

Center for
Electronic Correlations and Magnetism
University of Augsburg

Surprising Effects of the Interaction between Electrons in Matter

Dieter Vollhardt

Colloquium, University of Würzburg; July 6, 2009

Outline:

1. Peculiarities of many-particle systems
2. Correlations
3. Electronic correlations in solids
4. Dynamical Mean-Field Theory:
Models vs. materials
5. New Developments & Perspectives

Supported by Deutsche Forschungsgemeinschaft (SFB 484)

1.

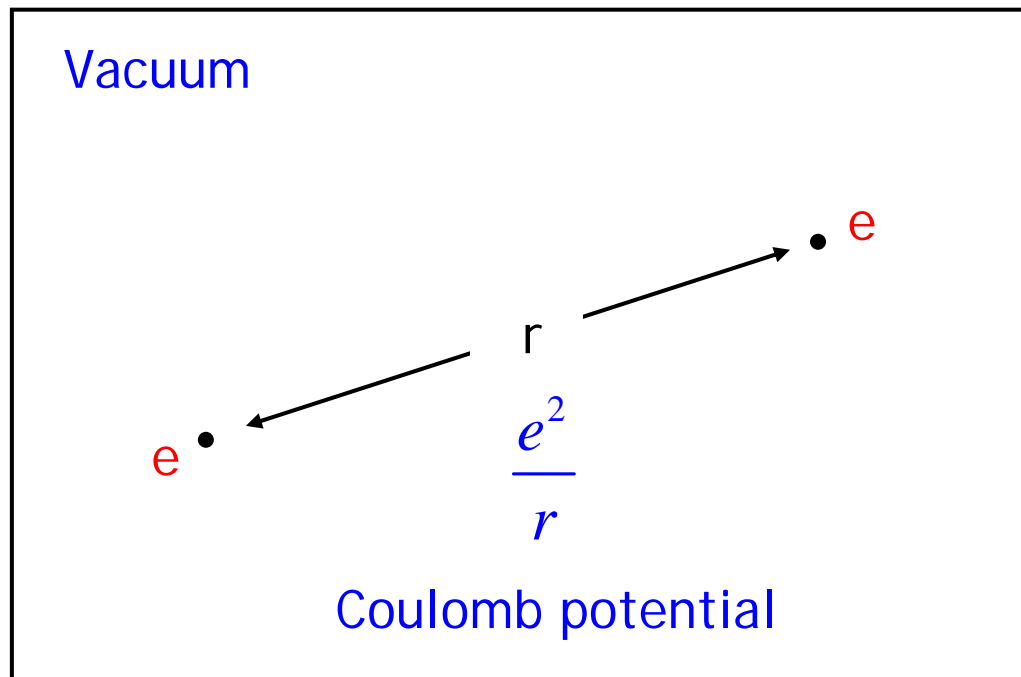
Peculiarities of Many-Particle Systems

Interacting many-particle systems

Elementary ("bare") particles + interactions



effective ("quasi") particles + effective interactions



Interacting many-particle systems

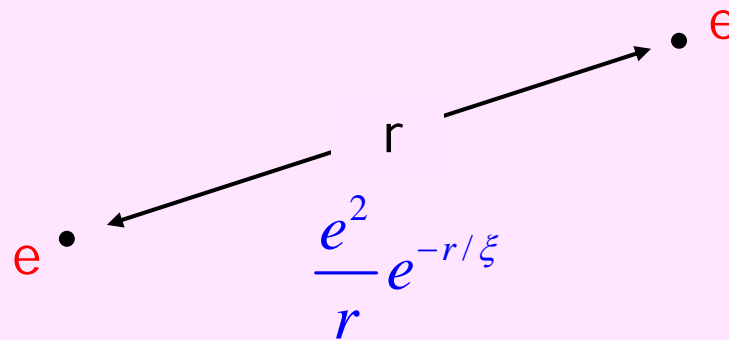
Elementary ("bare") particles + interactions



