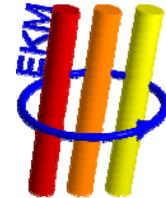




Center for Electronic Correlations and Magnetism  
University of Augsburg



# Surprising effects of the interaction between electrons in solids

Dieter Vollhardt



Inauguration Symposium of the Wolfgang Pauli Centre  
DESY Hamburg; April 17, 2013



Supported by **DFG**

TRR 80



FOR 1346



## Outline:

- “Physics of dirt” (Pauli)
- Peculiarities of quantum many-particle systems
- Electronic correlations in solids
- Dynamical Mean-Field Theory: Models vs. materials
- Developments & Perspectives

# Solids

Example: **Magnetite** ( $\text{Fe}_3\text{O}_4$ )

Macroscopic view:



Microscopic view:  $O(10^{23})$  interacting electrons + ions

→ quantum many-particle problem

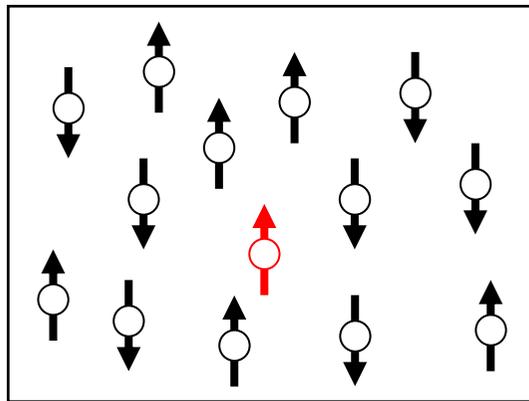


$\text{Fe}_3\text{O}_4$

- “Die Festkörperphysik ist eine Schmutzphysik” (Pauli)
- “One shouldn’t wallow in dirt” (Pauli to Peierls)

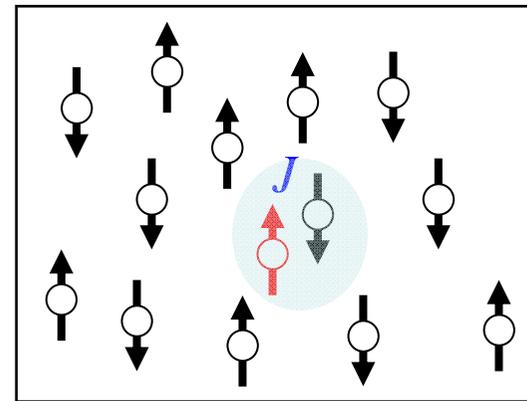
... but “dirt physics” can be fundamental and universal

**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”

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

Prototypical interaction problem with “running coupling constant”  $J(\Lambda)$   
→ QED, QCD

# Peculiarities of Interacting Many-Particle Systems

# Interacting many-particle systems

Elementary (“bare”) particles + fundamental interactions

↓ # particles  $N \rightarrow \infty$

effective (“quasi”) particles + effective interactions

## Non-interacting electrons

$$\text{Spin} = \frac{1}{2}\hbar \quad \text{Fermion}$$

$$N \rightarrow \infty$$



Pauli exclusion principle  
(Hamburg, 1925)

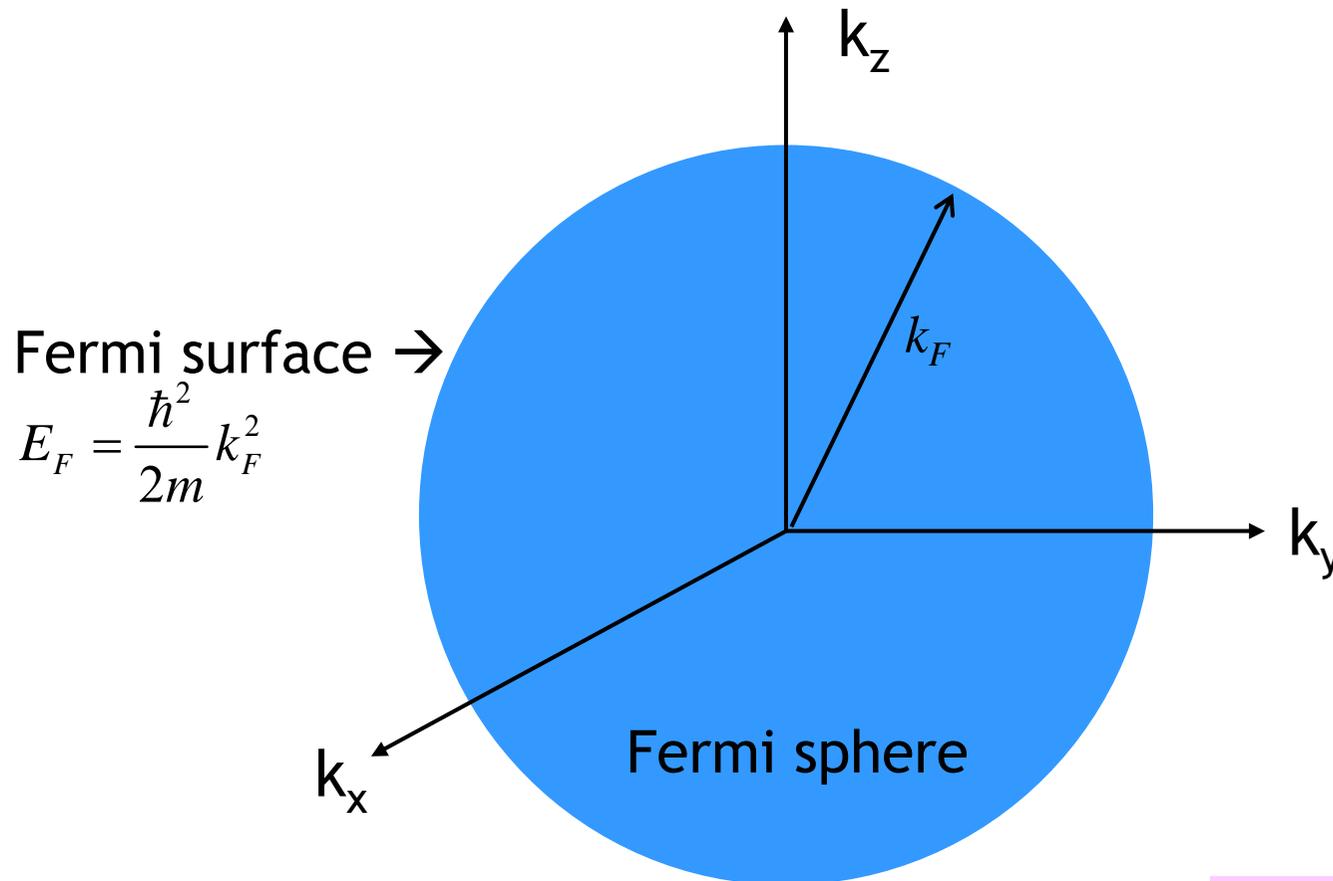
Fermi-Dirac statistics



Ground state:

