

Center for
Electronic Correlations and Magnetism
University of Augsburg

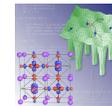
Dynamical Mean-Field Approach for Strongly Correlated Materials

Dieter Vollhardt

Autumn School 2011: Hands-on LDA+DMFT
Forschungszentrum Jülich
October 4, 2011

Supported by **DFG**

FOR 1346



Outline:

- Electronic correlations
- Dynamical Mean-Field Theory (DMFT)
- Applications of DMFT to models and materials

Correlations

Correlation [lat.]: *con* + *relatio* ("with relation")

Correlations in mathematics, natural sciences:

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

e.g., densities:

$$\langle \rho(\mathbf{r})\rho(\mathbf{r}') \rangle \neq \langle \rho(\mathbf{r}) \rangle \langle \rho(\mathbf{r}') \rangle$$

Correlations (I):

Effects beyond factorization approximations (e.g., Hartree-Fock)

Temporal/spatial correlations in everyday life



Beware: External periodic potential \rightarrow long-range order enforced
 \rightarrow trivial correlations

Temporal/spatial correlations in everyday life



Time/space average inappropriate

Electronic Correlations in the Periodic Table

Periodic Table of the Elements

1 IA New Original	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 H Hydrogen 1.00794	2 He Helium 4.002602	3 Li Lithium 6.941	4 Be Beryllium 9.012182	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.00674	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797	11 Na Sodium 22.989770	12 Mg Magnesium 24.3050	13 Al Aluminum 26.981538	14 Si Silicon 28.0855	15 P Phosphorus 30.973761	16 S Sulfur 32.066	17 Cl Chlorine 35.4527	18 Ar Argon 39.948
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.29
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 to 71 Lanthanide series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.078	79 Au Gold 196.96655	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98038	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 to 103 Actinide series	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (262)	108 Hs Hassium (265)	109 Mt Meitnerium (268)	110 Uun Ununnilium (269)	111 Uuu Unununium (272)	112 Uub Ununbium (277)	113 Uuq Ununquadium (285)	114 Uuq Ununquadium (285)	115 Uuh Ununhexium (289)	116 Uuh Ununhexium (289)	117 Uue Ununseptium (289)	118 Uuo Ununoctium (293)
57 La Lanthanum 138.9055	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.5001	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93032	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.84
89 Ac Actinium (227)	90 Th Thorium 232.0381	91 Pa Protactinium 231.03588	92 U Uranium 238.0289	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)

Partially filled d-orbitals

Partially filled f-orbitals

Narrow d, f -orbitals → strong electronic correlations

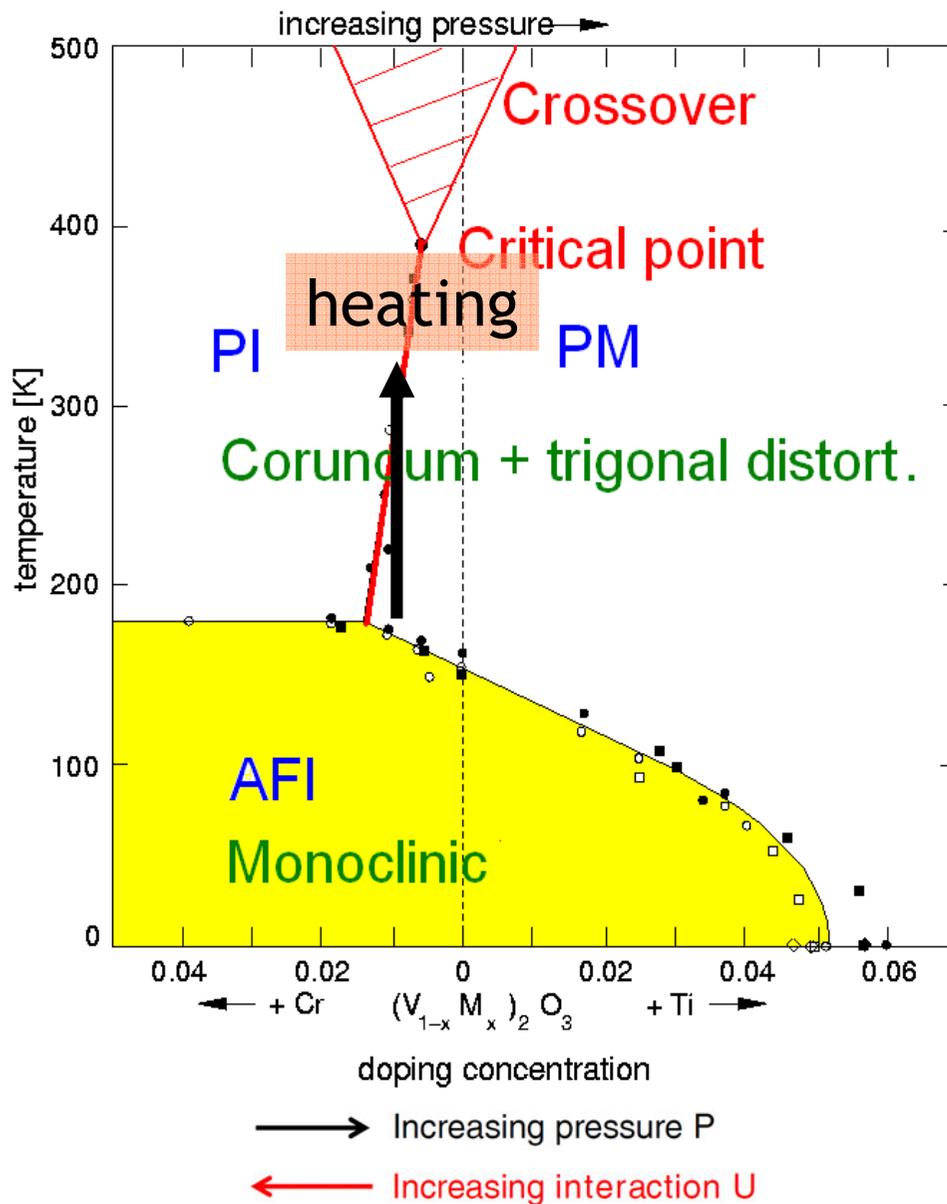
Note: The subgroup numbers 1-18 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 110-118 are the Latin equivalents of those numbers.

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Electronic Correlations in Solids

1.

Mott metal-insulator transition in V_2O_3



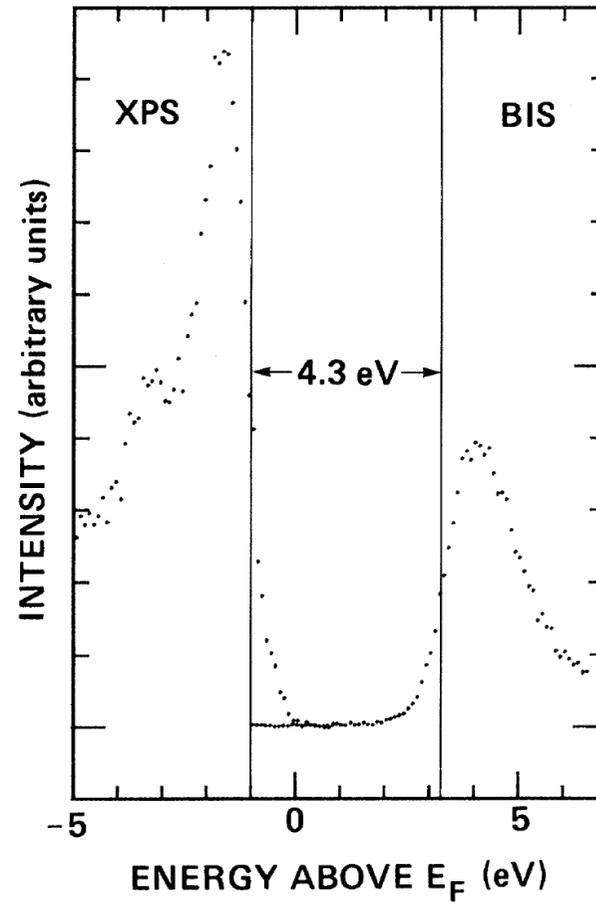
Rice, McWhan (1970); McWhan, Menth, Remeika, Brinkman, Rice (1973)

- PI ↔ PM: 1. order transition without lattice symmetry change
- Anomalous slope of P(T)
→ *Pomeranchuk effect* in ^3He

Microscopic explanation?

2.

Photoemission spectra of NiO

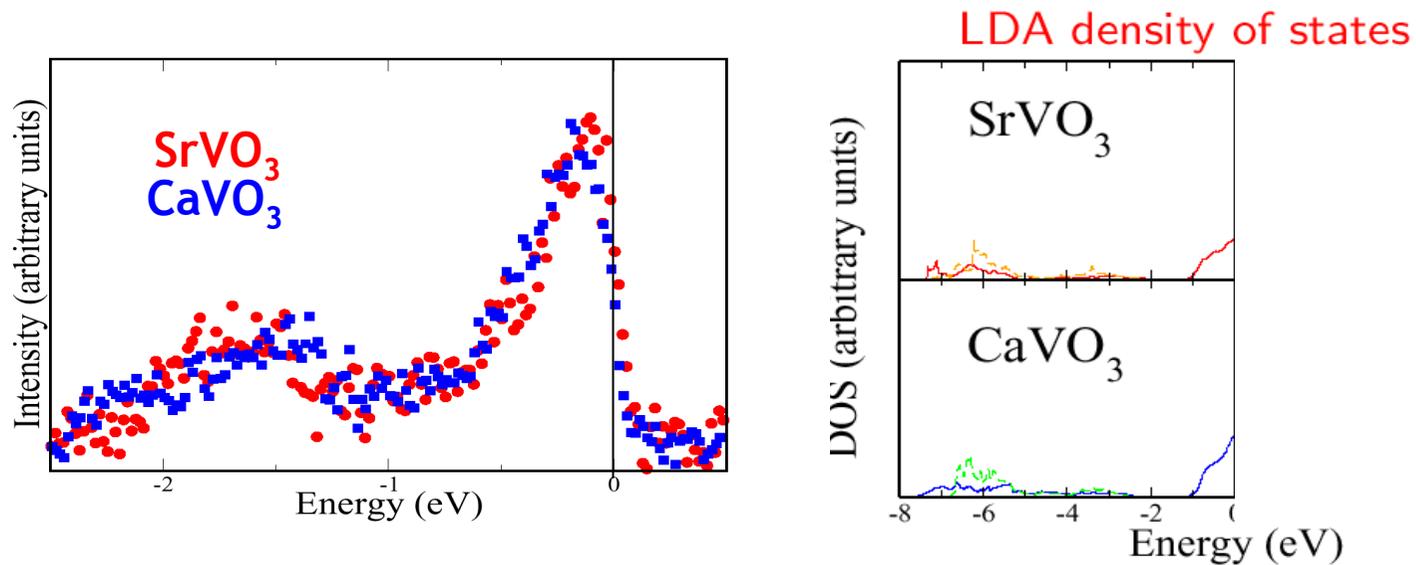


Sawatzky, Allen (1984)

Origin of gap
(antiferromagnetism)?

3.

Photoemission spectra of $(\text{Sr,Ca})\text{VO}_3$



Osaka - Augsburg - Ekaterinburg collaboration: Sekiyama *et al.*, 2004

Reason for shift of spectral weight?

Correlated electron materials

Fascinating topics for fundamental research

- large resistivity changes
- gigantic volume changes
- high- T_c superconductivity
- strong thermoelectric response
- colossal magnetoresistance
- huge multiferroic effects

} large
susceptibilities

with

Technological applications:

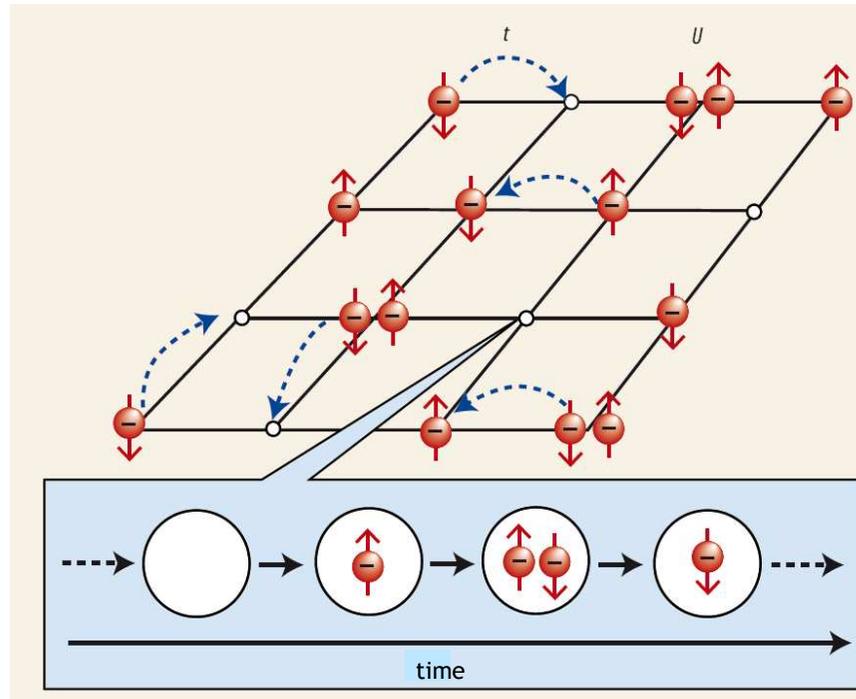
- sensors, switches
- magnetic storage
- refrigerators
- functional materials, ...

