Ulmke (1998)

Ferromagnetism of itinerant electrons

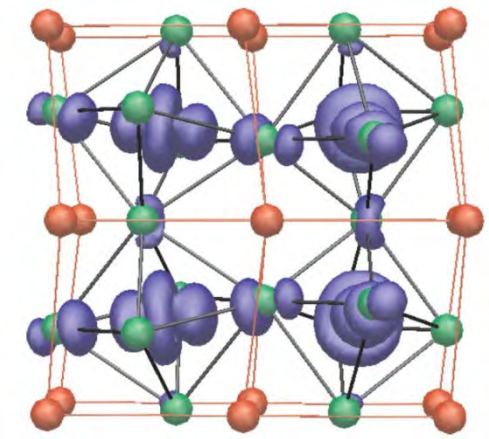


Lichtenstein, Katsnelson, Kotliar (2001)

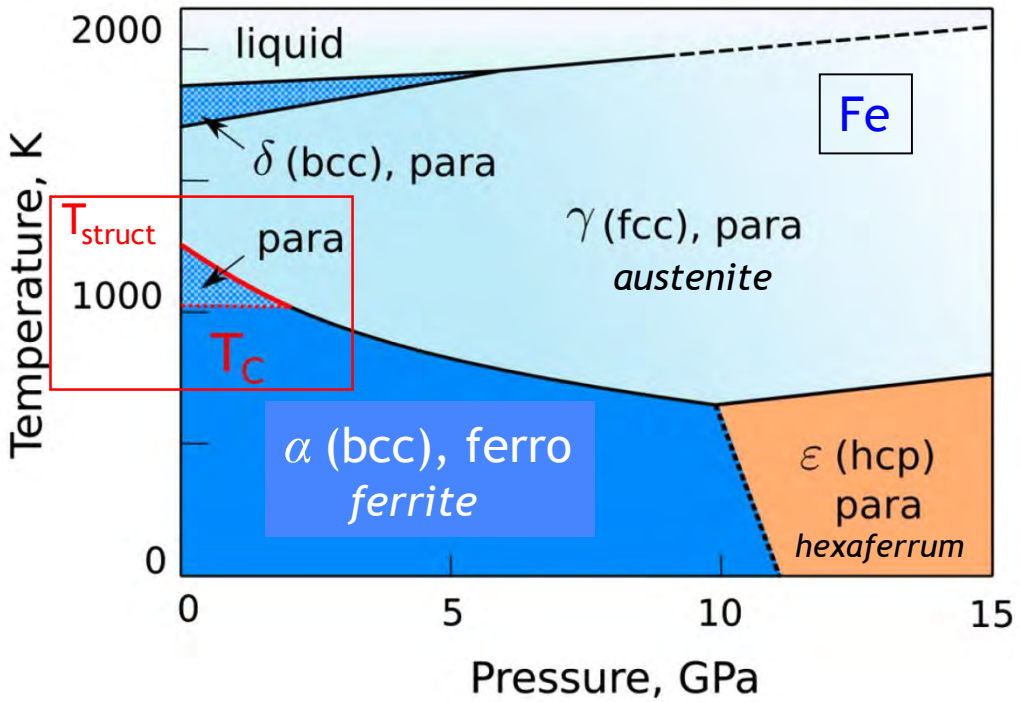
Microscopic origin of exchange interactions in Fe

Eriksson collaboration (2016)

Until recently:
DFT+DMFT investigations of correlated materials for
given lattice structure



- How do electrons + ions influence each other ?
- Which lattice structure is stabilized ?



DFT/GGA: Paramagnetic α-phase unstable

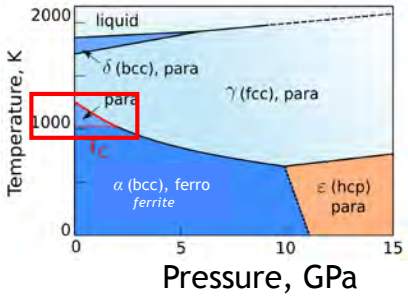
- Why is the paramagnetic α-phase stable?
- How to compute T_{struct} ?