Fermi body/surface

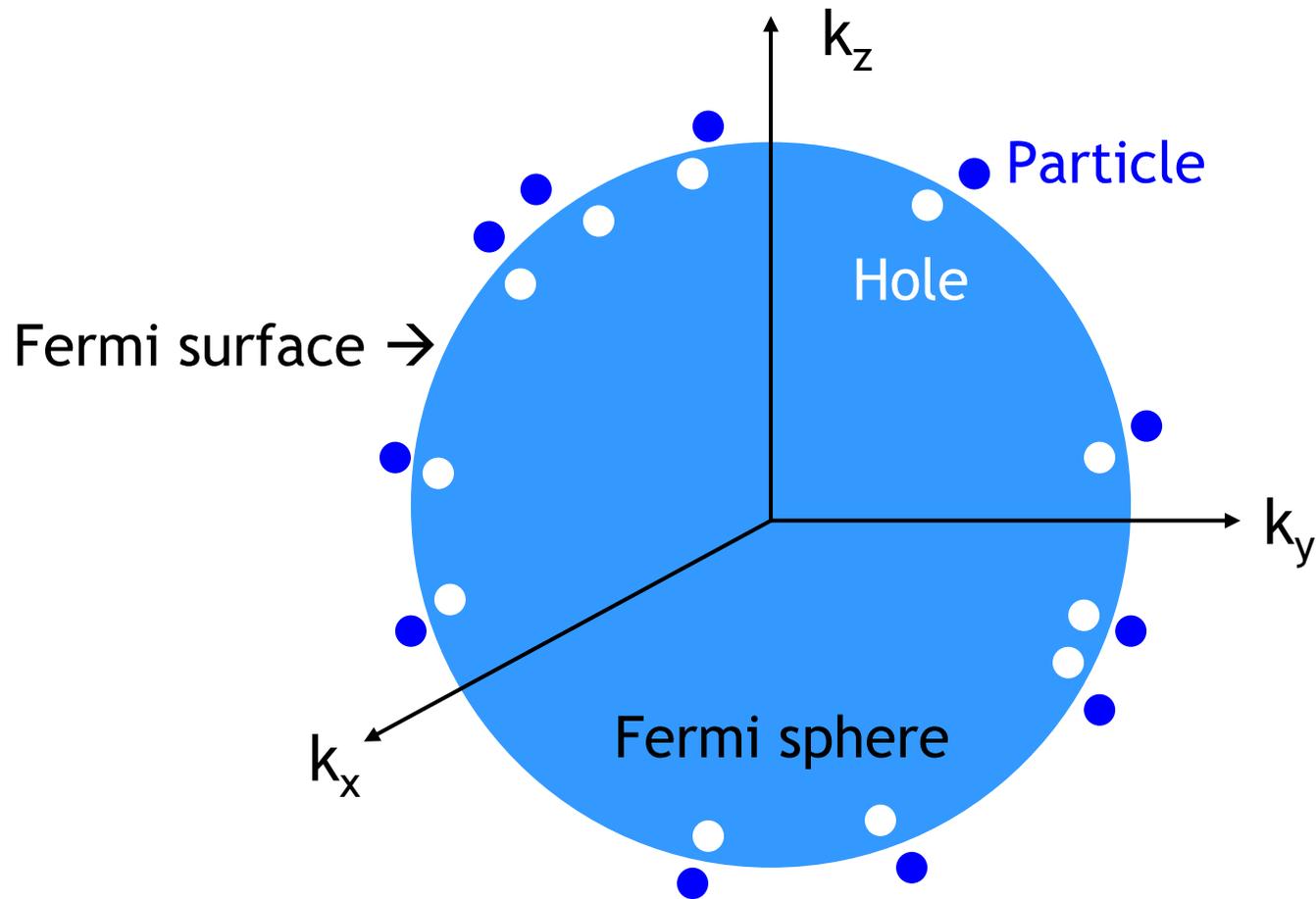
# Fermi gas: Ground state



$$\frac{E_0}{N} = \frac{3}{5} E_F \Rightarrow \text{Fermi pressure } P_{\text{Fermi}} = -\frac{\partial E_0}{\partial V} = \frac{2}{5} \frac{N}{V} E_F > 0$$

Incompressibility  
of ordinary matter  
due to **Pauli principle +  
uncertainty relation**

# Fermi gas: Excited state

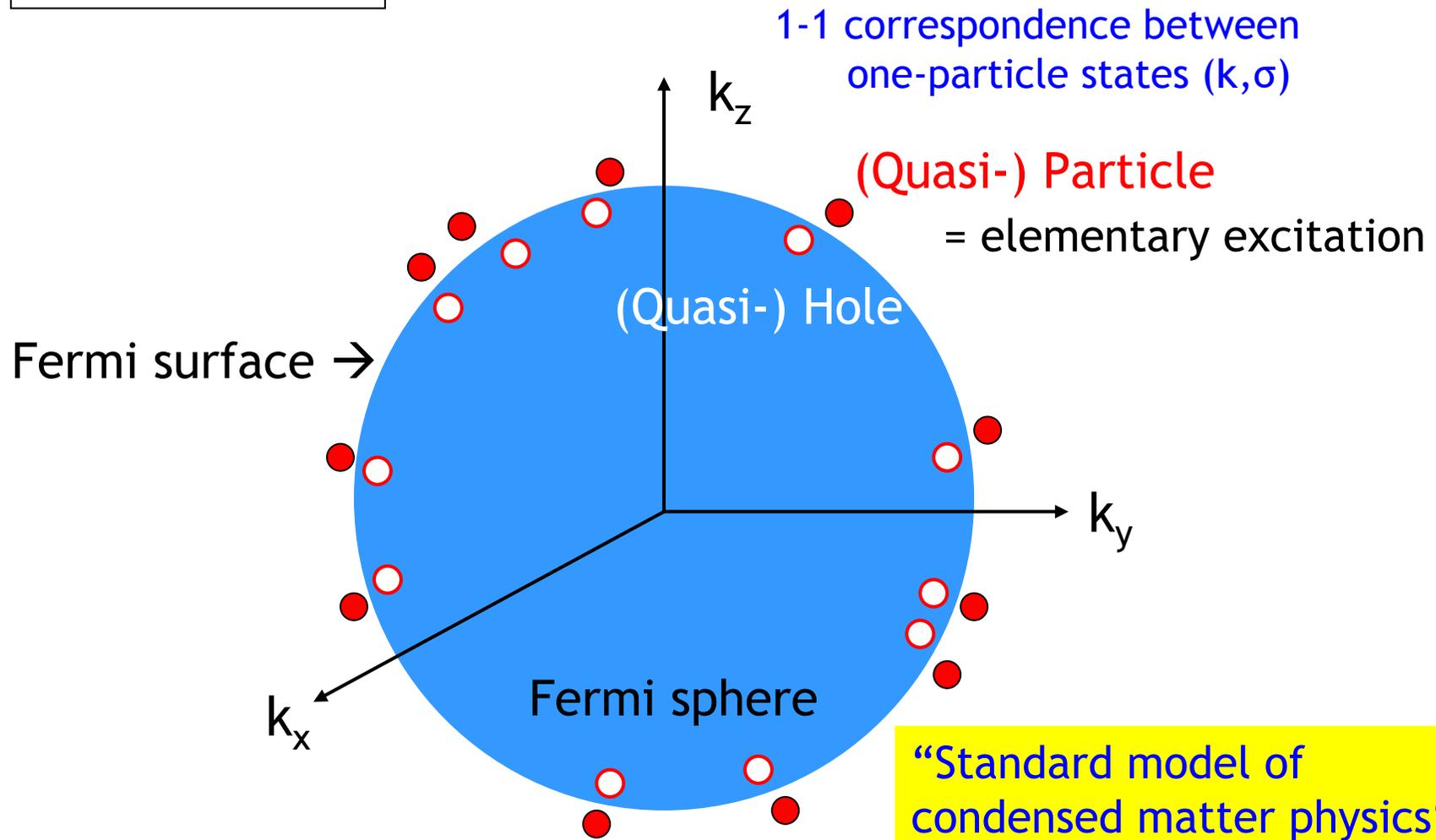


$k$ -eigenstates: **infinite** life time

**Switch on repulsive interaction**

# Fermi liquid

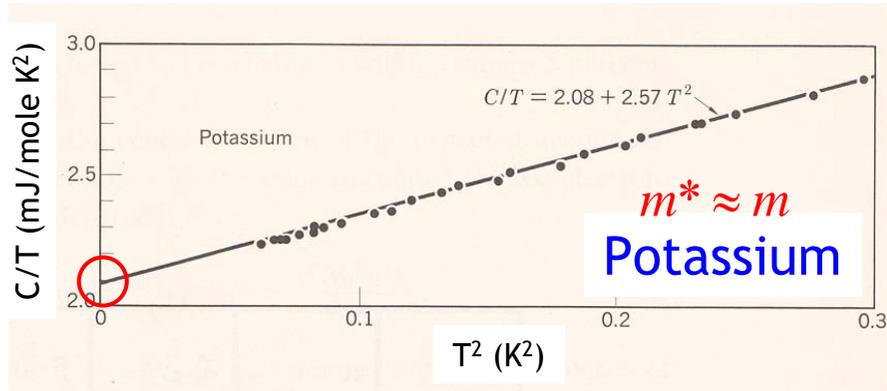
Landau (1956/58)



Well-defined  $k$ -states ("quasiparticles") with

- finite life time
- effective mass
- effective interaction

## Simple metals

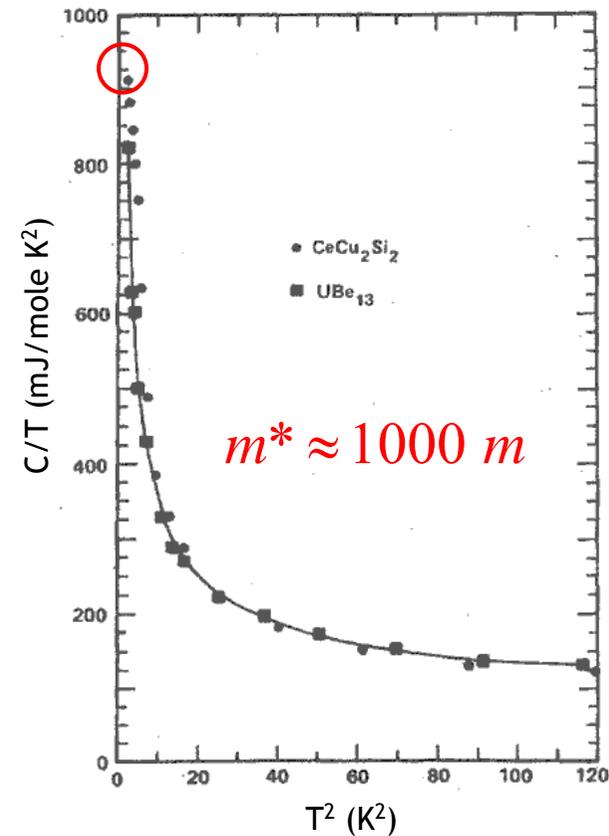


$$\lim_{T \rightarrow 0} \frac{c_V}{T} = \gamma \propto \frac{m^*}{m}$$

Result of elementary excitations (quasiparticles)