Electronic Correlations: Models

→ Lecture of F. Lechermann

Hubbard model

(tight binding approach)



Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

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

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle \neq \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle$$



Purely numerical approaches (d=2,3): hopeless

Theoretical challenge:

Construct reliable, comprehensive
non-perturbative approximation scheme

Static (Hartree-Fock-type)
mean-field theories
generally insufficient



WANTED
DEAD OR ALIVE

AND

Reliable
approximation scheme
for
correlated
models and materials

PROFESSORSHIP

REWARD \$10,000

Dynamical Mean-Field Theory (DMFT) of Correlated Electrons

What is a “mean-field theory (MFT)” ?

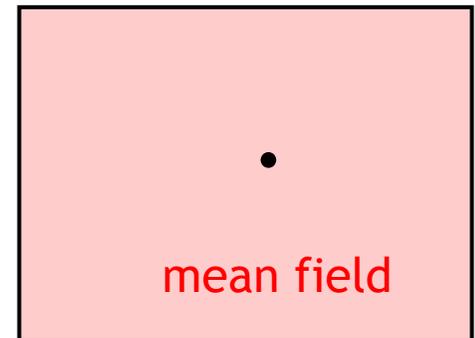
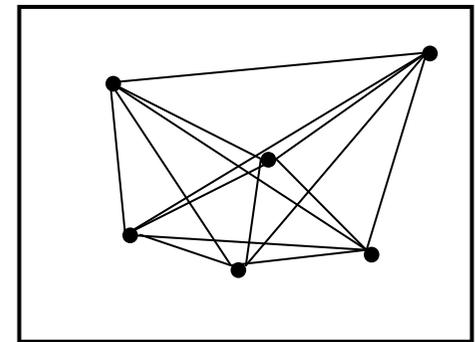
1) Construction by factorization

$$\langle AB \rangle \rightarrow \langle A \rangle \langle B \rangle$$

e.g., spins:

$$\langle S_i S_j \rangle \rightarrow \langle S_i \rangle \langle S_j \rangle$$

→ Weiss MFT



What is a “mean-field theory (MFT)” ?

2) Construction by exaggeration

For example:

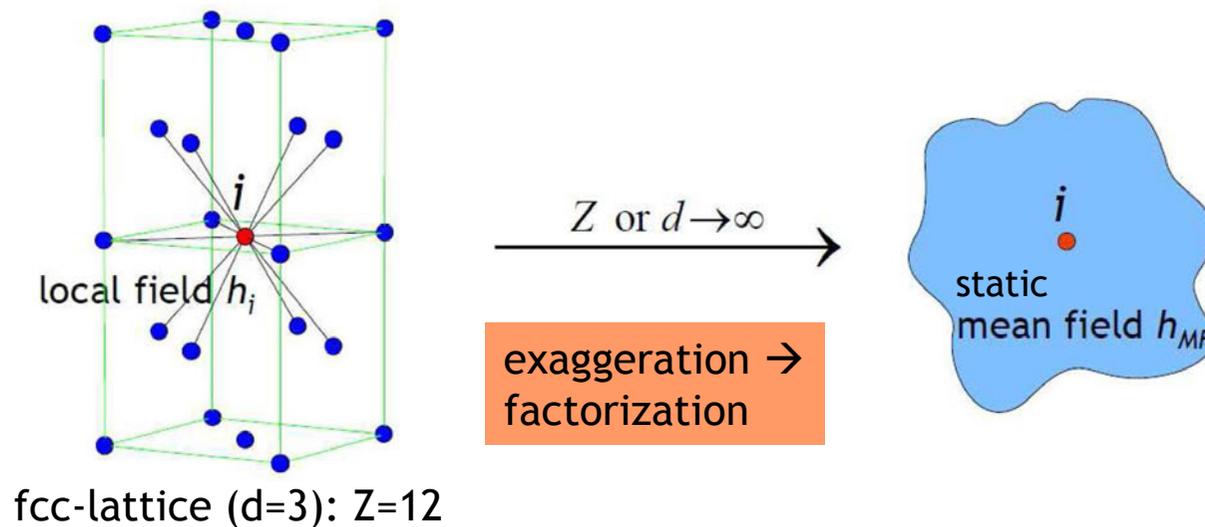
Spin S

Degeneracy N

Dimension d / coordination number Z

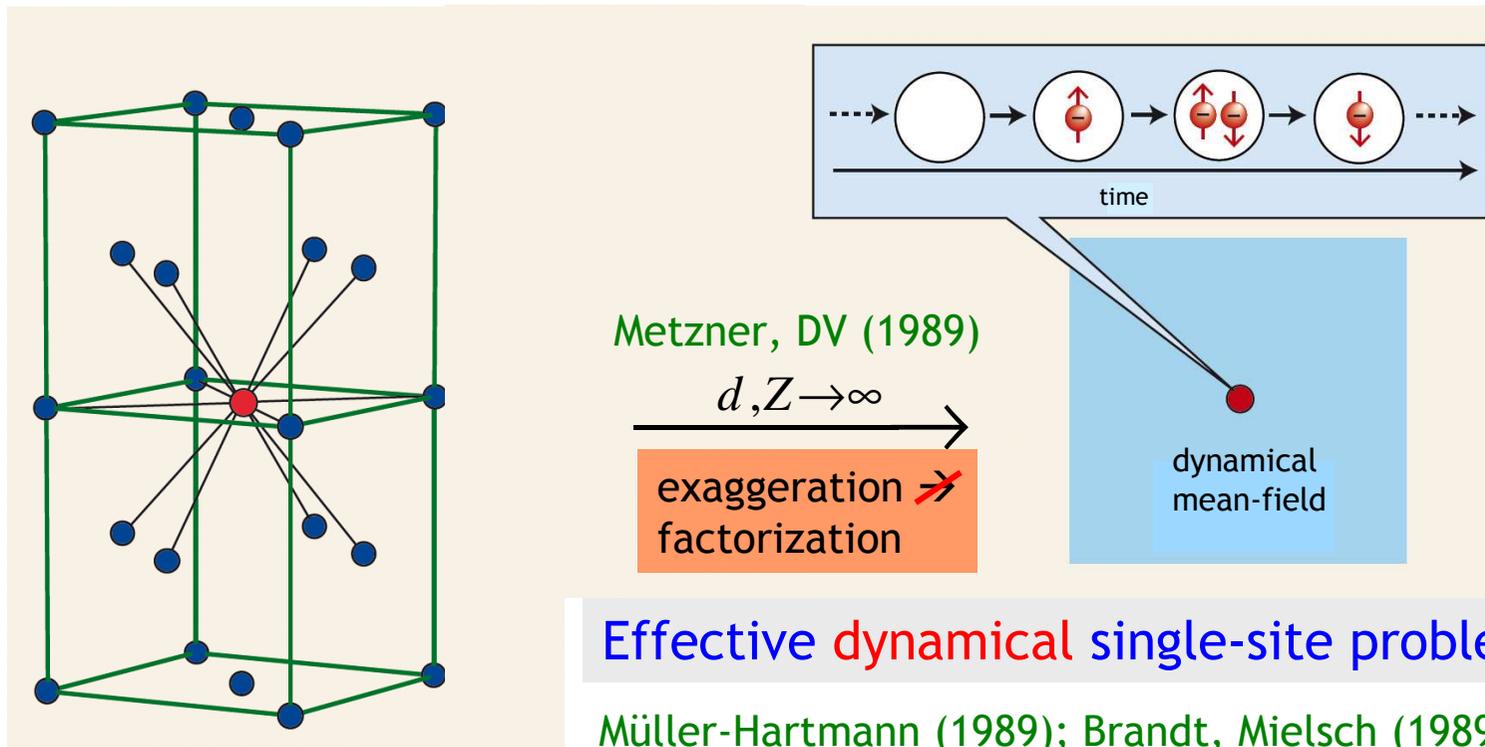
} $\rightarrow \infty$

Spin models:



Theory of correlated electrons

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad \text{Hubbard model}$$



Z=12

Effective dynamical single-site problem

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

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

Metzner, DV (1989)

$$\langle H_{kin} \rangle_0 = \underbrace{-t}_{\infty \frac{1}{\sqrt{Z}}} \sum_{i,\sigma} \underbrace{\sum_{j(NN i)}_{Z} \underbrace{\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_0}_{\infty \frac{1}{\sqrt{Z}}}$$

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

Amplitude for hopping $j \rightarrow NN i$

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

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

Metzner, DV (1989)

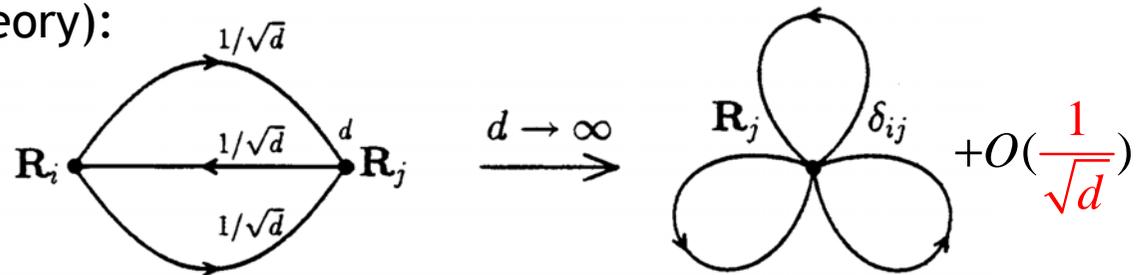
$$\langle H_{kin} \rangle_0 = \underbrace{-t}_{\infty \frac{1}{\sqrt{Z}}} \sum_{i,\sigma} \sum_{\substack{j(NN \ i) \\ Z}} \underbrace{\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_0}_{\infty \frac{1}{\sqrt{Z}}}$$

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

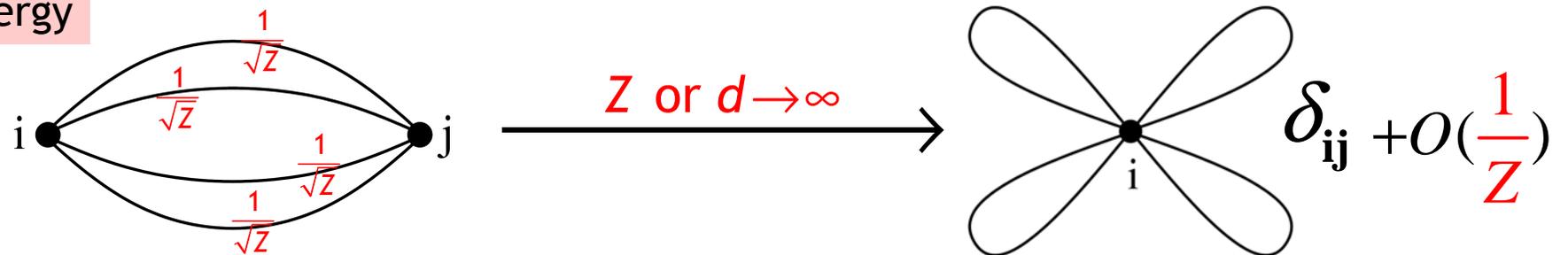
Z or $d \rightarrow \infty \rightarrow$ Collapse of irreducible diagrams in position space
 \rightarrow great simplifications

Examples (2. order pert. theory):