effective ("quasi") particles + effective interactions

Electron gas: **Screening**

Simplest approximation: Thomas-Fermi



Effective Yukawa potential

Interacting many-particle systems

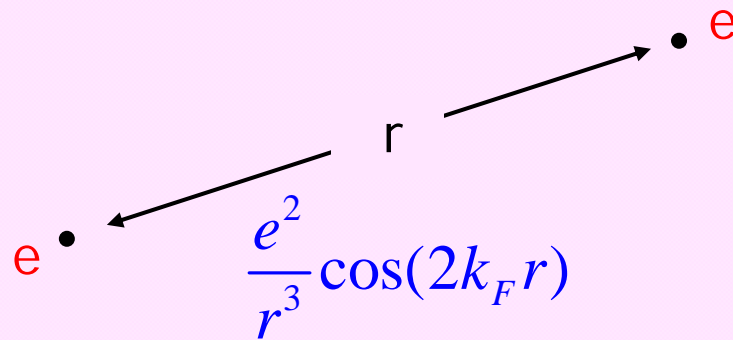
Elementary ("bare") particles + interactions



effective ("quasi") particles + effective interactions

Electron gas: **Screening**

Better approximation: Lindhard



Friedel oscillations

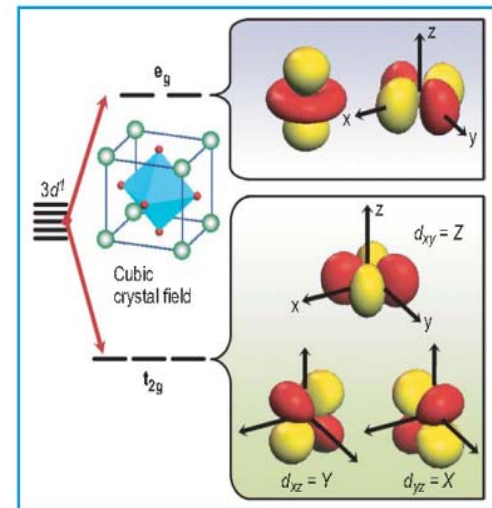
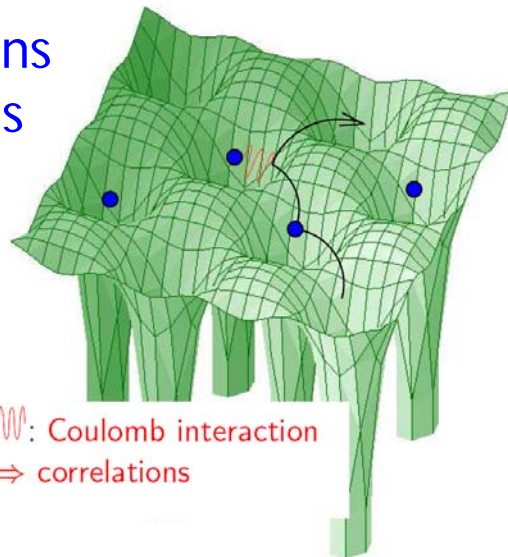
Interacting many-particle systems