## "Heavy Fermions"

Steglich *et al.* (1979)



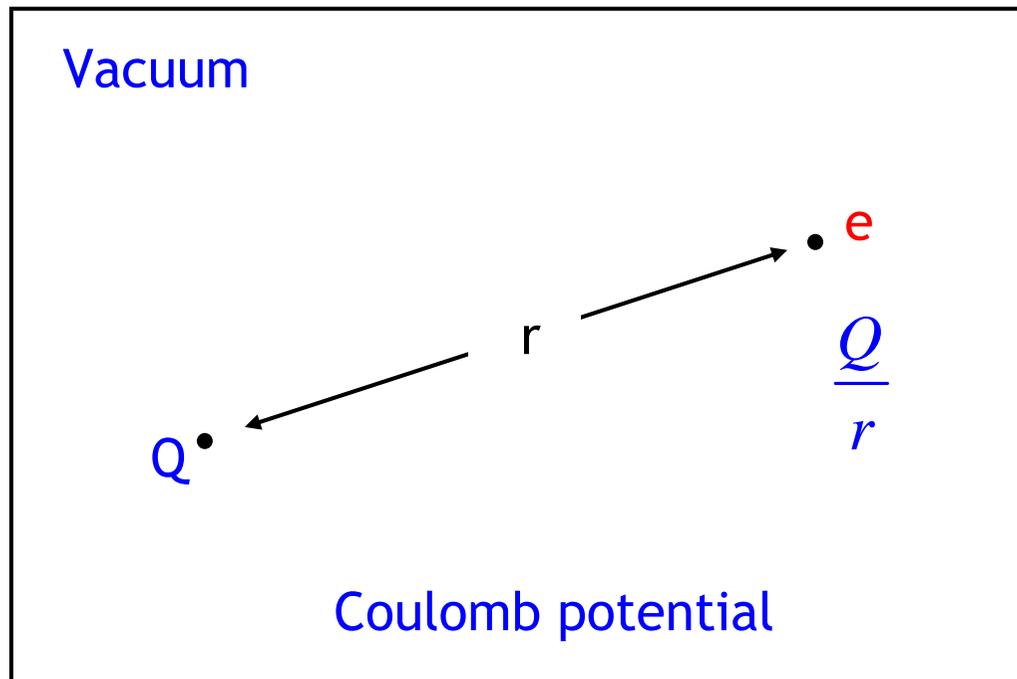
CeCu<sub>2</sub>Si<sub>2</sub>, UBe<sub>13</sub>:  
very heavy quasiparticles:  
Kondo impurity physics

# Interacting many-particle systems

Elementary (“bare”) particles + fundamental interactions

↓ # particles  $N \rightarrow \infty$

effective (“quasi”) particles + effective interactions



# Interacting many-particle systems

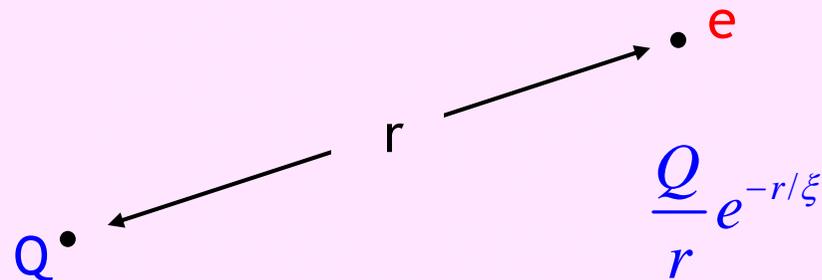
Elementary (“bare”) particles + fundamental interactions

↓ # particles  $N \rightarrow \infty$

effective (“quasi”) particles + effective interactions

Electron gas: Screening

Simplest approximation: Thomas-Fermi



Effective Yukawa potential

# Interacting many-particle systems

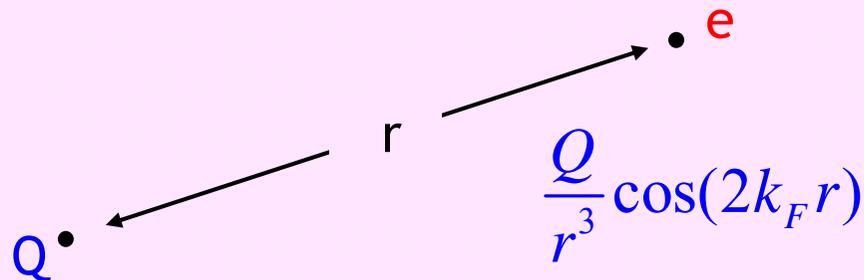
Elementary (“bare”) particles + fundamental interactions

↓ # particles  $N \rightarrow \infty$

effective (“quasi”) particles + effective interactions

Electron gas: Screening

Better approximation: Lindhard



Friedel oscillations

# Interacting many-particle systems

Elementary (“bare”) particles + fundamental interactions

↓ # particles  $N \rightarrow \infty$

effective (“quasi”) particles + effective interactions

Electrons in real solids

Heid (2004)

$Q$

$r$

$e$

Cubic crystal field

$e_g$

$t_{2g}$

$3d^1$

$d_{xy} = Z$

$d_{xz} = Y$

$d_{yz} = X$

“Strong effective interaction”  
of electrons in localized orbitals

# Interacting many-particle systems

↓ # particles  $N \rightarrow \infty$

Entirely new phenomena, e.g., phase transitions



Unpredicted behavior “emerges”

We used to think that if we knew one, we knew two,  
because one and one are two.

We are finding out that we must learn a great deal more about 'and'.

Eddington (1882-1944)

“More is different”

Anderson (1972)

# Interacting many-particle systems

↓ # particles  $N \rightarrow \infty$

Entirely new phenomena, e.g., **phase transitions**



Unpredicted behavior **“emerges”**

Examples:

Superconductivity

Magnetism

Metal-insulator transition

Traffic

Weather

Stock market

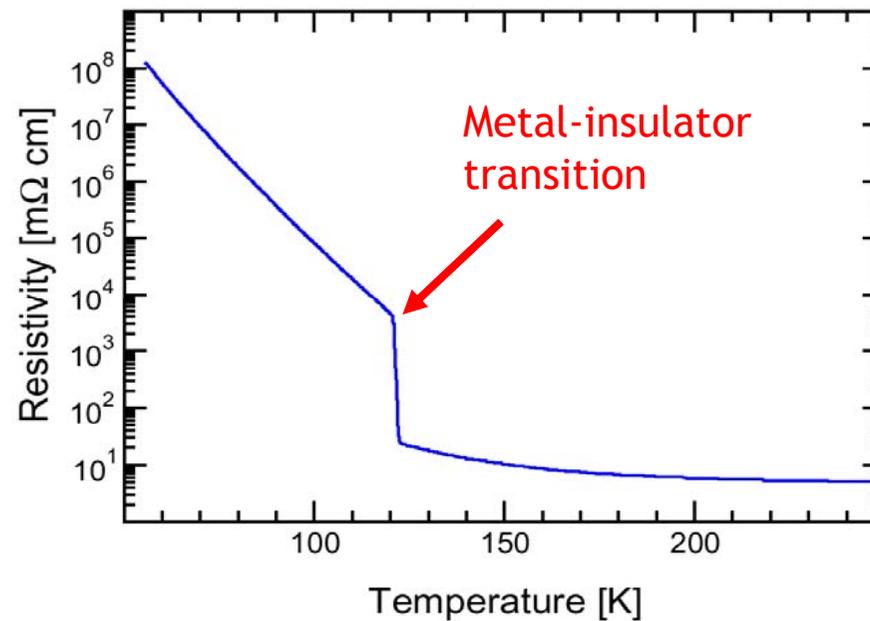
# Interacting many-particle systems

↓ # particles  $N \rightarrow \infty$

Entirely new phenomena, e.g., **phase transitions**



$\text{Fe}_3\text{O}_4$



Why?

Electrons interact by **strong effective repulsion**

# Correlations

Correlations in mathematics, natural sciences:

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

e.g., densities:

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

### Correlations (I):

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

→ The Fermi gas  $\psi(1, \dots, N) = \mathcal{A} \prod_{i=1}^N \psi_{v_i}(i)$  is uncorrelated,  
but is **spatially correlated** due to the **Fermi statistics** (“Pauli hole”)

## Temporal/spatial correlations in everyday life



Time/space average insufficient

# Electronic Correlations in Solids

# 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 1.00794	2 He 4.002602	3 Li 6.941	4 Be 9.012182	5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797	11 Na 22.989770	12 Mg 24.3050	13 Al 26.981538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955912	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938045	26 Fe 55.845	27 Co 58.933195	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90584	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 101.07	46 Pd 106.36	47 Ag 107.8682	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	57 to 71 Lanthanide series	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.222	78 Pt 195.078	79 Au 196.96655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.98038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 to 103 Actinide series	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Uun (269)	111 Uuu (272)	112 Uub (277)	113 Uut (284)	114 Uuq (285)	115 Uuh (288)	116 Uuq (289)	117 Uue (289)	118 Uuo (293)

Partially filled d-orbitals

Atomic masses in parentheses are those of the most stable or common isotope.