Self-energy

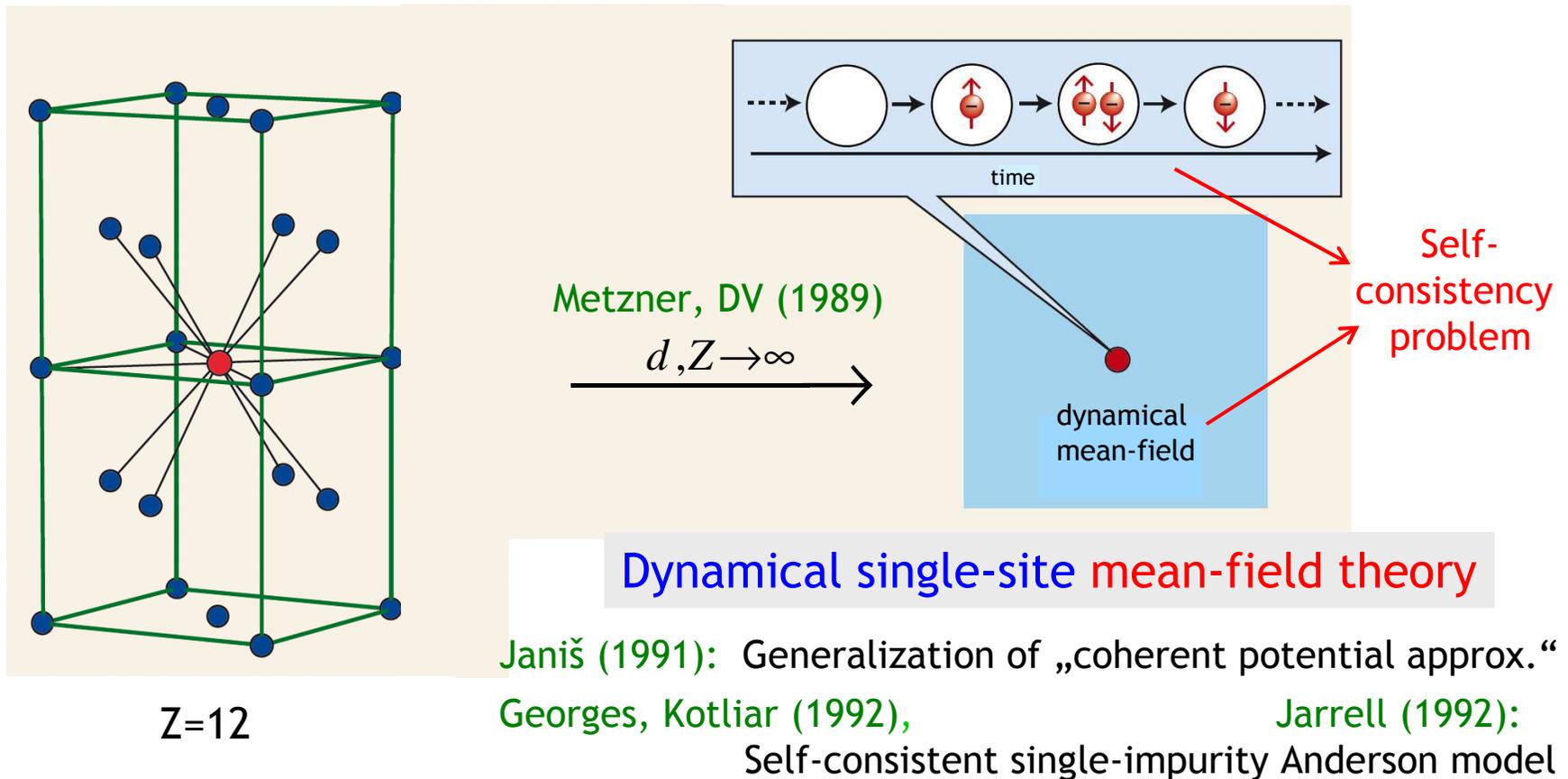


Energy



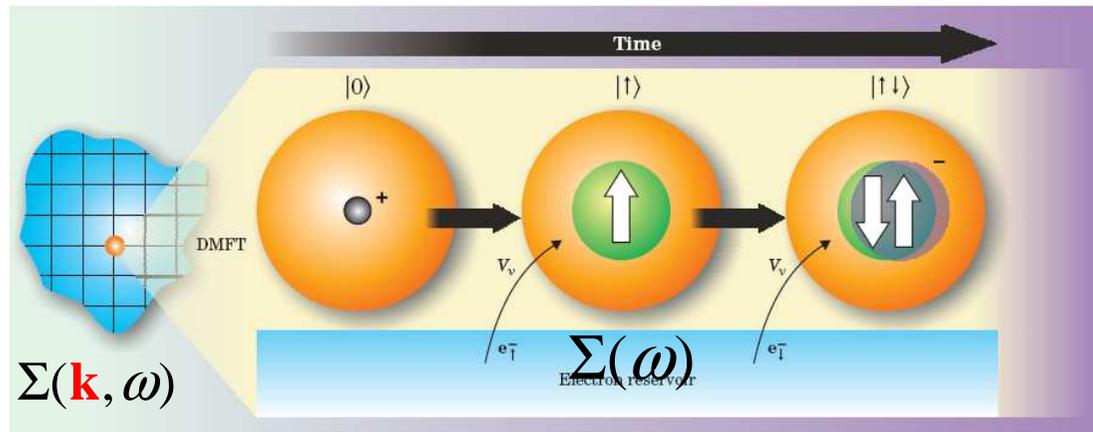
Theory of correlated electrons

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



Useful physical *interpretation*:

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

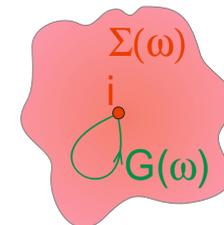


Kotliar, DV (2004)

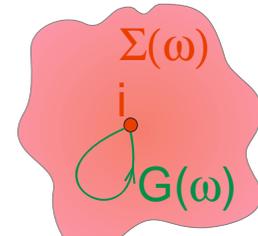
Proper **time** resolved treatment of **local** electronic interactions

“**Dynamical** Mean-Field Theory (DMFT)“

Local many-body problem with full dynamics



DMFT self-consistency equations



$\Sigma(\omega)$: “effective medium”

(i) Effective **single impurity** problem: “local propagator” $G_{\sigma n} = -\langle \psi_{\sigma n} \psi_{\sigma n}^* \rangle_A$.

$$G = -\frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \psi^*] \psi \psi^* e^{\underbrace{\psi^* [G^{-1} + \Sigma] \psi - U \psi^* \psi \psi^* \psi}_{\text{single-site ("impurity") action } A}}$$

(ii) **k-integrated Dyson equation** (“lattice Green function”: **lattice enters**)

$$G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \Sigma(\omega) - \varepsilon} = G^0(\omega - \Sigma(\omega))$$

→ free electrons in a dynamic potential $\Sigma(\omega)$

→ Lecture of M. Kollar

DMFT: Search for the “best” impurity solver

Hubbard I

IPT

NCA

QMC (Hirsch-Fye)

→ Lecture of N. Blümer

ED

Lanczos

→ Lecture of E. Koch

NRG

Recent:

PQMC

DDMRG

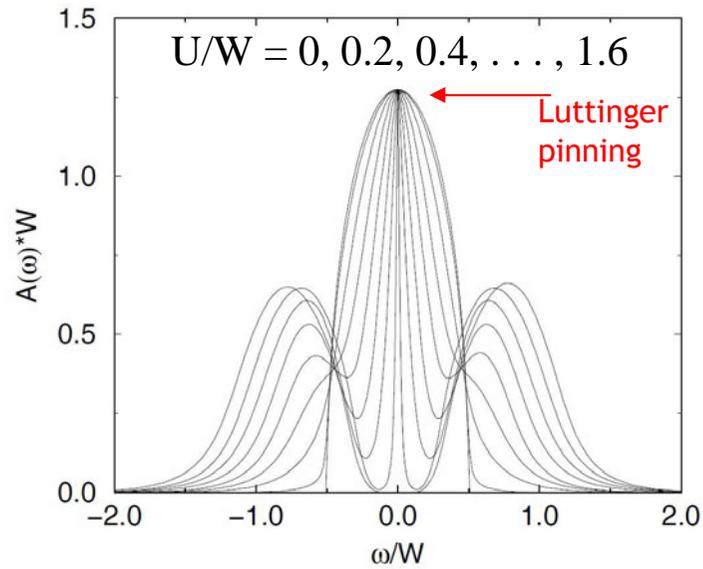
CT-QMC

→ Lecture of P. Werner

Application of DMFT:

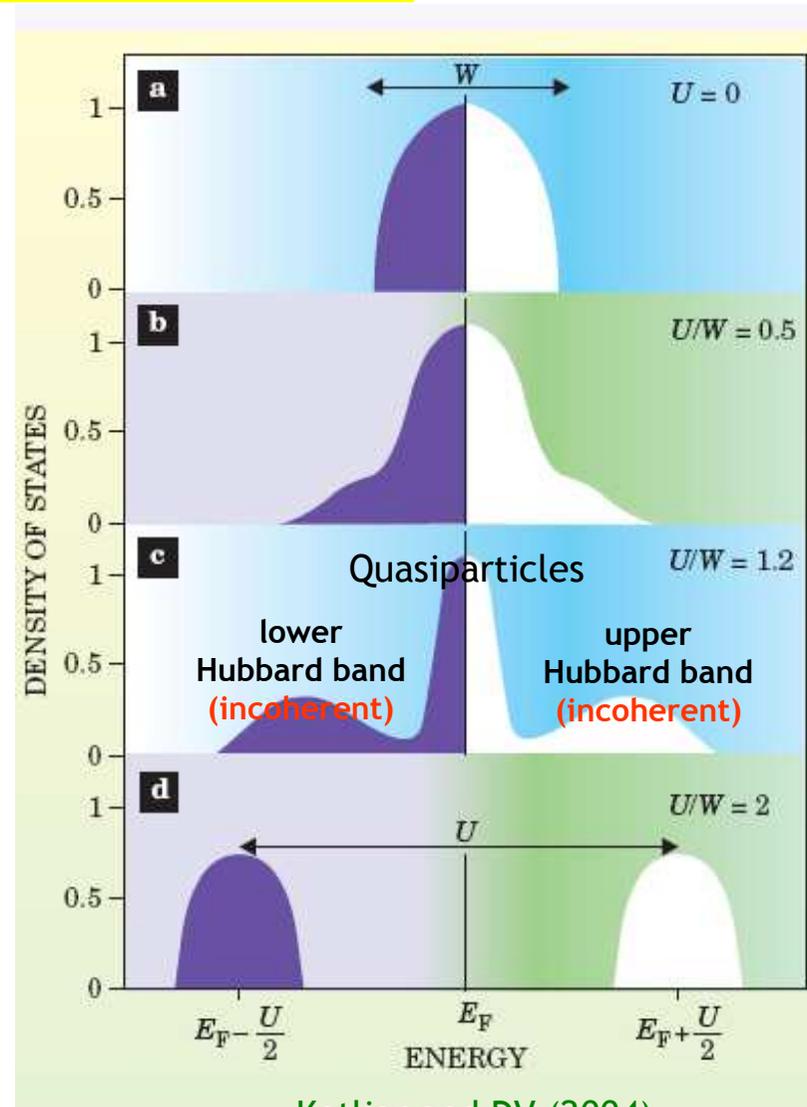
1. Mott-Hubbard metal-insulator transition

Mott-Hubbard metal-insulator transition



Bethe lattice, $T=0$

Bulla (1999)



Kotliar and DV (2004)