Elementary ("bare") particles + interactions

↓ $N \rightarrow \infty$

effective ("quasi") particles + effective interactions

Electrons
in solids



"Strong interaction" of
electrons in localized orbitals

Quasiparticles

Electrons

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



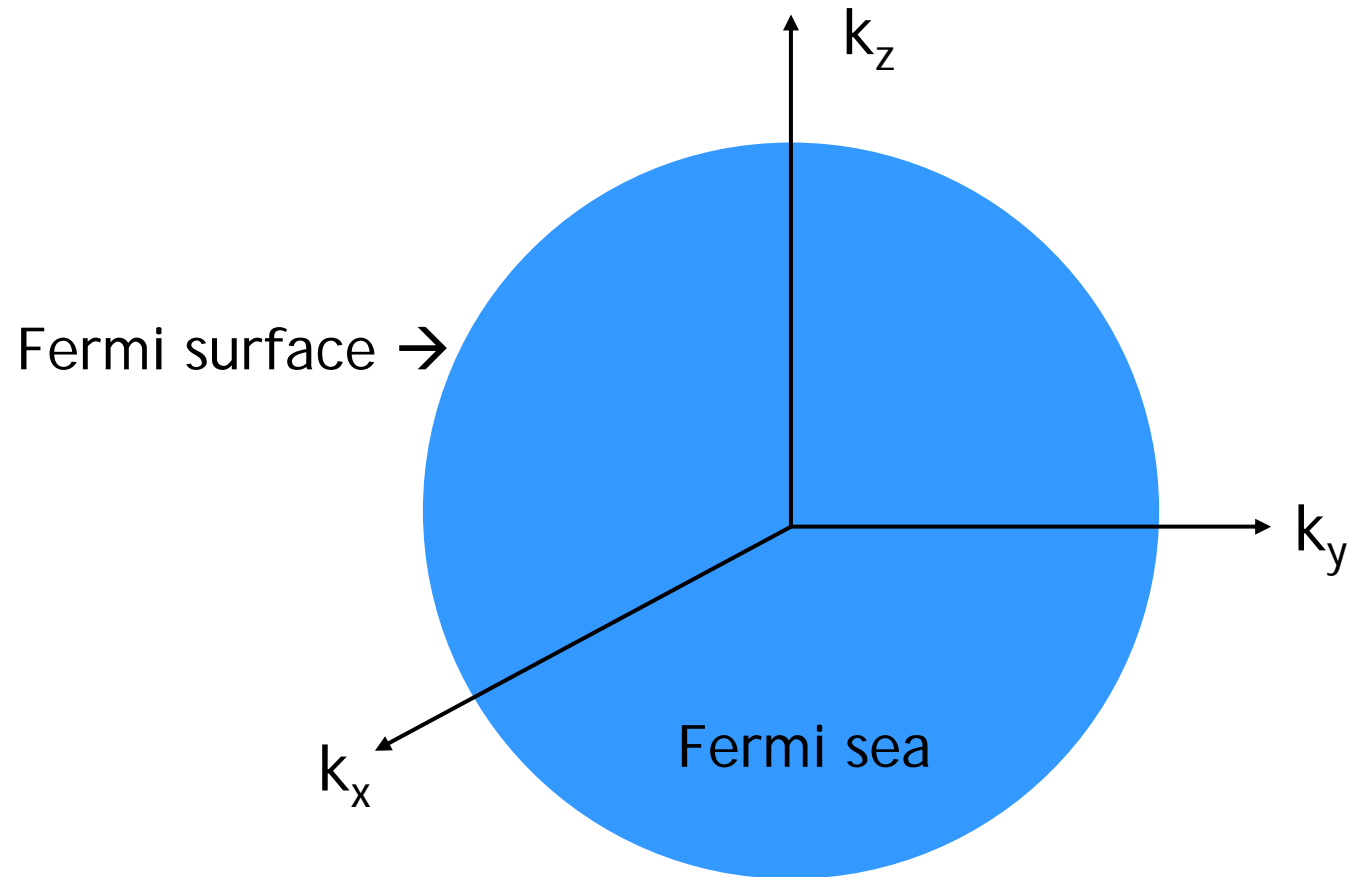
Fermi-Dirac statistics



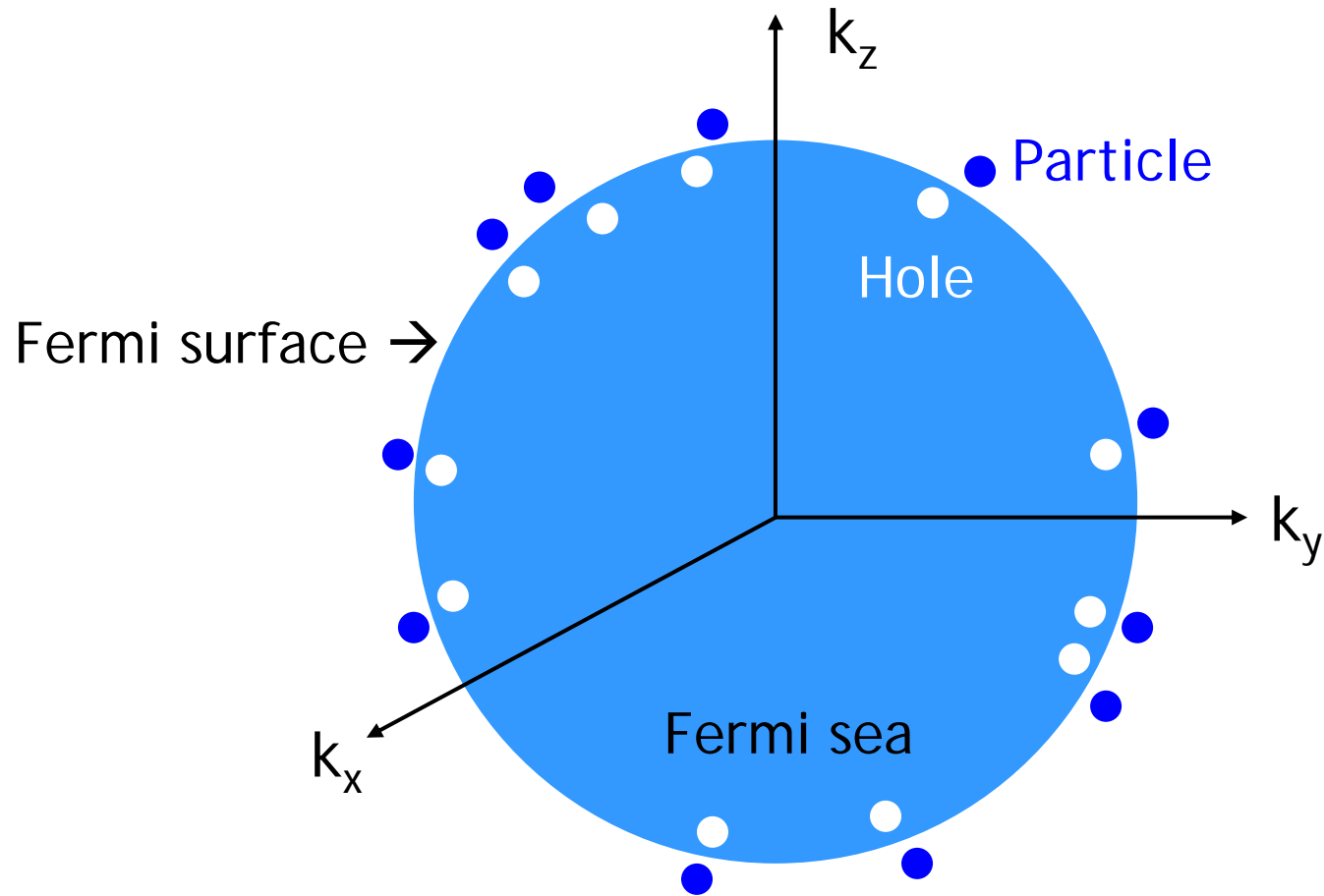
Pauli exclusion principle
of many fermions

Fermi body/surface

Fermi gas: Ground state



Fermi gas: Excited states ($T > 0$)