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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.

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
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)

Partially filled f-orbitals

Narrow d,f-orbitals/bands → strong electronic correlations

# Correlated electron materials have unusual properties

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

## With potential for technological applications:

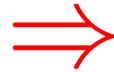
- sensors, switches, Mottronics
- spintronics
- thermoelectrics
- high- $T_c$  superconductors
- functional materials:  
oxide heterostructures ...

How to study  
correlated systems  
theoretically?

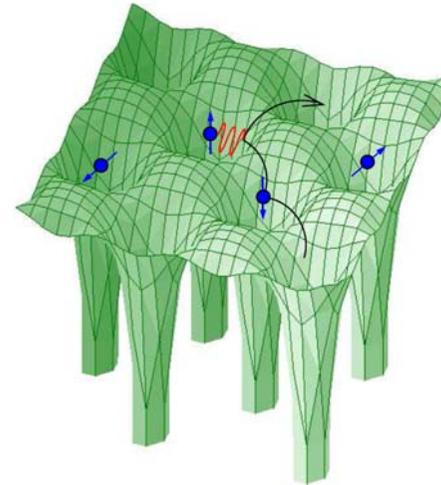
material



modeling



realistic model



quantum many-particle problem

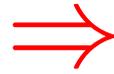
“The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.”

Dirac (1929)

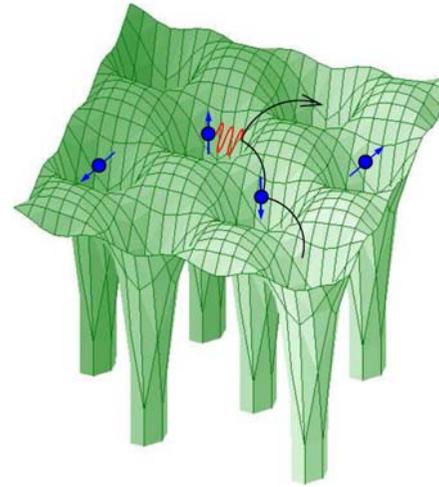
material



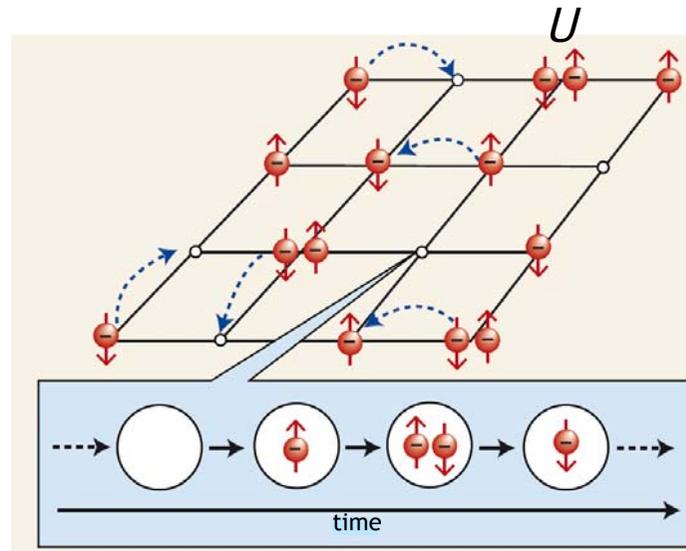
modeling



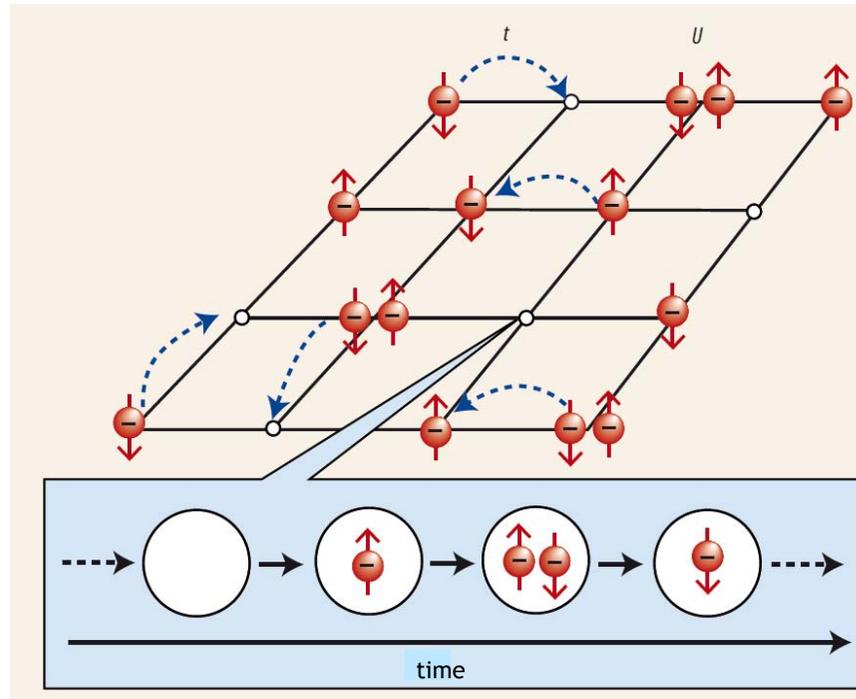
realistic model



maximal reduction: Hubbard model



# Hubbard model



Gutzwiller, 1963  
Hubbard, 1963  
Kanamori, 1963

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

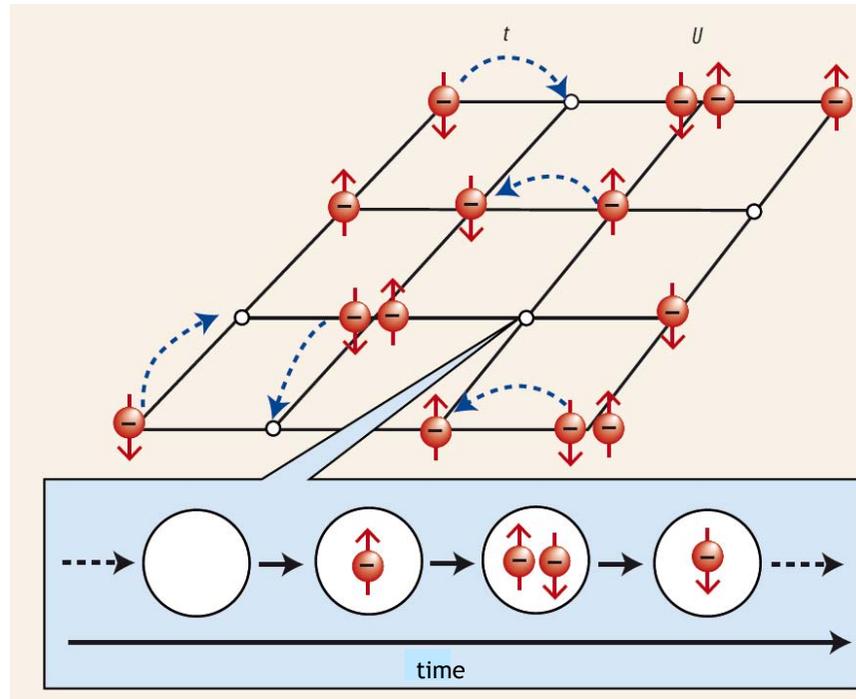
$$\langle n_{i\uparrow} n_{i\downarrow} \rangle \neq \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle$$

Dimension of Hilbert space  $\sim O(L^4)$   
 $L$ : # lattice sites

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

Computational time for  $N_2$  molecule:  
ca. 1 year with 50.000 compute nodes

# Hubbard model



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 of many-fermion problems:  
 Construct reliable, comprehensive  
**non-perturbative** approximation schemes