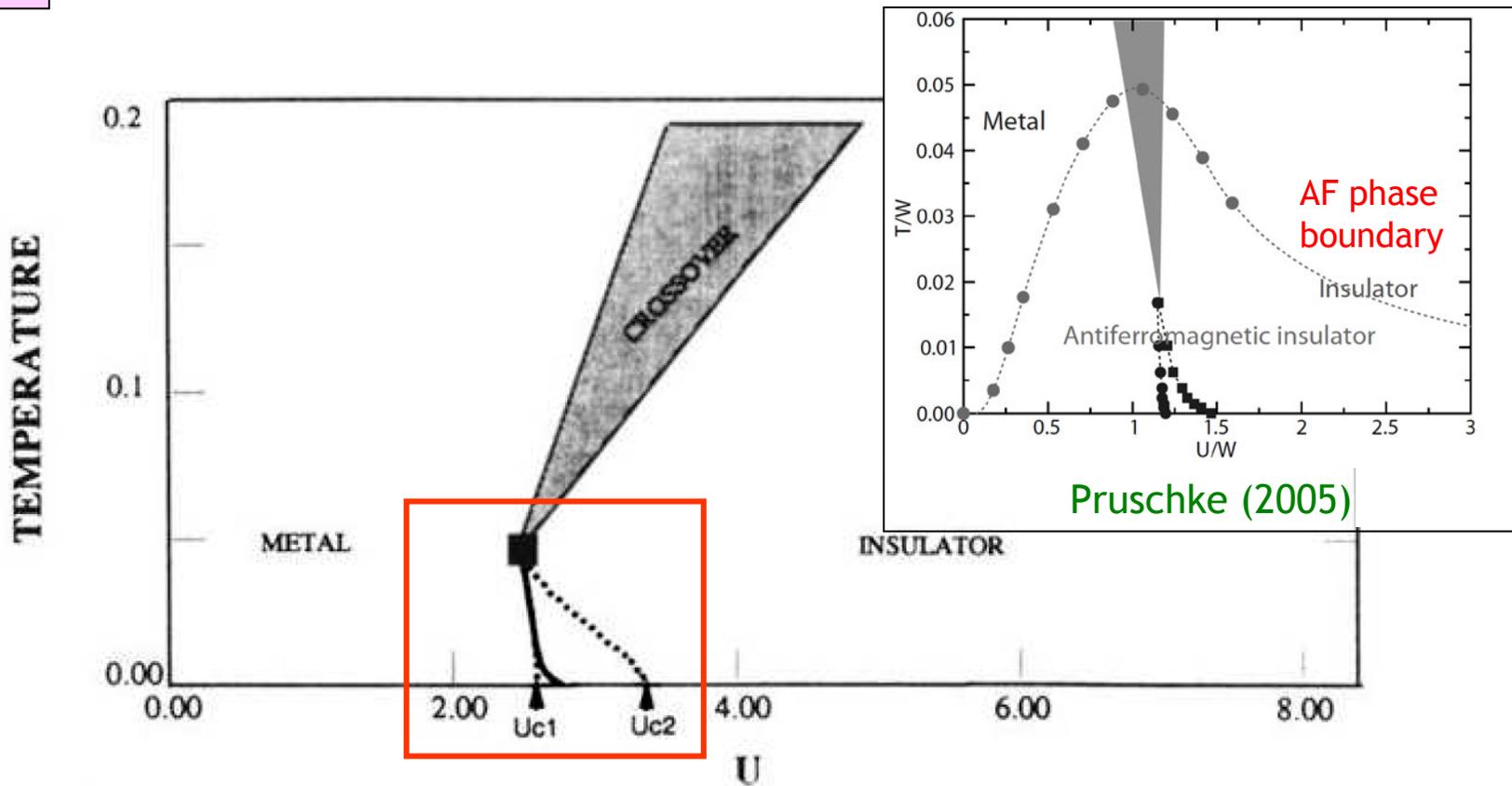
Correlations (II): lead to transfer of spectral weight

Experimentally detectable ?

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

1994

paramagnetic solution (“frustrated antiferromagnetism“)

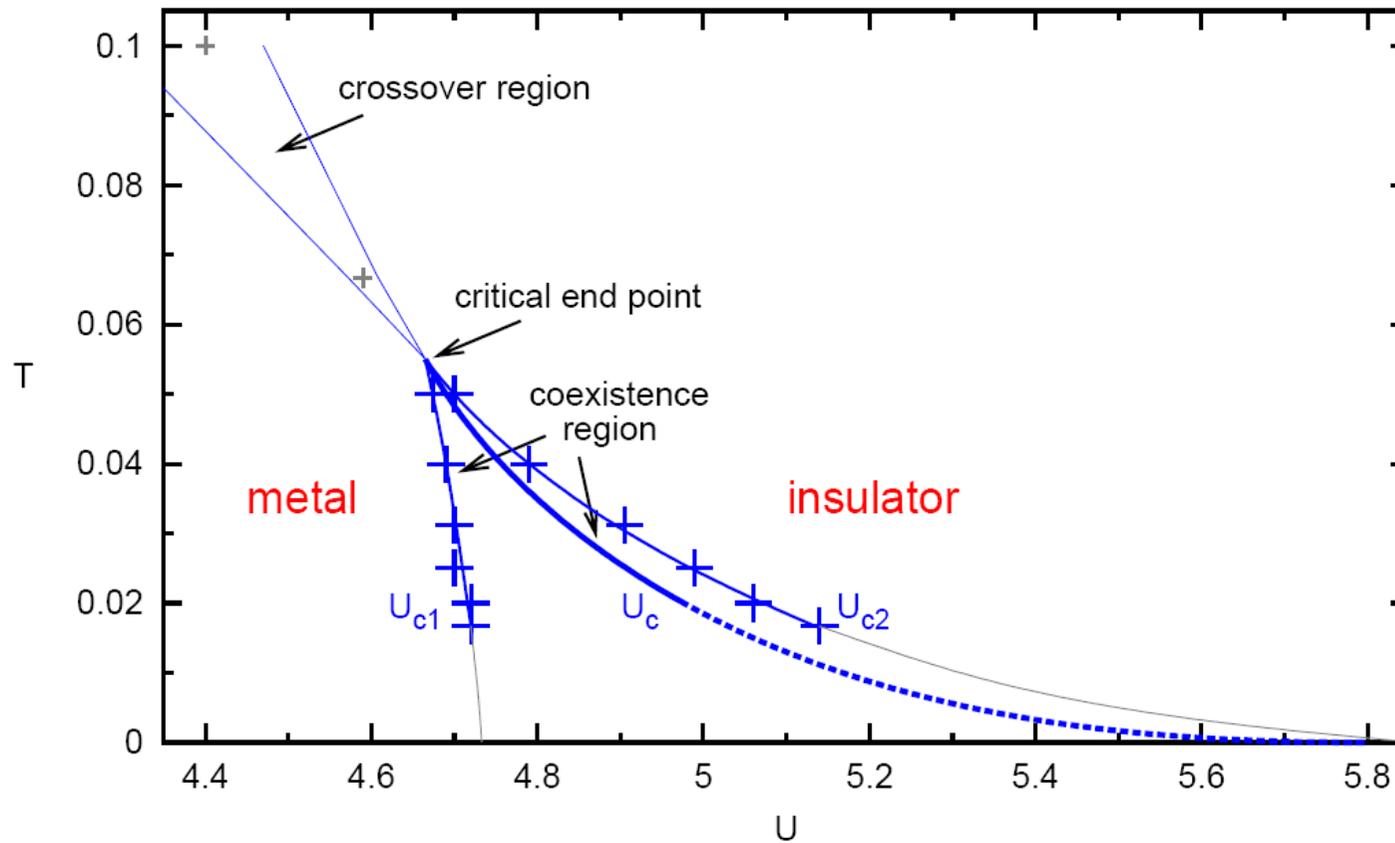


Iterated perturbation theory Rozenberg *et al.* (1994)

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

2002

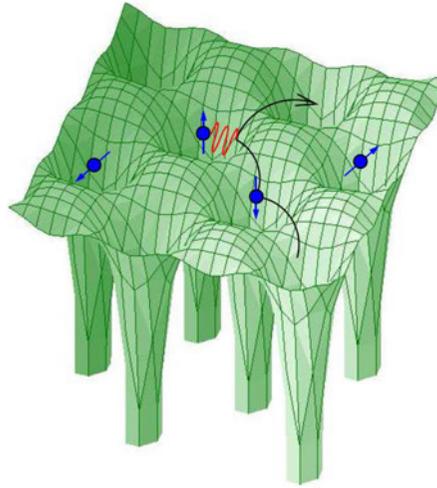
paramagnetic solution (“frustrated antiferromagnetism“)



Blümer (2002)

Application of DMFT:

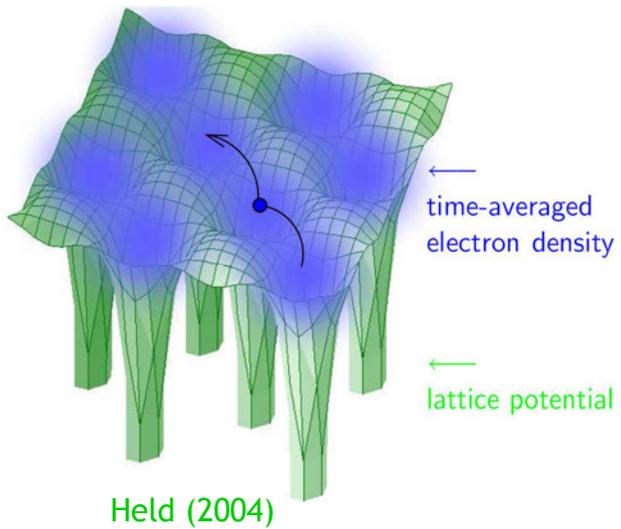
2. Electronically Correlated Materials

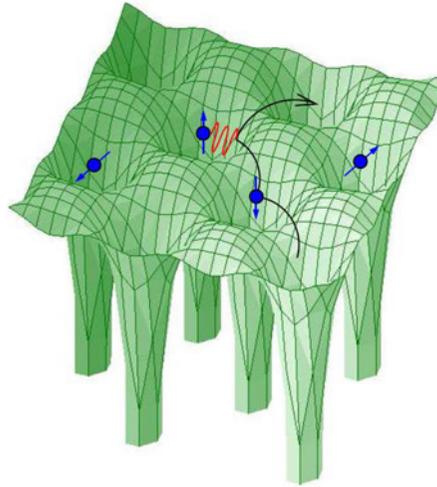


DFT/LDA

- + material specific: “ab initio”
- fails for strong correlations
- + fast code packages

→ Lecture of P. Blöchl



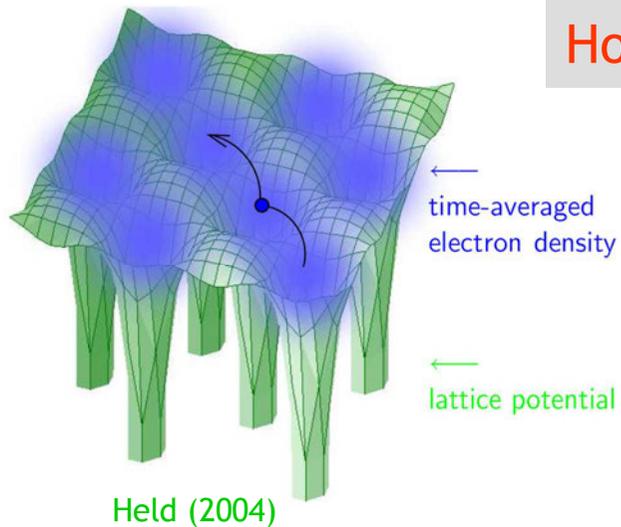


DFT/LDA

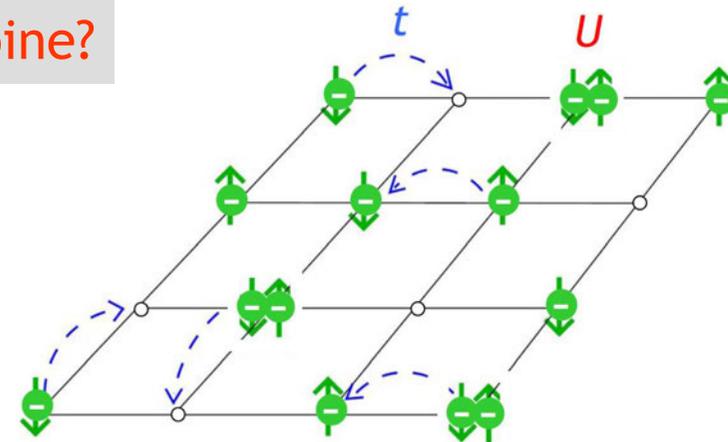
- + material specific: “ab initio”
- fails for strong correlations
- + fast code packages

Model Hamiltonians

- input parameters unknown
- + systematic many-body approach
- computationally expensive



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 of E. Pavarini

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

Combination with KKR (“KKR+DMFT“)

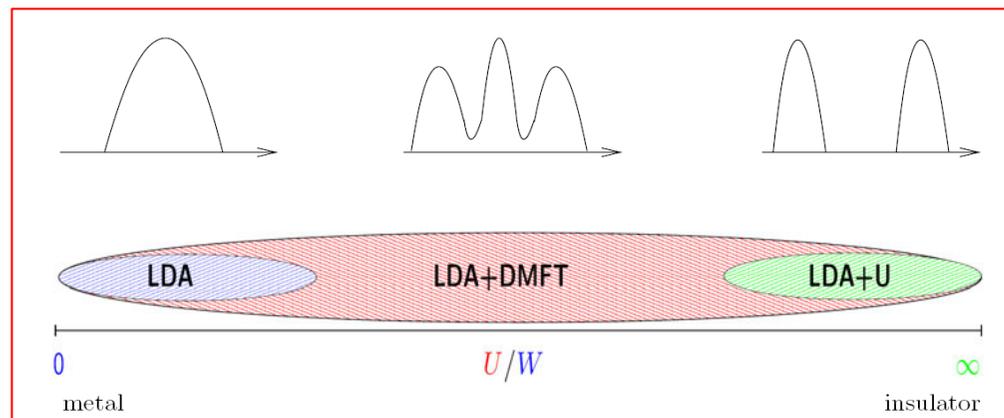
→ Lecture of H. Ebert

Computational scheme for correlated electron materials:

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

+

Local electronic correlations
(Many-body theory: DMFT)



Held *et al.* (Psi-k 2003)

LDA+DMFT (simplest version)

- 1) Calculate LDA band structure: $\epsilon_{lm'l'm'}(k) \rightarrow \hat{H}_{LDA}$
- 2) Supplement LDA by local Coulomb interaction (only for correlated bands)

$$\hat{\mathcal{H}} = \underbrace{\sum_{\mathbf{k}lm'l'm'\sigma} \epsilon_{lm'l'm'}(\mathbf{k}) \hat{c}_{\mathbf{k}lm\sigma}^\dagger \hat{c}_{\mathbf{k}l'm'\sigma}}_{\text{LDA}}$$

$$+ \underbrace{\sum_{\substack{i=i_d, m\sigma, m'\sigma' \\ l=l_d}} \sum' \frac{U_{mm'}^{\sigma\sigma'}}{2} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}}_{\text{local Coulomb interaction}}$$

local Coulomb interaction

$$- \underbrace{\sum_{\substack{i=i_d, m\sigma, m'\sigma' \\ l=l_d}} \sum' J_{mm'} \hat{c}_{ilm\sigma}^\dagger \hat{c}_{ilm'\sigma'}^\dagger \hat{c}_{ilm'\sigma} \hat{c}_{ilm\sigma'}}_{\text{Hund's rule coupling}}$$

Hund's rule coupling

→ Lecture of F. Aryasetiawan

LDA+DMFT (simplest version)

- 1) Calculate LDA band structure: $\epsilon_{lm'l'm'}(k) \rightarrow \hat{H}_{LDA}$
- 2) Supplement LDA by local Coulomb interaction (only for correlated bands)

$$\hat{\mathcal{H}} = \underbrace{\sum_{\mathbf{k}lm'l'm'\sigma} \epsilon_{lm'l'm'}(\mathbf{k}) \hat{c}_{klm\sigma}^\dagger \hat{c}_{kl'm'\sigma}}_{\text{LDA}} - \underbrace{\sum_{\substack{i=i_d, m\sigma \\ l=l_d}} \Delta\epsilon_d \hat{n}_{ilm\sigma}}_{\text{double counting correction}}$$

$$+ \underbrace{\sum_{\substack{i=i_d, m\sigma, m'\sigma' \\ l=l_d}} \sum' \frac{U_{mm'}^{\sigma\sigma'}}{2} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}}_{\text{local Coulomb interaction}} - \underbrace{\sum_{\substack{i=i_d, m\sigma, m'\sigma' \\ l=l_d}} \sum' J_{mm'} \hat{c}_{ilm\sigma}^\dagger \hat{c}_{ilm'\sigma'}^\dagger \hat{c}_{ilm'\sigma} \hat{c}_{ilm\sigma'}}_{\text{Hund's rule coupling}}$$

→ Lecture of F. Aryasetiawan

Contact with experiment, e.g., via

Spectral function (“interacting DOS”) in DMFT

k-integrated spectral function
→ PES

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

k-resolved spectral function
→ ARPES

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

Matrices in orbital space

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

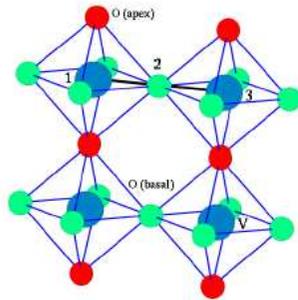
Application of LDA+DMFT

a) (Sr,Ca)VO₃: 3d¹ system

Electronic structure

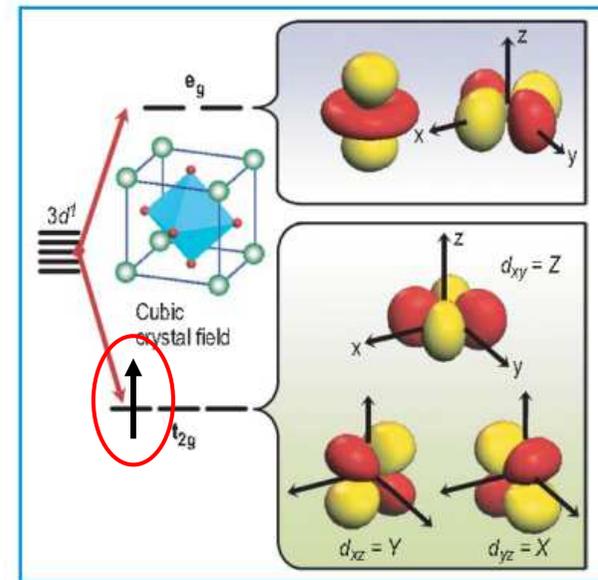
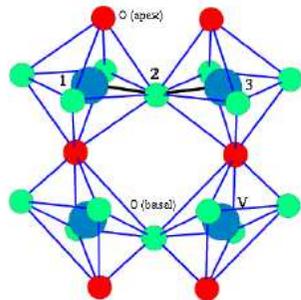
Crystal structure

SrVO_3 : $\angle V-O-V = 180^\circ$

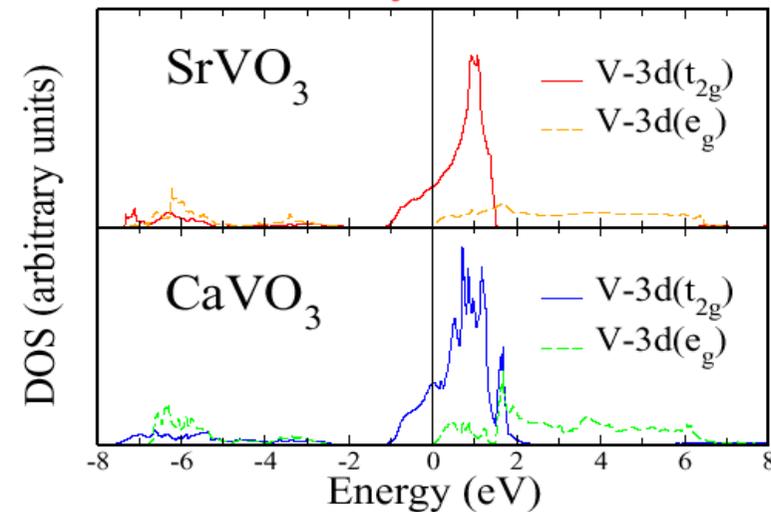


orthorhombic distortion

CaVO_3 : $\angle V-O-V \approx 162^\circ$



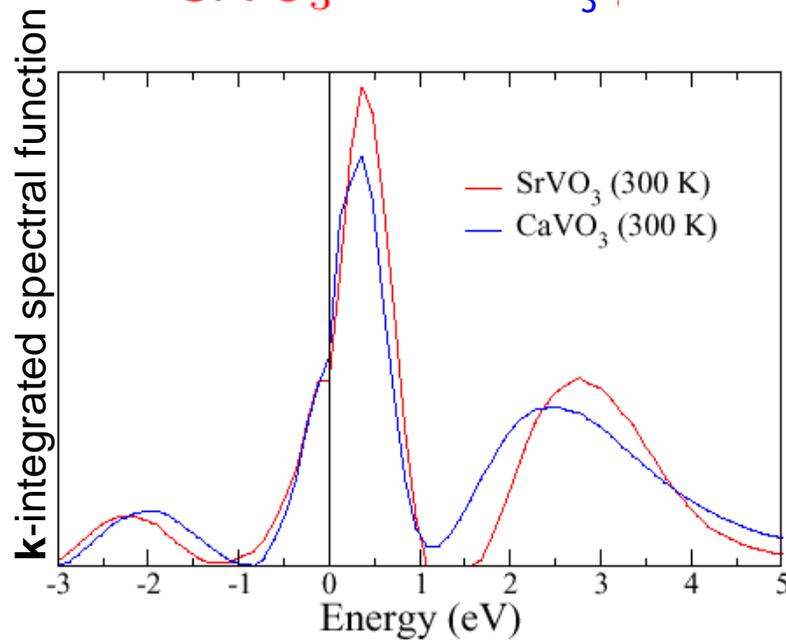
LDA density of states



No correlation effects/spectral transfer

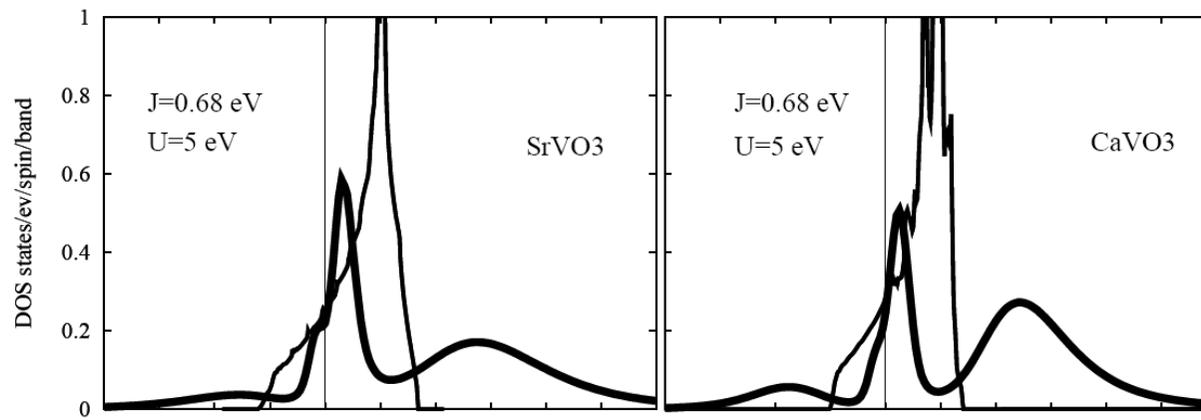
LDA+DMFT results

SrVO₃ and CaVO₃



Constrained LDA:
U=5.55 eV, J=1.0 eV

Sekiyama et al., (2004)



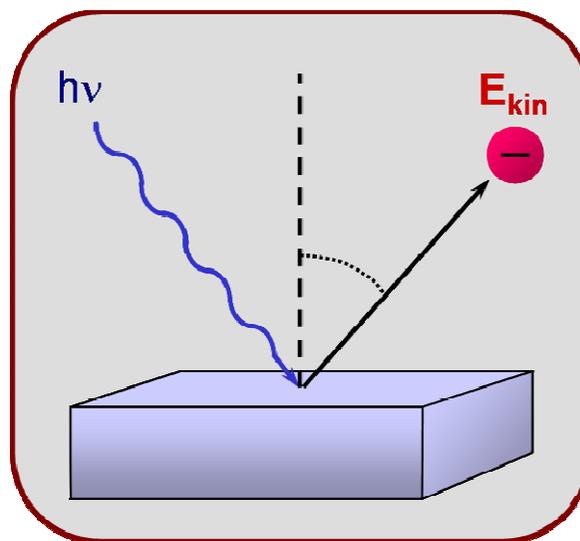
Pavarini et al. (2004)

How to measure ?