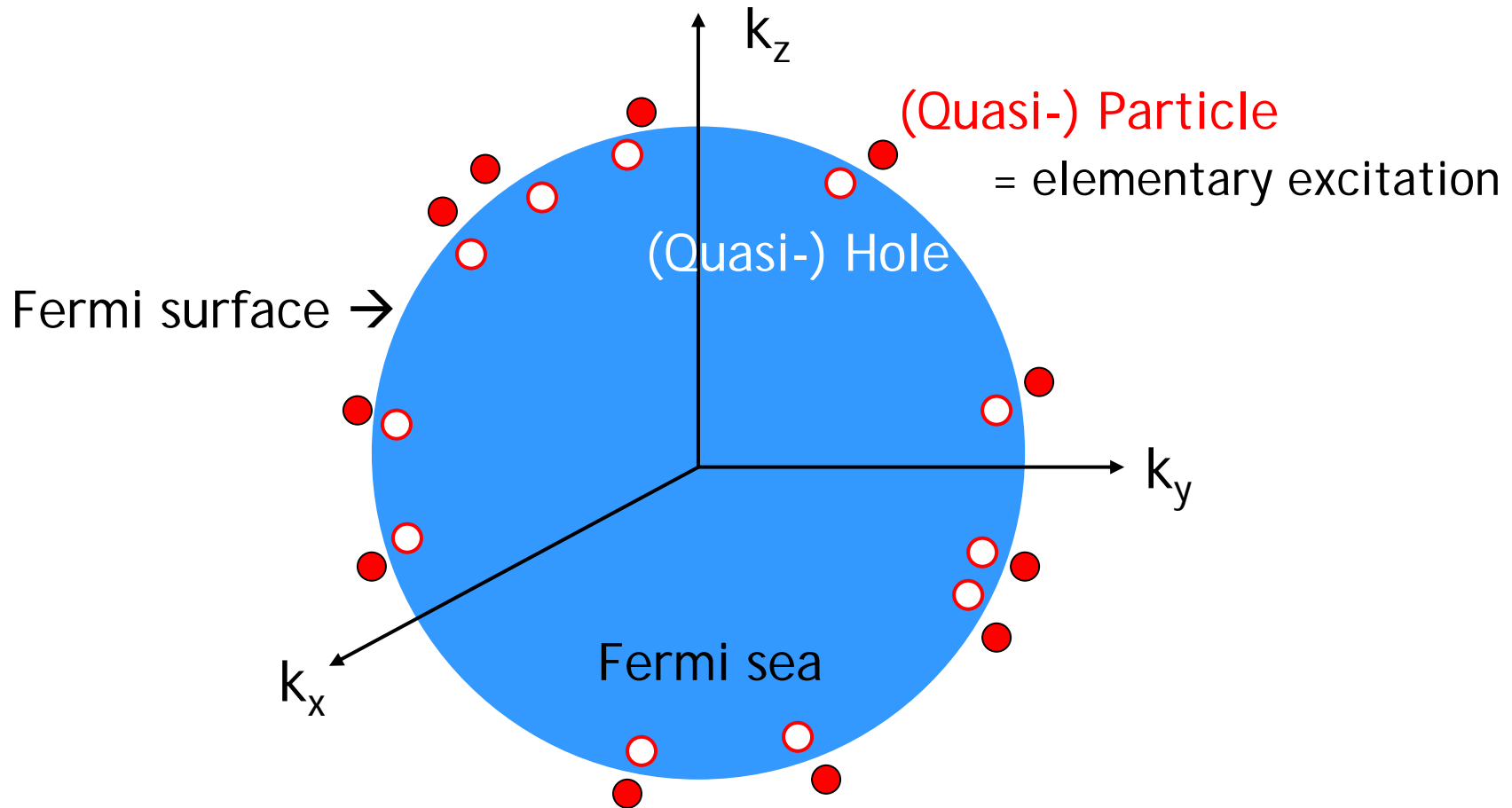
Exact k -states ("particles"): infinite life time

Switch on interaction adiabatically ($d=3$)

Landau Fermi liquid

Landau (1956/58)