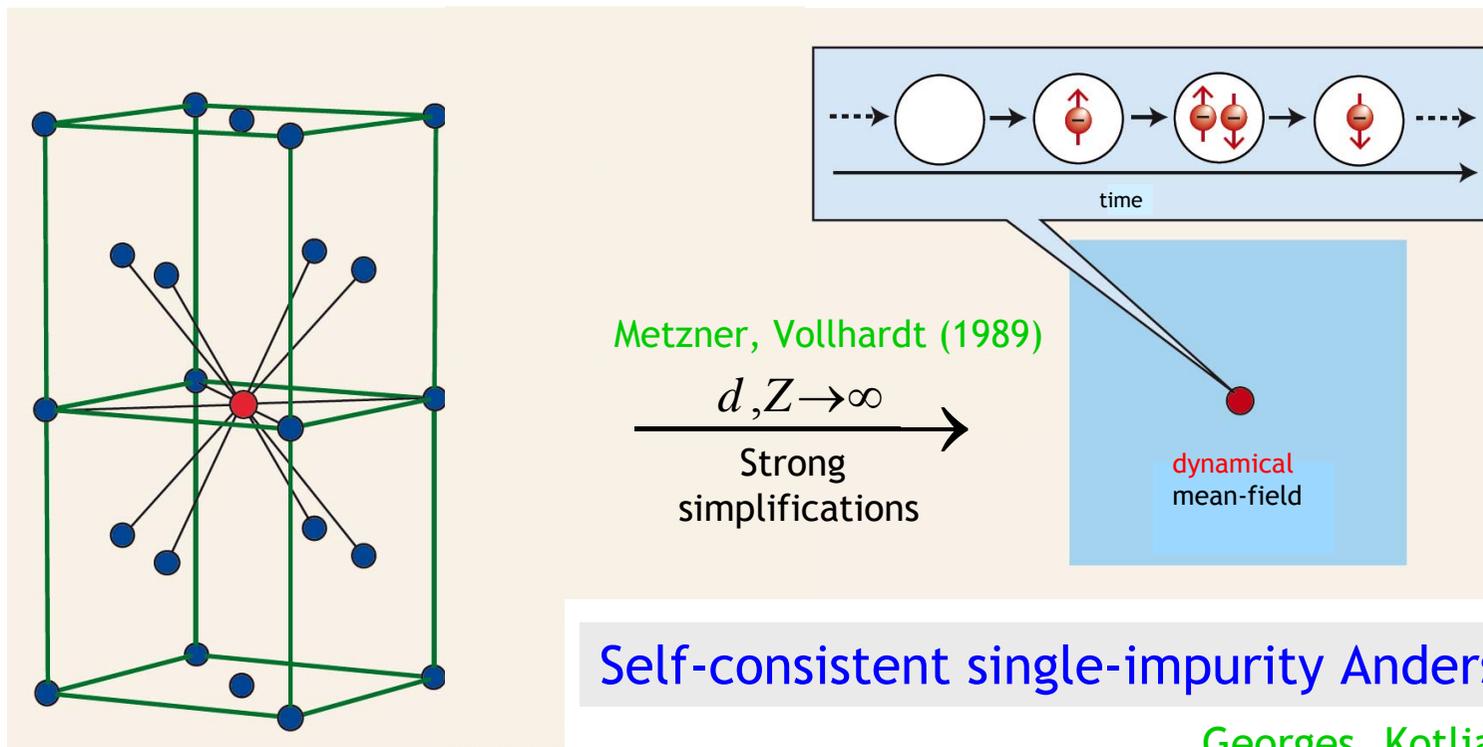
Static (Hartree-Fock-type)  
 mean-field theories  
 generally insufficient

# Dynamical Mean-Field Theory (DMFT) of Correlated Electrons

# Theory of correlated electrons

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

Face-centered cubic lattice (d=3)



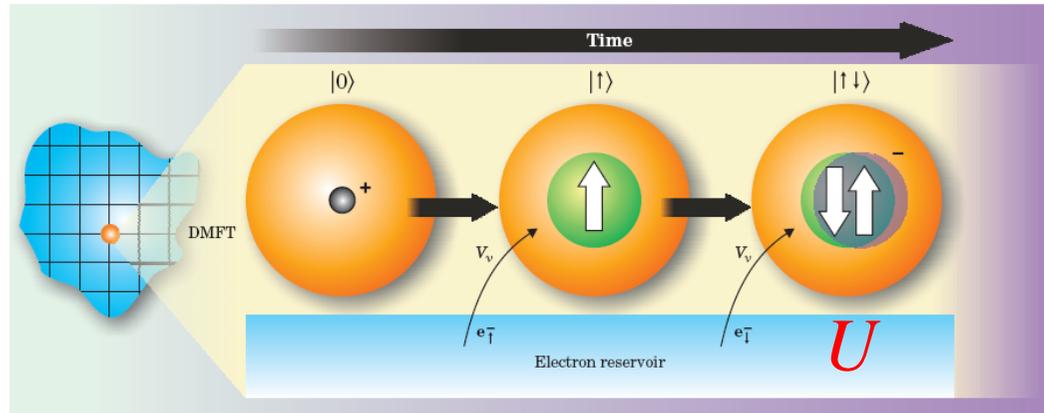
Self-consistent single-impurity Anderson model

Georges, Kotliar (1992))

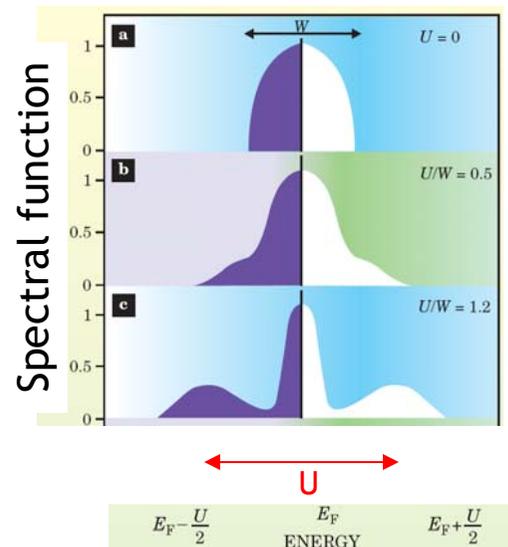
$Z=12$

Solve with an „impurity solver“, e.g., QMC, NRG, ED,...

# Dynamical mean-field theory (DMFT) of correlated electrons



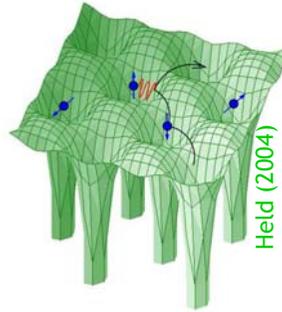
Exact **time** resolved treatment of **local** electronic interactions



**Correlations (II):**  
Transfer of spectral weight

Experimentally  
detectable ?

# Correlated Electron Materials



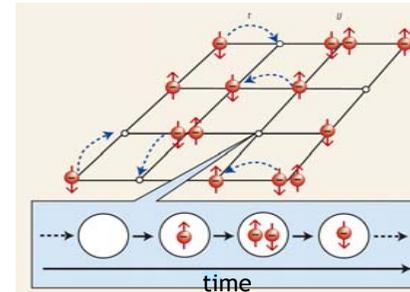
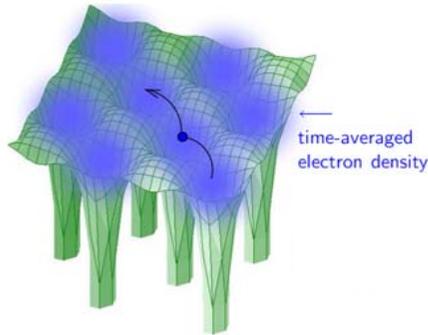
Comprehensive, non-perturbative approximation scheme needed

DFT/LDA

Model Hamiltonians

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

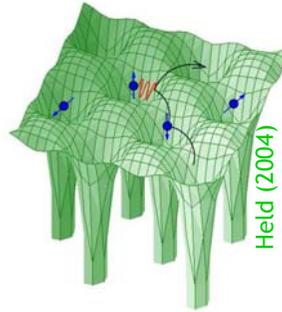
- input parameters unknown: unrealistic
- + systematic many-body approach



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

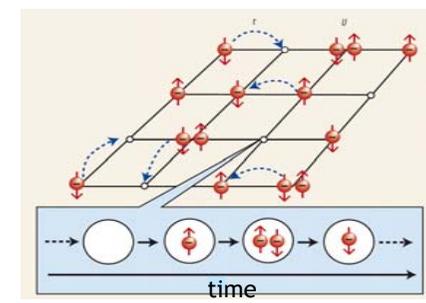
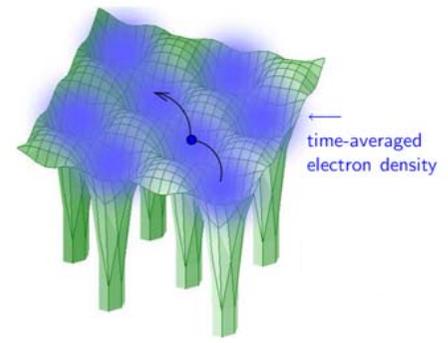


Electronic correlations  
Many-body theory



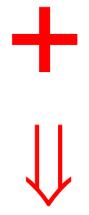
Comprehensive, non-perturbative approximation scheme needed

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



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

Electronic correlations  
Many-body theory  
(DMFT)



LDA+DMFT

Anisimov *et al.* (1997)  
Lichtenstein, Katsnelson (1998)