Excursion: Spectroscopy

→ Lecture of H. Tjeng

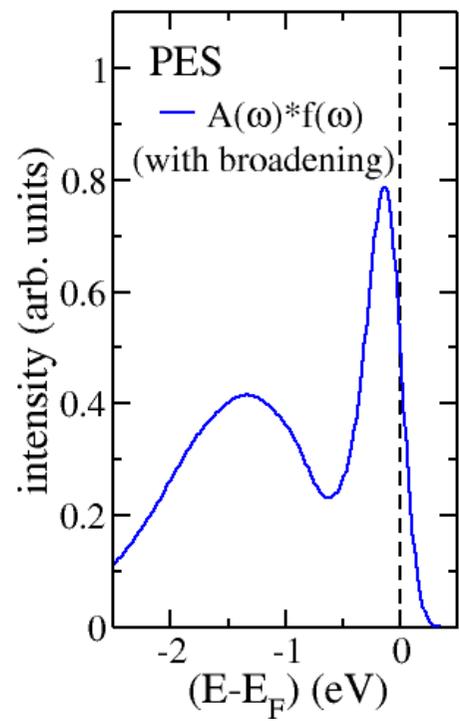
Photoemission Spectroscopy (PES)



Angular Resolved PES = ARPES

Measures **occupied** states of electronic spectral function

PES



Occupied states
(experiment)

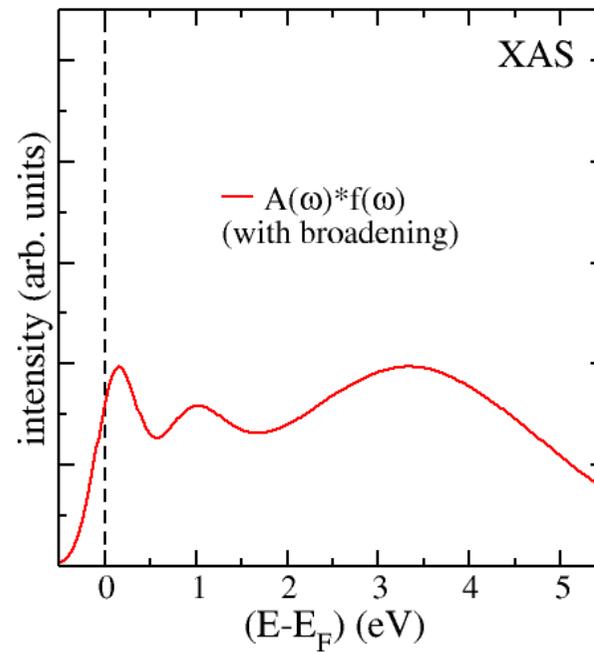
Inverse Photoemission Spectroscopy (IPES)

Measures **unoccupied** states of electronic spectral function

Information also available by:

X-ray absorption spectroscopy (XAS)

IPES/XAS

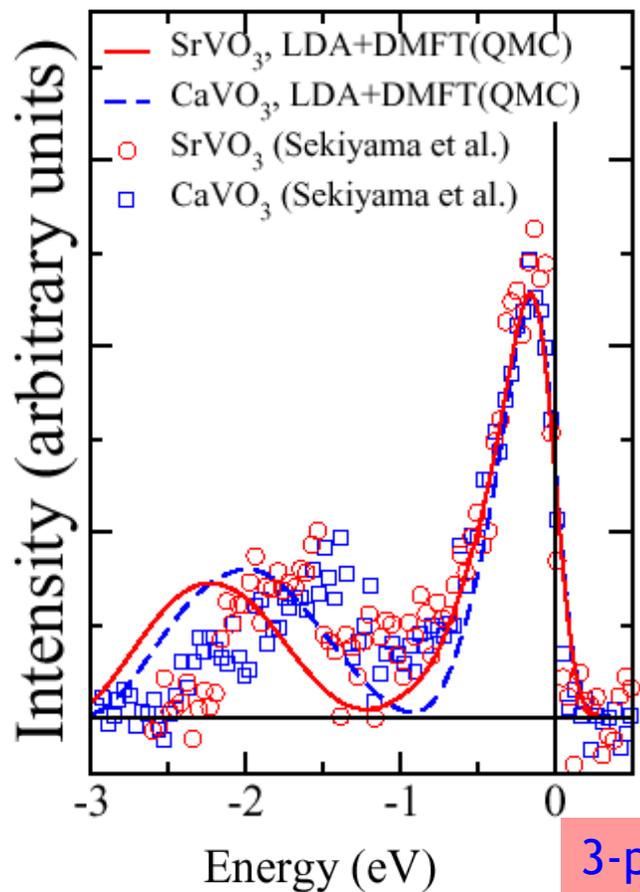


Unoccupied states
(measured)

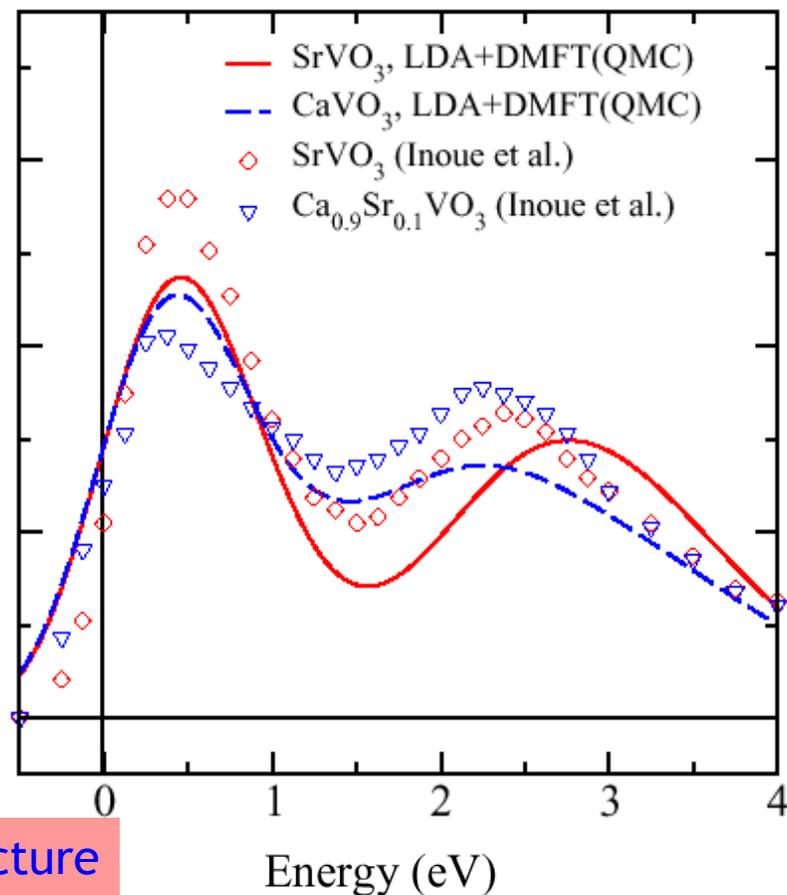
Comparison with experiment

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

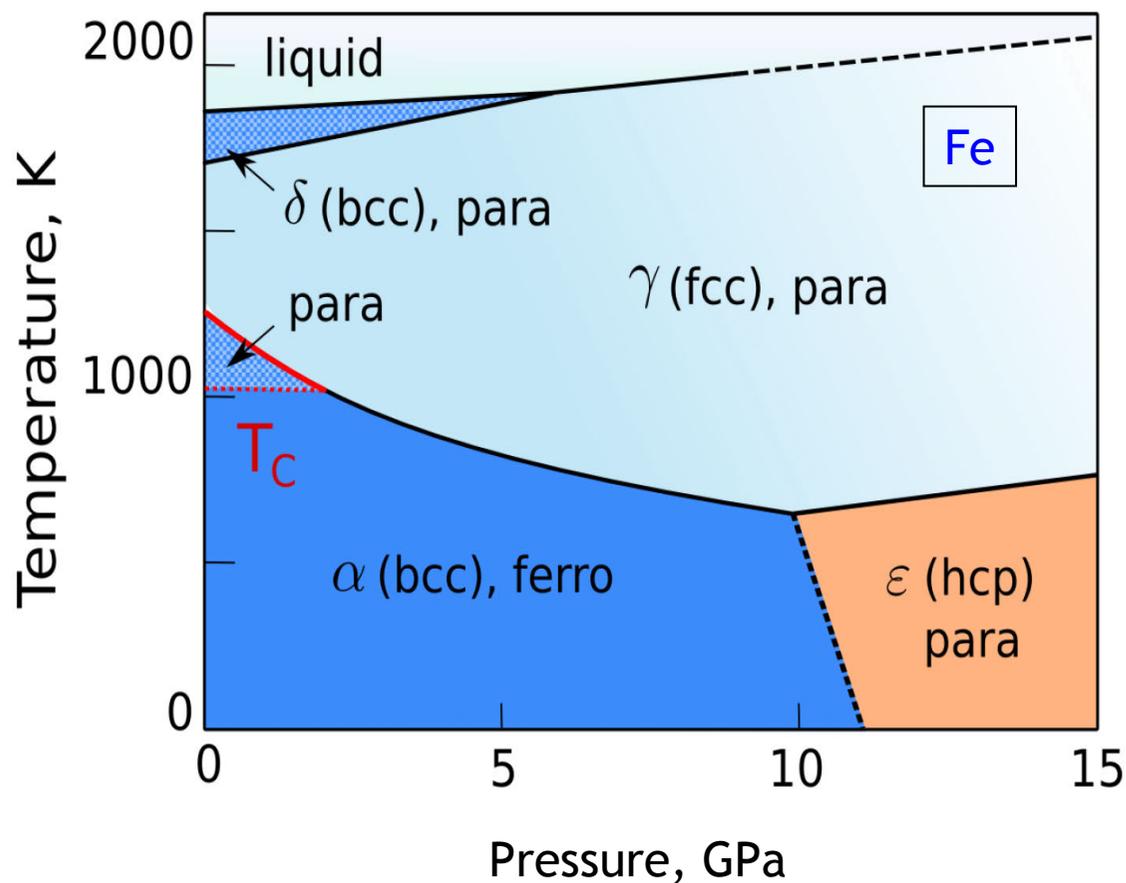


3-peak structure
detected



New developments in LDA+DMFT: Electronic correlations & structural transformations

Electron correlations can induce structural transformations



Leonov *et al.* (2011)

Beyond DMFT

Cluster Extensions

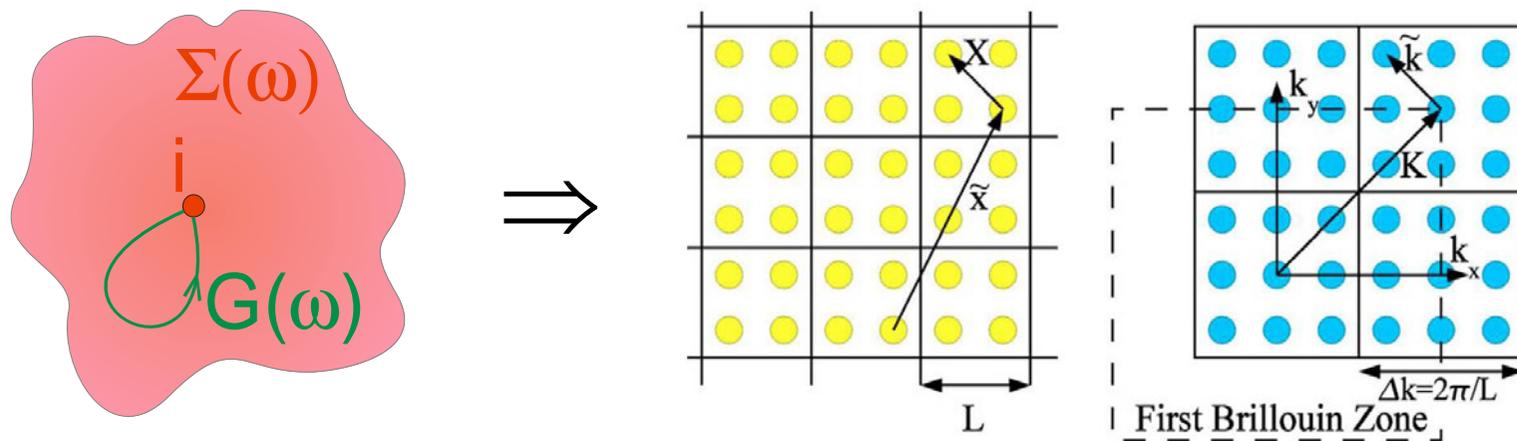
- Dynamical cluster approx. (DCA)
- Cluster DMFT (CDMFT)
- Self-energy functional theory

→ Lecture of A. Lichtenstein

Hettler *et al.* (1998, 2000)

Kotliar *et al.* (2001)

Potthoff (2003)