GGA+DMFT: Electronic correlations (local repulsion)

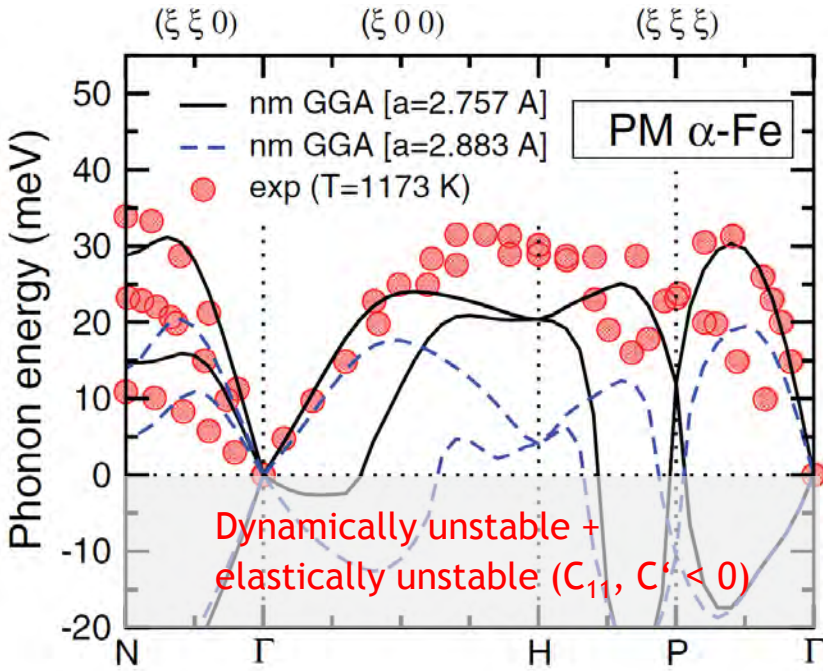
- increase unit cell volume → correct density & compressibility
- stabilize paramagnetic α-phase → $T_{struct} > T_C$

Leonov, Poteryaev, Anisimov, DV (2011)

Lattice dynamics of paramagnetic α-Fe

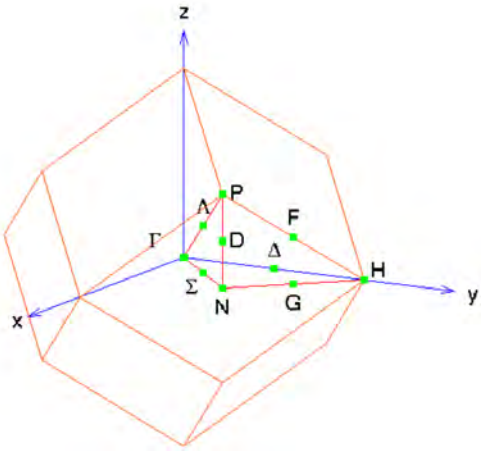


Non-magnetic GGA phonon dispersion



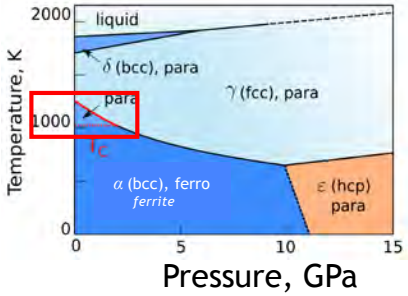
Experiment:
Neuhaus, Petry, Krimmel (1997)