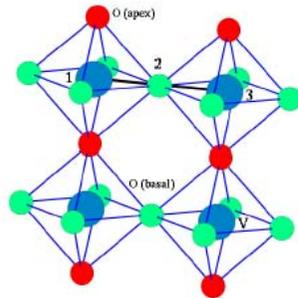
# Application of LDA+DMFT

(Sr,Ca)VO<sub>3</sub>: 3d<sup>1</sup> system

# Electronic structure

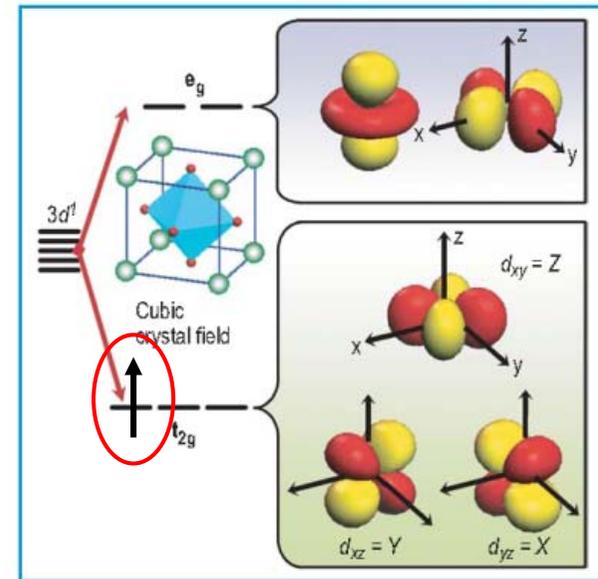
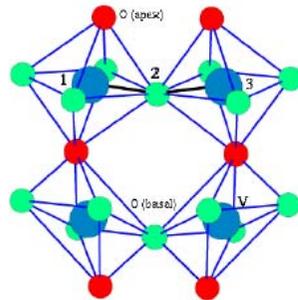
## Crystal structure

$\text{SrVO}_3$ :  $\angle V-O-V = 180^\circ$

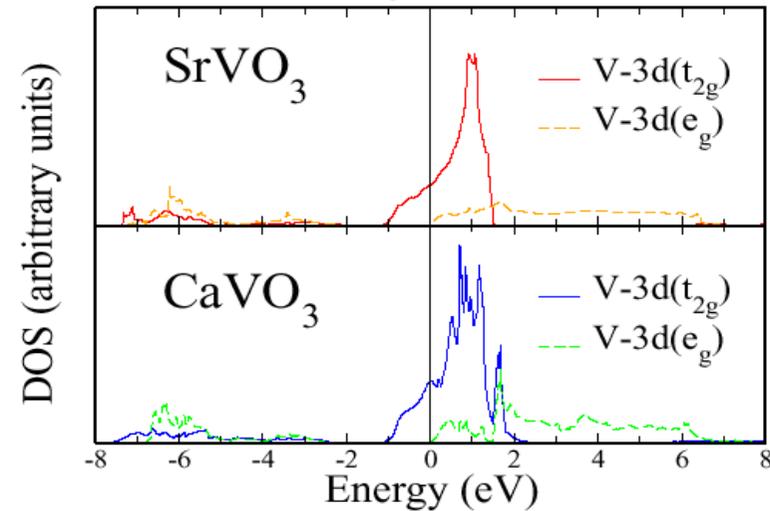


orthorhombic distortion

$\text{CaVO}_3$ :  $\angle V-O-V \approx 162^\circ$

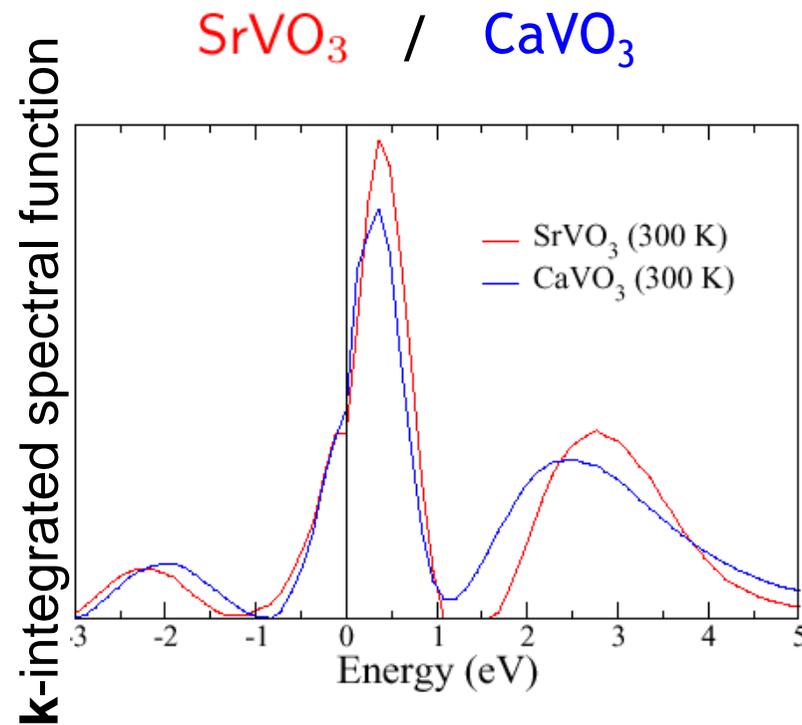


## LDA density of states



No correlation effects/spectral transfer

# LDA+DMFT results



constrained LDA:  
 $U=5.55$  eV,  $J=1.0$  eV

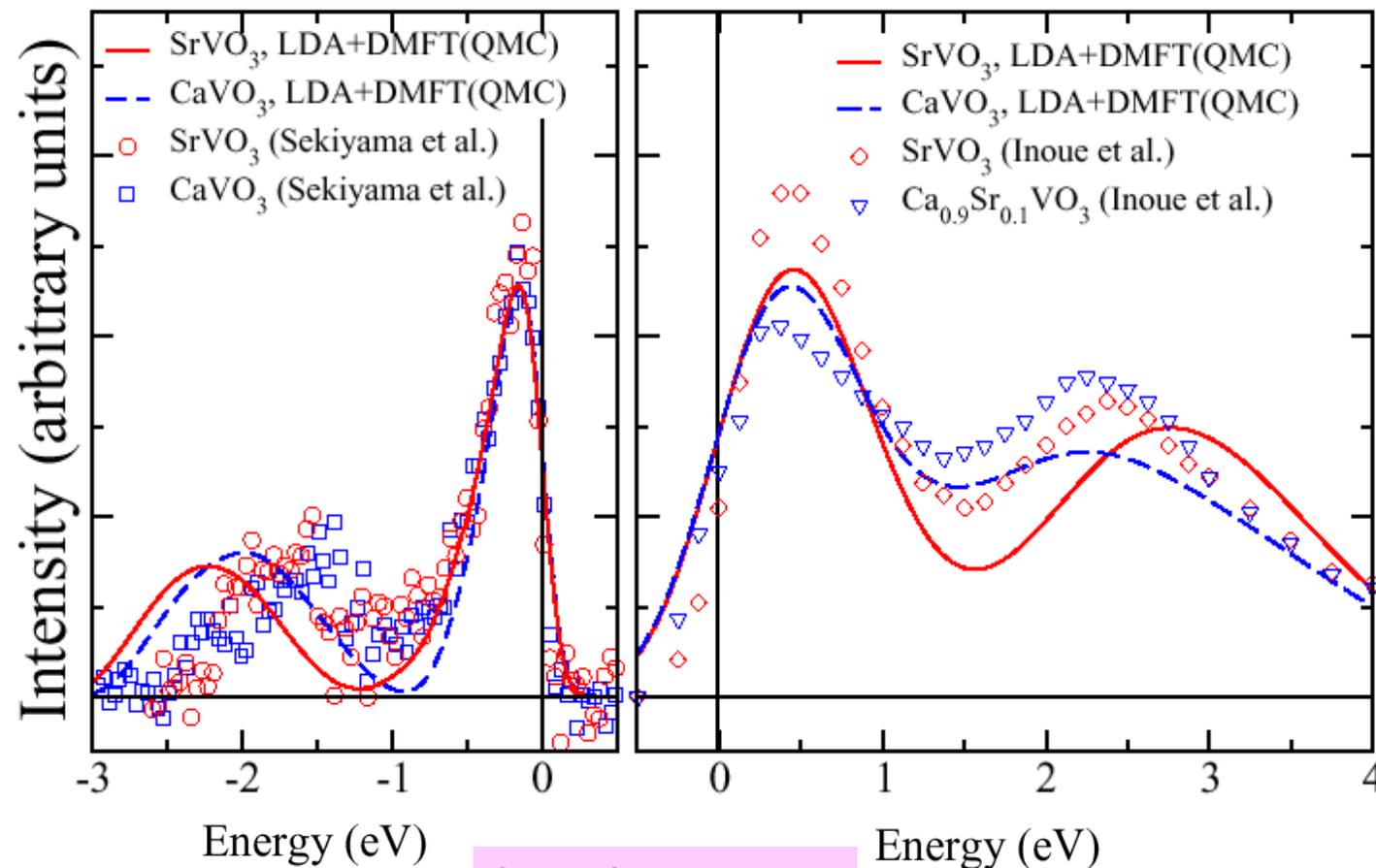
Osaka - Augsburg - Ekaterinburg collaboration: [Sekiyama \*et al.\* \(2004\)](#)

# Comparison with experiment

Osaka - Augsburg -  
Ekaterinburg collaboration,  
(2004, 2005)