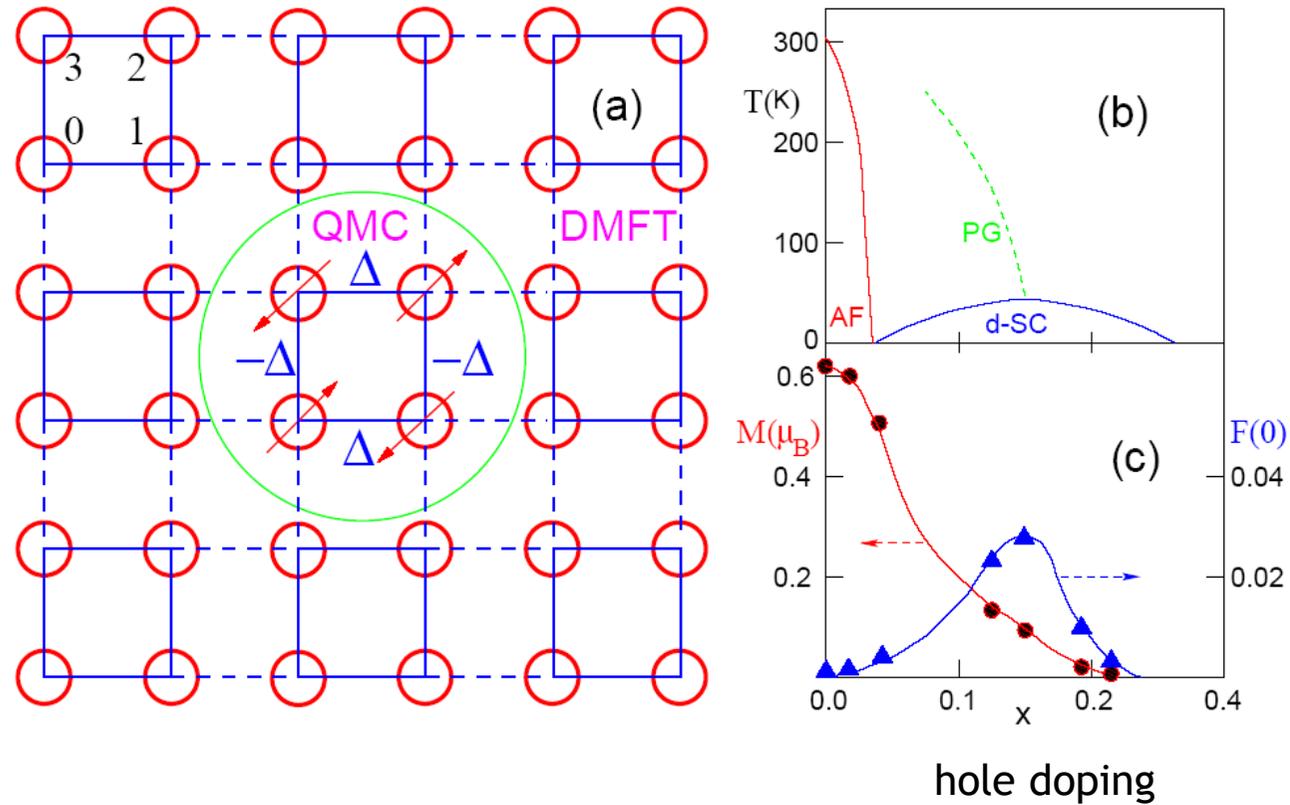
Dynamical vertex approximation (D Γ A)

→ Lecture of K. Held

Local + non-local self-energy diagrams from local irreducible vertex

Toschi, Katanin, Held (2006)

Antiferromagnetic d -wave 2×2 periodically repeated cluster

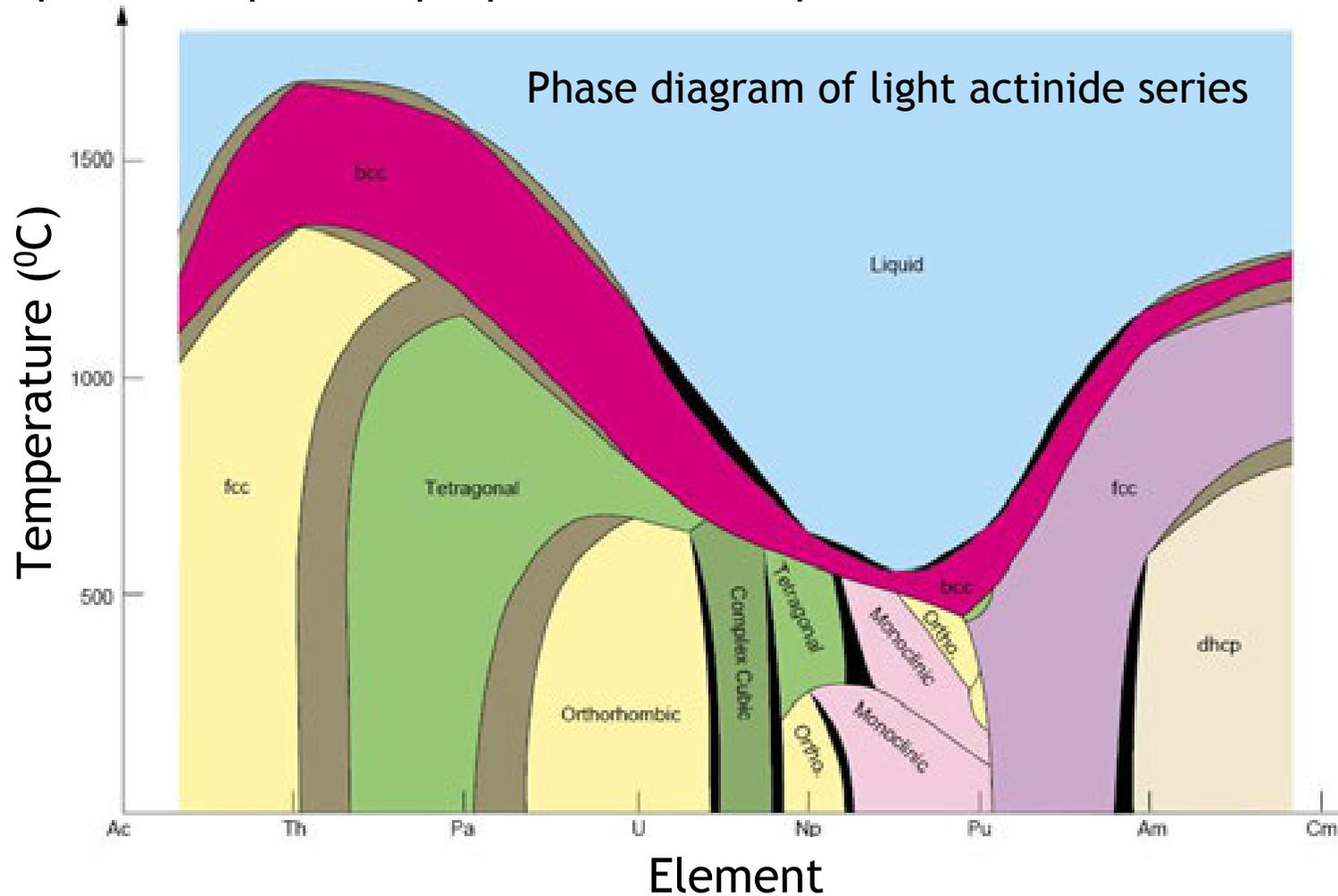


Lichtenstein, Katsnelson (2000)

Perspectives of the LDA+DMFT approach

Perspectives of the LDA+DMFT approach

Explain and predict properties of complex correlated materials:

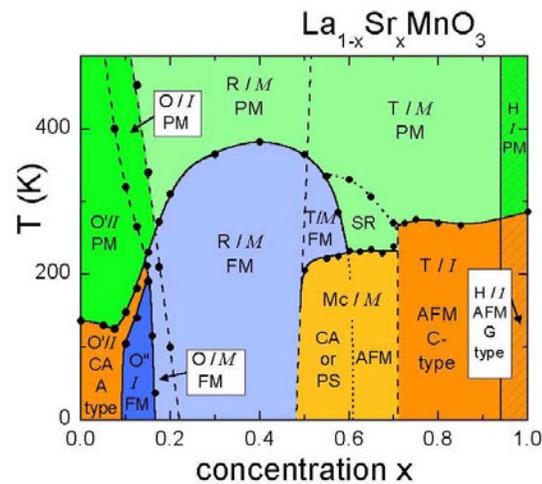


Phase diagram connecting individual binary alloy diagrams
Black: two-phase regions; Brown : details unknown

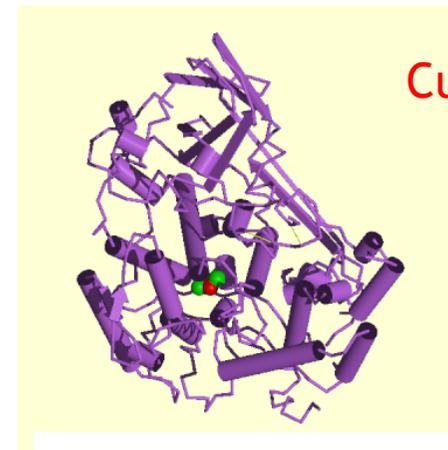
Boring and Smith (2000)

Perspectives of the LDA+DMFT approach

Explain and predict properties of complex correlated materials:



Phase diagram of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$
Hemberger *et al.* (2002)

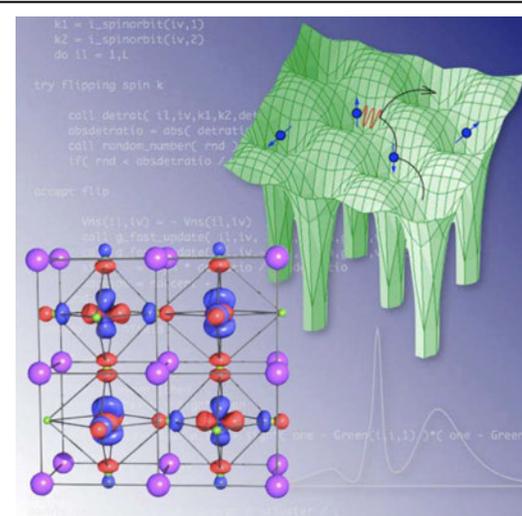


1, 2, ... multi-electron
transfer in
metalloprotein
complexes
→ Photosynthesis

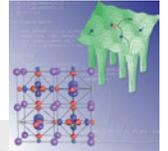
Goal: Dynamical mean-field approach with predictive power for strongly correlated materials

DFG Research Unit FOR 1346

Operates since July 2010



Projects of the DFG Research Unit FOR 1346

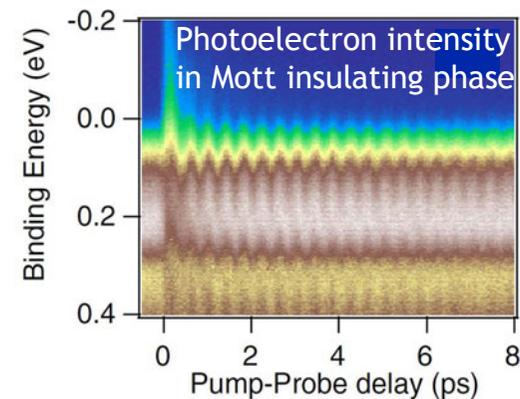
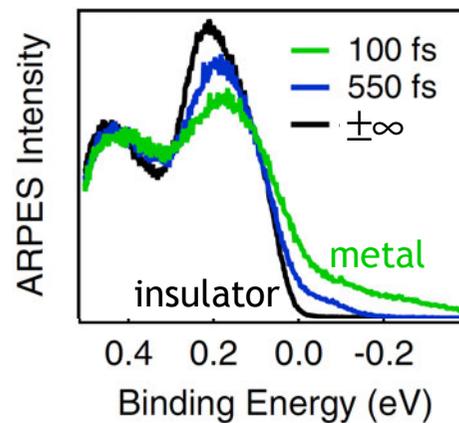
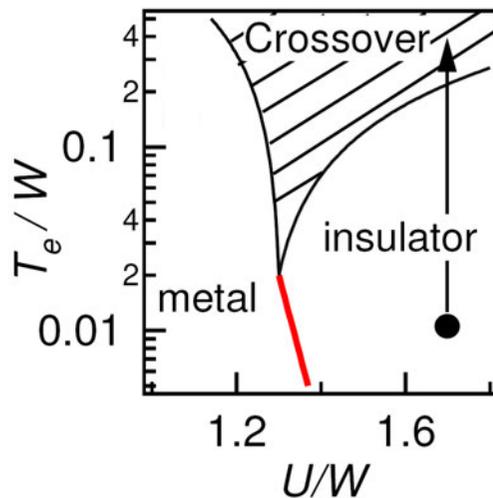


- P1** Realistic many-body approach to materials with strong nonlocal correlations
(Lechermann, Potthoff, Lichtenstein)
- P2** LDA+DMFT approach to multi-band correlation phenomena:
Susceptibilities and structural relaxation
(Kollar, Kuneš, Vollhardt)
- P3** A self-consistent, relativistic implementation of the LSDA+DMFT method
(Ebert, Minár)
- P4** Massively parallel simulations of strong electronic correlations:
Realistic Coulomb vertex and multiplet effects
(Pavarini, Koch, Blügel)
- P5** Doping of prototypical Mott insulators:
Correlations, electronic structure, and electron-lattice effects
(Claessen, Valentí, Jeschke)
- P6** Electronic structure of exemplary correlated materials
(Haverkort, Khomskii, Tjeng)
- P7** Merging GW and dynamical mean-field theory
(Held, Toschi, Kresse) [Austria]
- P8** Quantum Monte Carlo impurity solvers for multi-orbital problems
and frequency dependent interactions
(Assaad, Blümer, Werner [Switzerland])
- P9** Energies and forces for materials with strong correlations
(Blöchl, Pruschke)