1. Brillouin zone

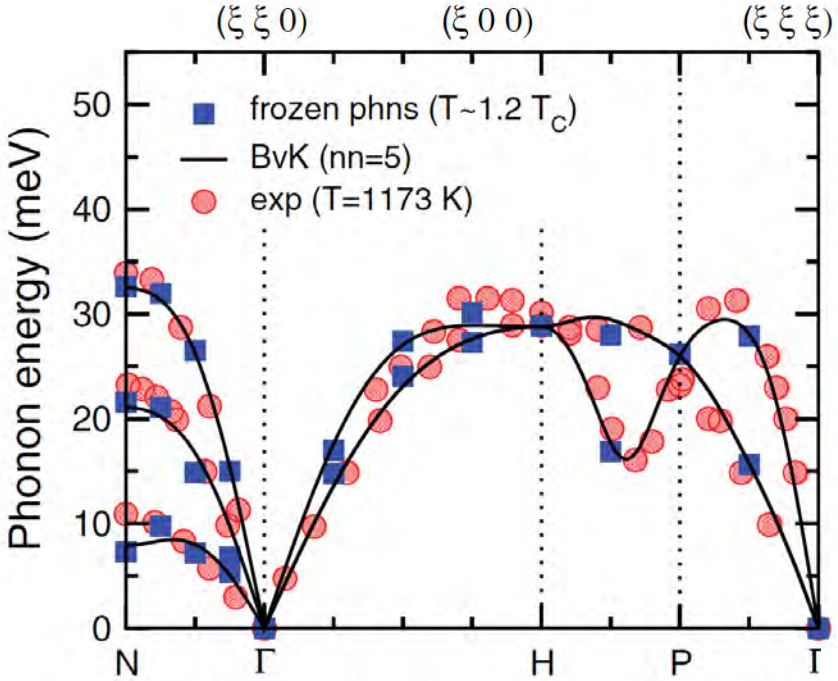


Lattice dynamics of paramagnetic α-Fe

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



GGA+DMFT phonon dispersion at 1.2 T_C



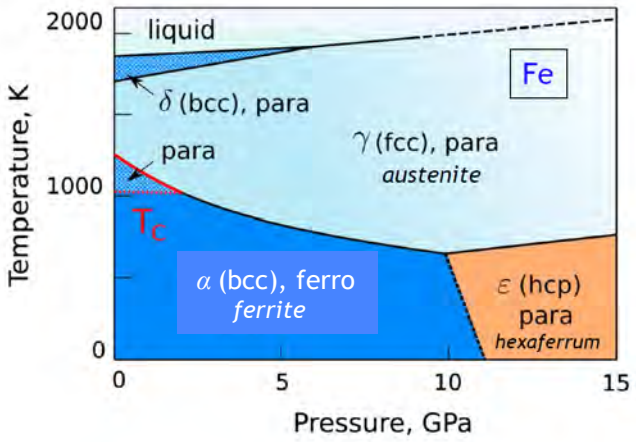
Experiment:
Neuhaus, Petry, Krimmel (1997)

Calculated:
- equilibrium lattice constant a~2.883 Å (a_{exp}~2.897 Å)
- Debye temperature Θ~458 K

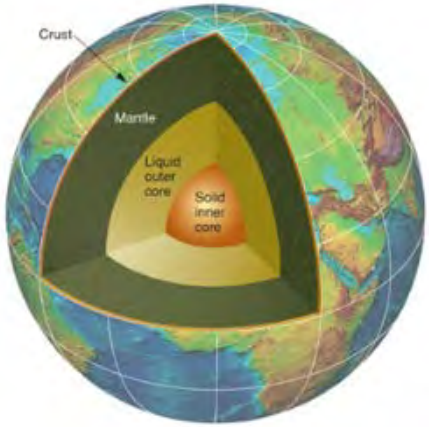
Theory:
Leonov, Poteryaev, Anisimov, DV (2012)

Further applications of DFT+DMFT to Fe

Phase diagram of iron



Behavior at high pressures and temperatures?

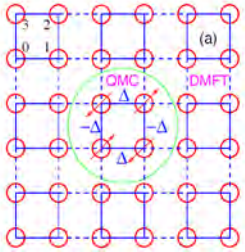


Respiration:
Binding of heme on
O_2 and CO

Weber *et al.* (2013)

Application of DMFT:
Need for improved realism

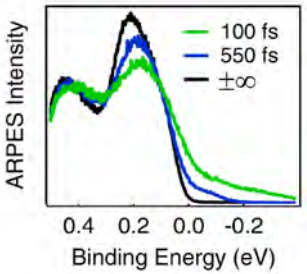
- Beyond single-site DMFT



→ Lectures by M. Potthoff, H. Hafermann, T. Maier, K. Held

- Correlated electrons in non-equilibrium

→ Lecture by M. Eckstein



Wide field of applications for DMFT based techniques