Bulk sensitive  
photoemission spectroscopy  
→ occupied states

X-ray absorption spectroscopy  
→ unoccupied states

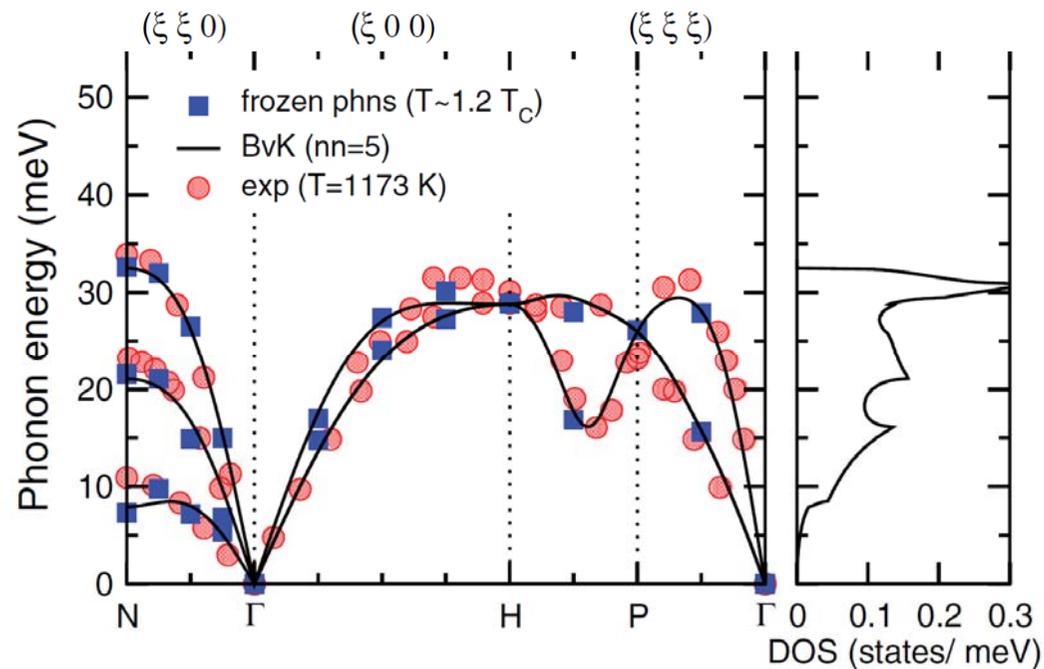


3-peak structure  
detected

# State-of-the-art LDA+DMFT: Correlation-induced structural transformations

Lattice dynamics of paramagnetic *bcc* iron Leonov *et al.* (2012)

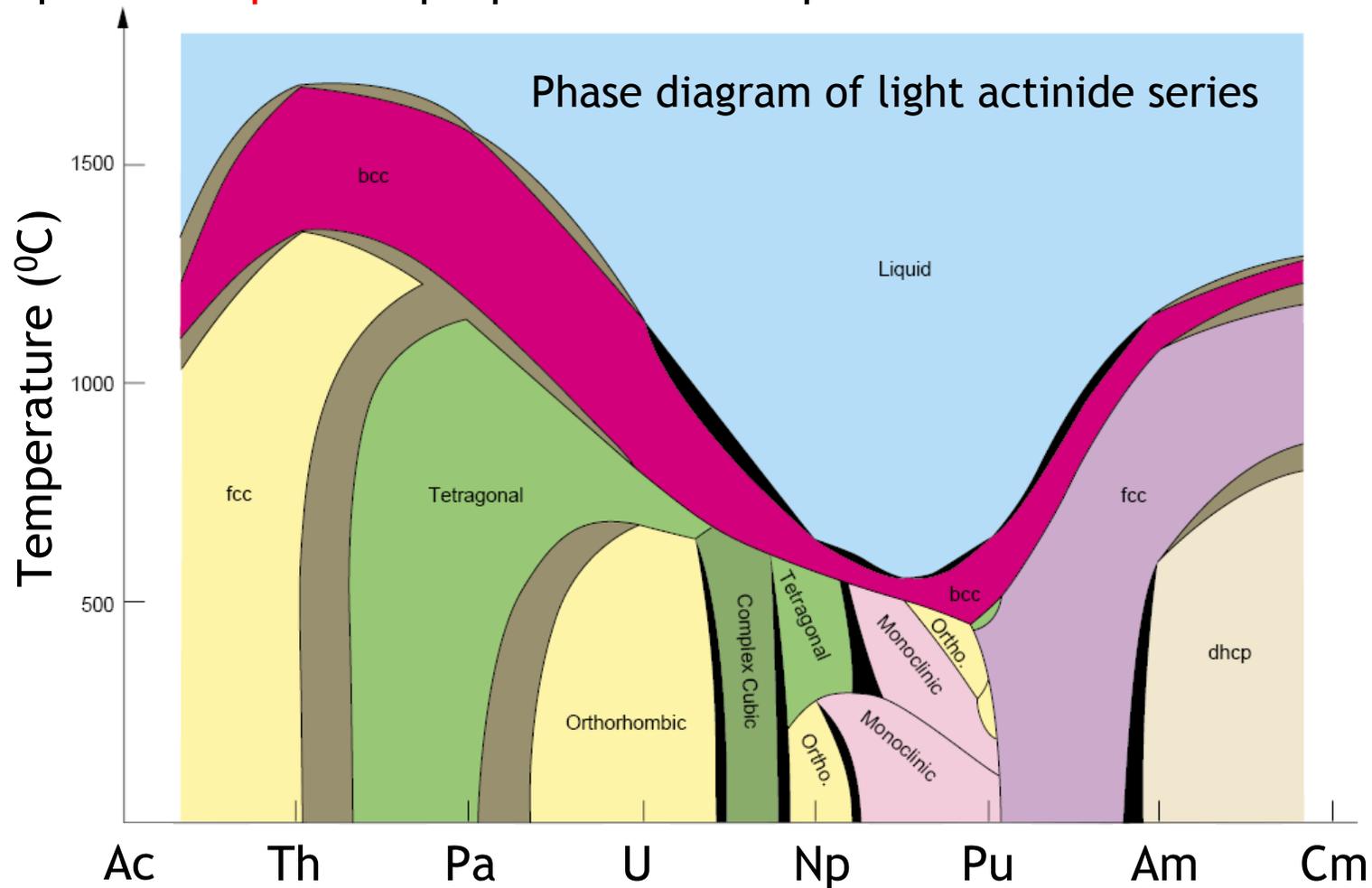
GGA+DMFT phonon dispersion at  $1.2 T_C$



Exp.: Neuhaus, Petry, Krimmel (1997)

# Perspective of the LDA+DMFT approach

Explain and **predict** properties of complex correlated materials



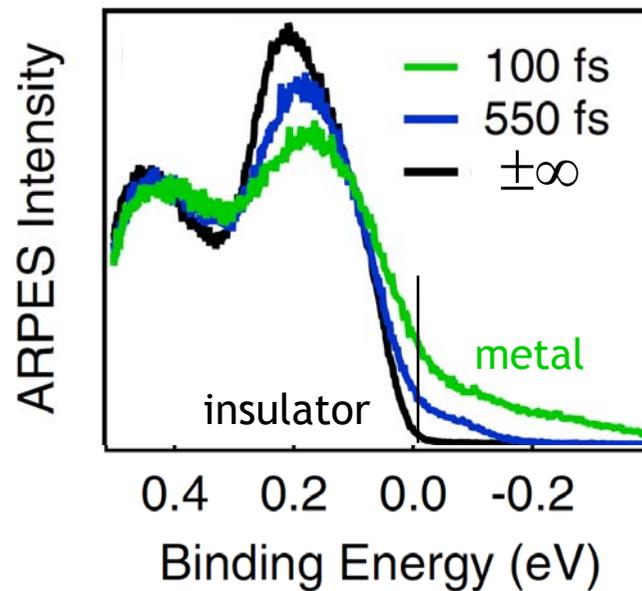
Phase diagram connecting individual binary alloy diagrams  
Black: two-phase regions; Brown : details unknown

Boring, Smith (2000)