Application of DMFT:
3. Recent Developments

a. Correlated electrons in non-equilibrium

Real-time evolution of correlation phenomena, e.g.,
time-resolved photoemission spectroscopy



Perfetti *et al.* (2006)

Required: Theory of non-equilibrium beyond
linear response in correlated bulk materials

a. Correlated electrons in non-equilibrium

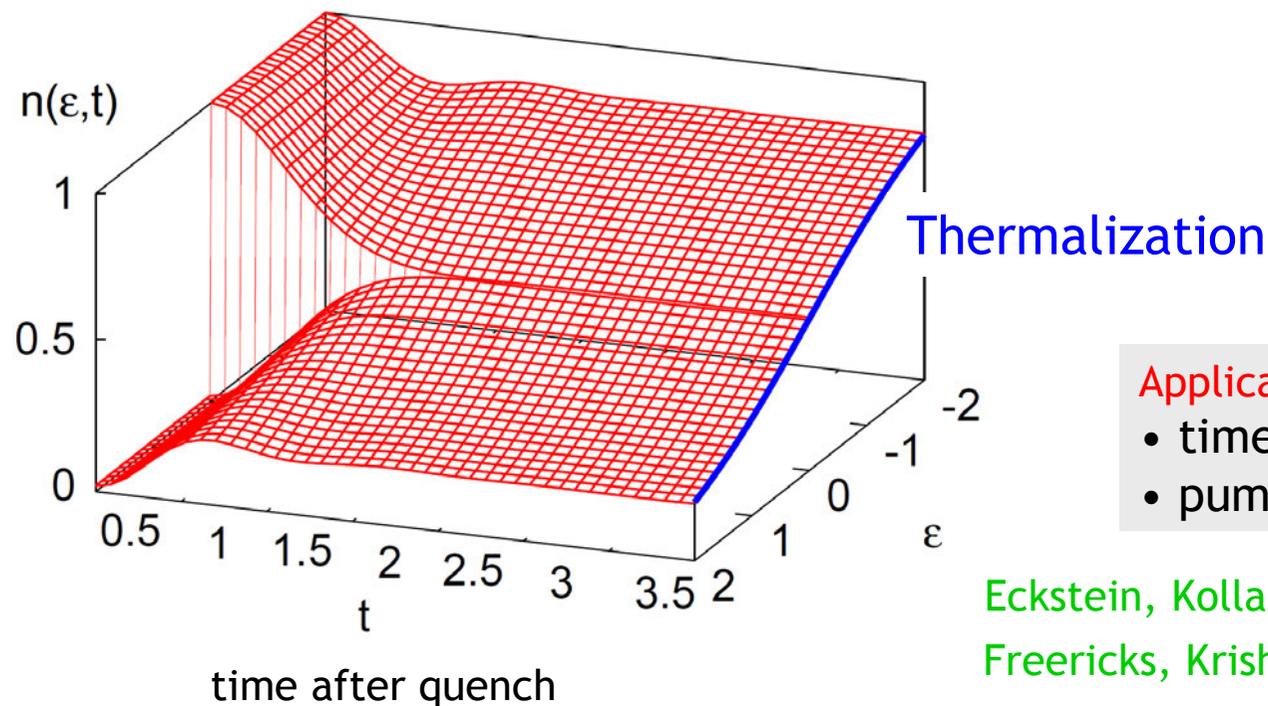
Non-equilibrium DMFT

Freericks, Turkowski (2006)

Quench in Hubbard model from $U=0$ to $U>0$

Eckstein, Kollar, Werner (2009)

Momentum distribution ($U=3.3$)



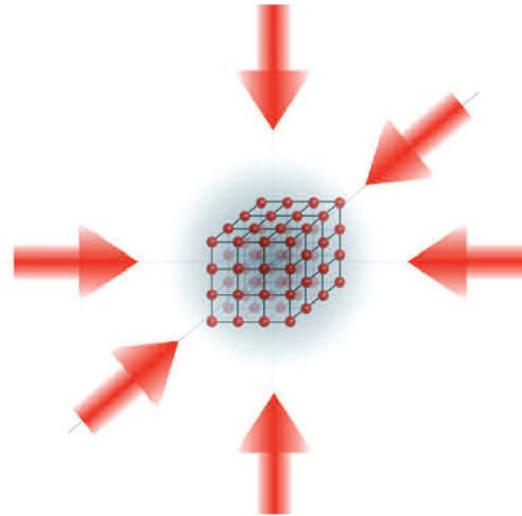
Application, e.g.

- time resolved PES
- pump-probe experiments

Eckstein, Kollar (2008)

Freericks, Krishnamurthy, Pruschke (2008)

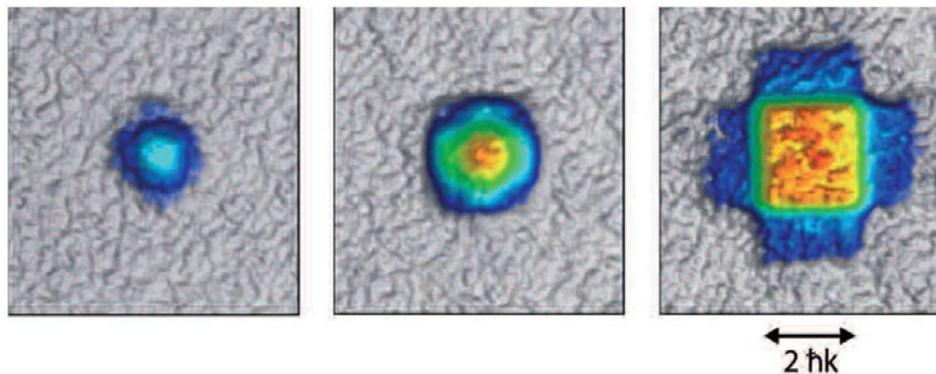
b. Correlated cold atoms in optical lattices



Greiner *et al.* (2002)

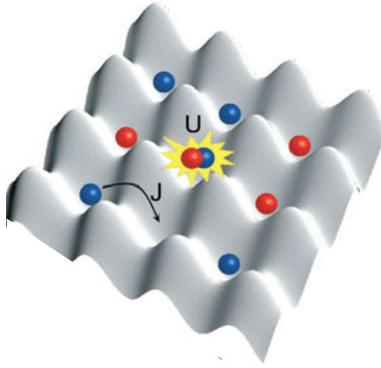
Bosonic/fermionic atoms in optical lattices: Exp. realization of models

High degree of tunability: “quantum simulator”



Observation of Fermi surface (^{40}K atoms) Köhl, Esslinger (2006)

b. Correlated cold atoms in optical lattices



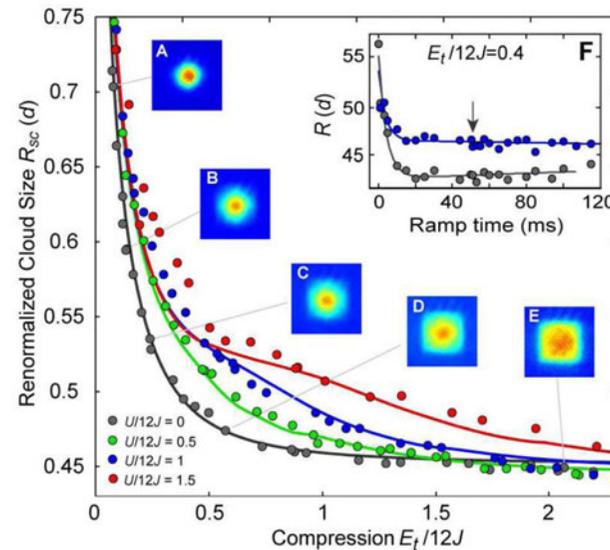
Hubbard model with ultracold atoms Jaksch *et al.*, (1998)

Atomic total angular momentum $L^{\text{tot}} = F \rightarrow N=2F+1$ hyperfine states

\rightarrow SU(N) Hubbard models

Honerkamp and Hofstetter (2004)

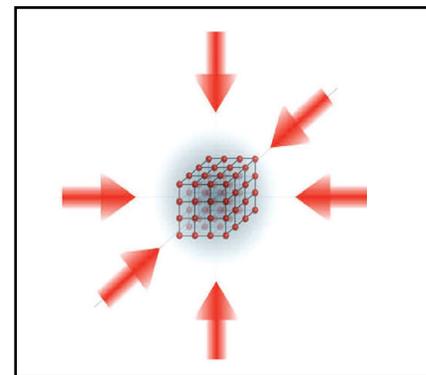
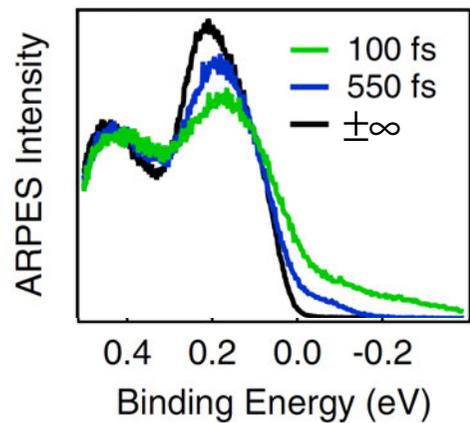
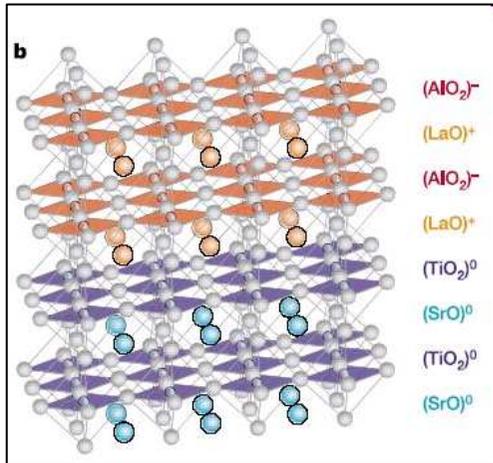
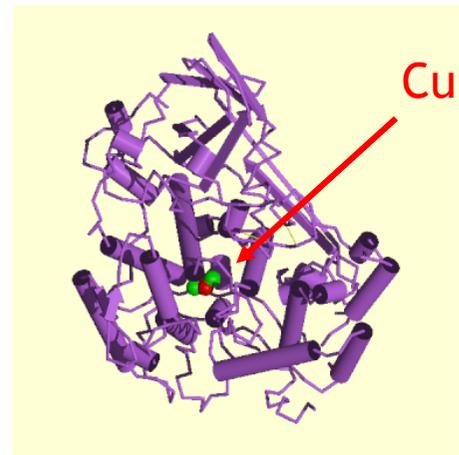
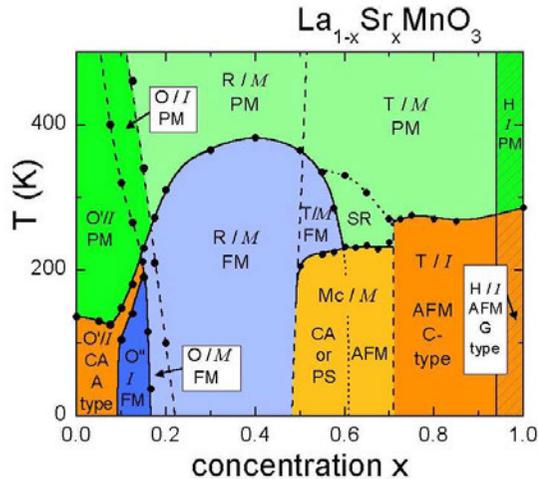
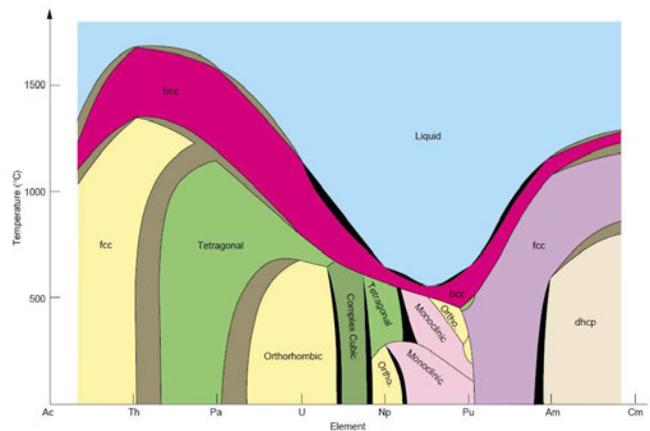
^{40}K atoms



DMFT results
experimentally confirmed

Metallic and Insulating Phases of Repulsively Interacting Fermions in a 3D Optical Lattice

Schneider *et al.*, (2008)



Wide field of applications for DMFT based techniques