# Developments & Perspectives

# 1. 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 in correlated bulk materials

# 1. Correlated electrons in non-equilibrium

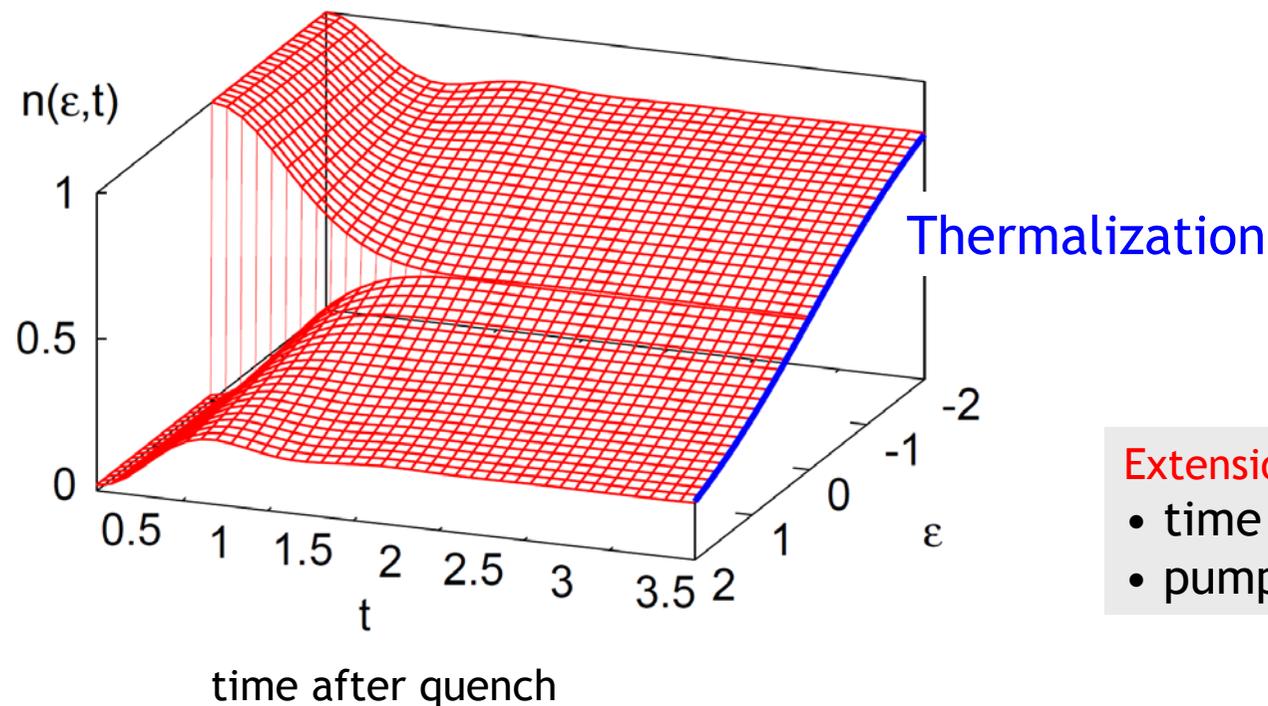
Non-equilibrium DMFT

Freericks, Turkowski (2006)  
Eckstein (2009)

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

Eckstein, Kollar, Werner (2009)

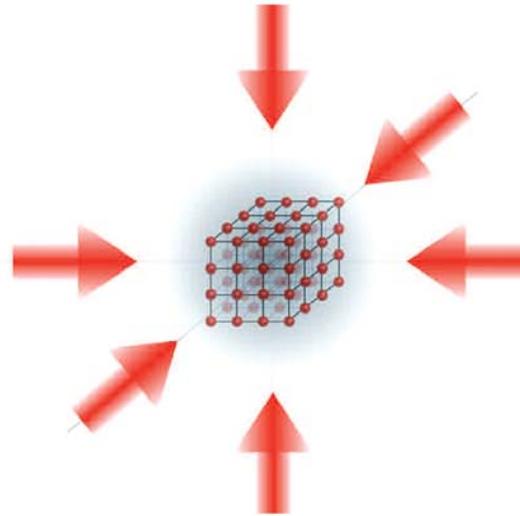
Momentum distribution ( $U=3.3$ )



Extension, e.g.

- time resolved PES
- pump-probe experiments

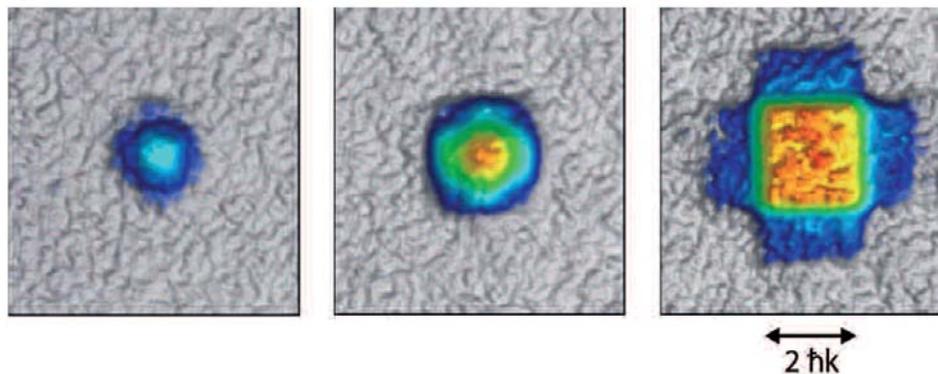
## 2. Correlated cold atoms in optical lattices



Greiner *et al.* (2002)

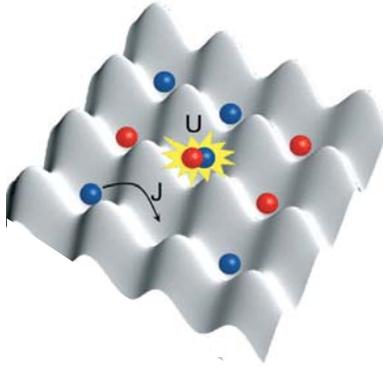
Bosonic/fermionic atoms in optical lattices: Exp. realization of models

High degree of tunability: “quantum simulator”



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

## 2. Correlated cold atoms in optical lattices



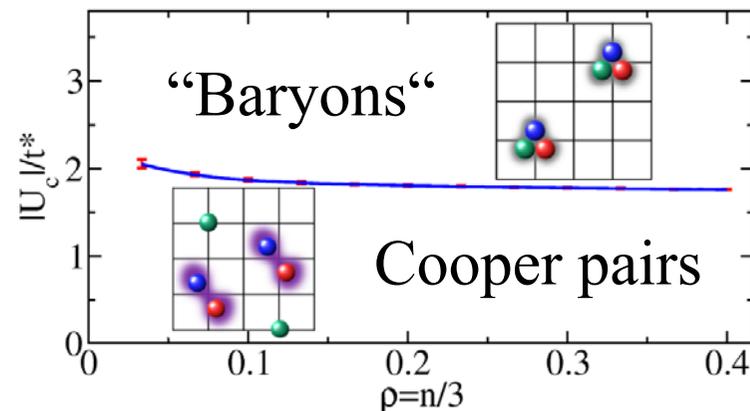
Hubbard model with ultracold atoms Jaksch *et al.* (1998)

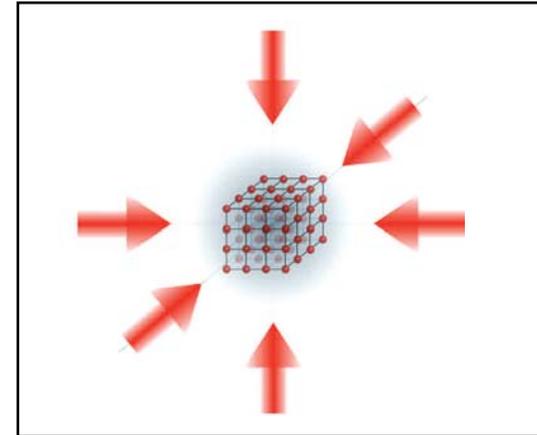
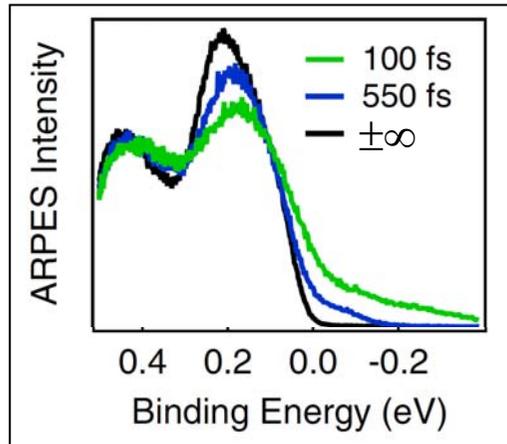
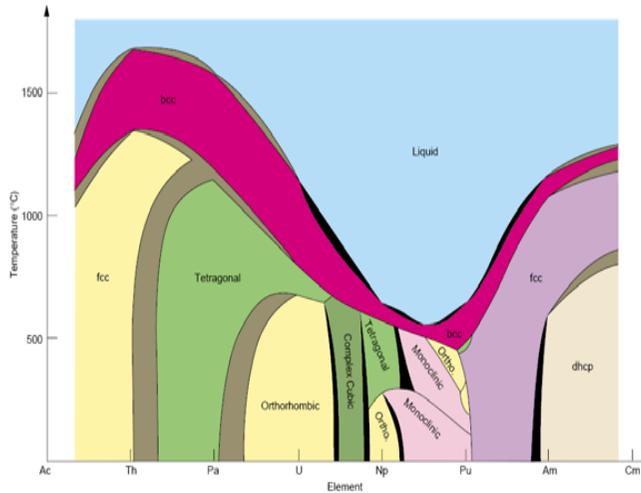
Atomic total angular momentum  $L^{\text{tot}} = F \rightarrow N=2F+1$  hyperfine states

→ SU(N) Hubbard models

$N=3$ , e.g.  ${}^6\text{Li}$ ,  $U < 0$ : Color superconductivity, “baryon formation (QCD)”

Rapp *et al.* (2006)





Correlated many-particle systems:  
**More fascinating than ever**

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