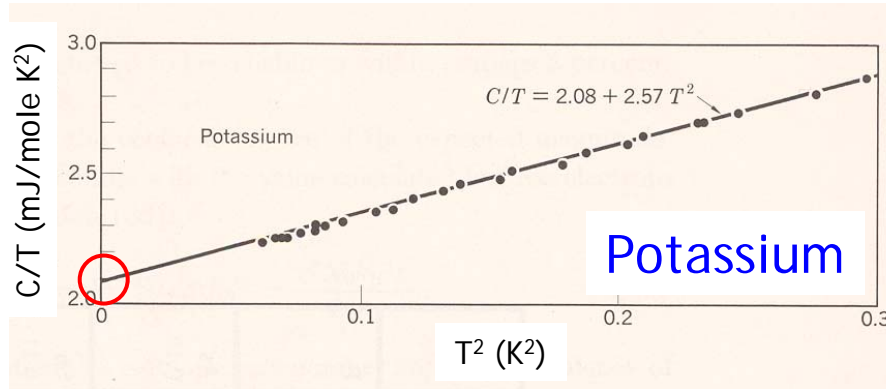
1-1 correspondence between k-states



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

- finite life time
- effective mass
- effective interaction

Simple metals

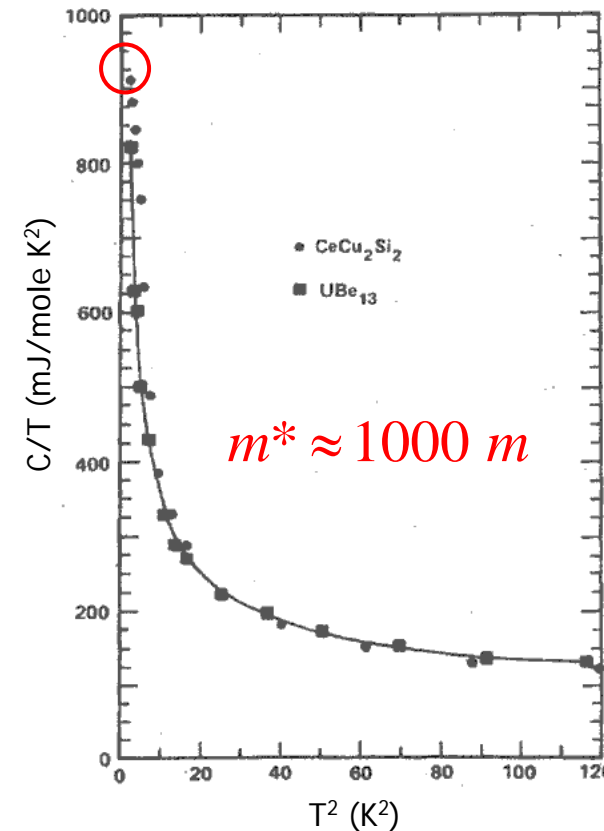


Consequence of elementary excitations (quasiparticles)

$$\lim_{T \rightarrow 0} \frac{c_V}{T} \approx \gamma_0 \Rightarrow m^* \approx m$$

"Heavy Fermions"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

$CeCu_2Si_2$, UBe_{13} :
strongly interacting electrons

$$\lim_{T \rightarrow 0} \frac{c_V}{T} = \gamma \propto \frac{m^*}{m}, \quad v_F = \frac{\hbar k_F}{m^*}$$

Interacting many-particle systems

↓ $N \rightarrow \infty$

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

↓

Unpredicted **"emergent"** behavior

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'.

Arthur Eddington (1882-1944)

"More is different"

Anderson (1972)

Interacting many-particle systems

↓ $N \rightarrow \infty$

Emergence

Examples:

Superconductivity
Magnetism
Galaxy formation

Traffic
Weather
Stock market

Ants
Human body
Consciousness

2. Correlations

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

Grammar: *either ... or*

Mathematics, natural sciences:

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

e.g., densities:

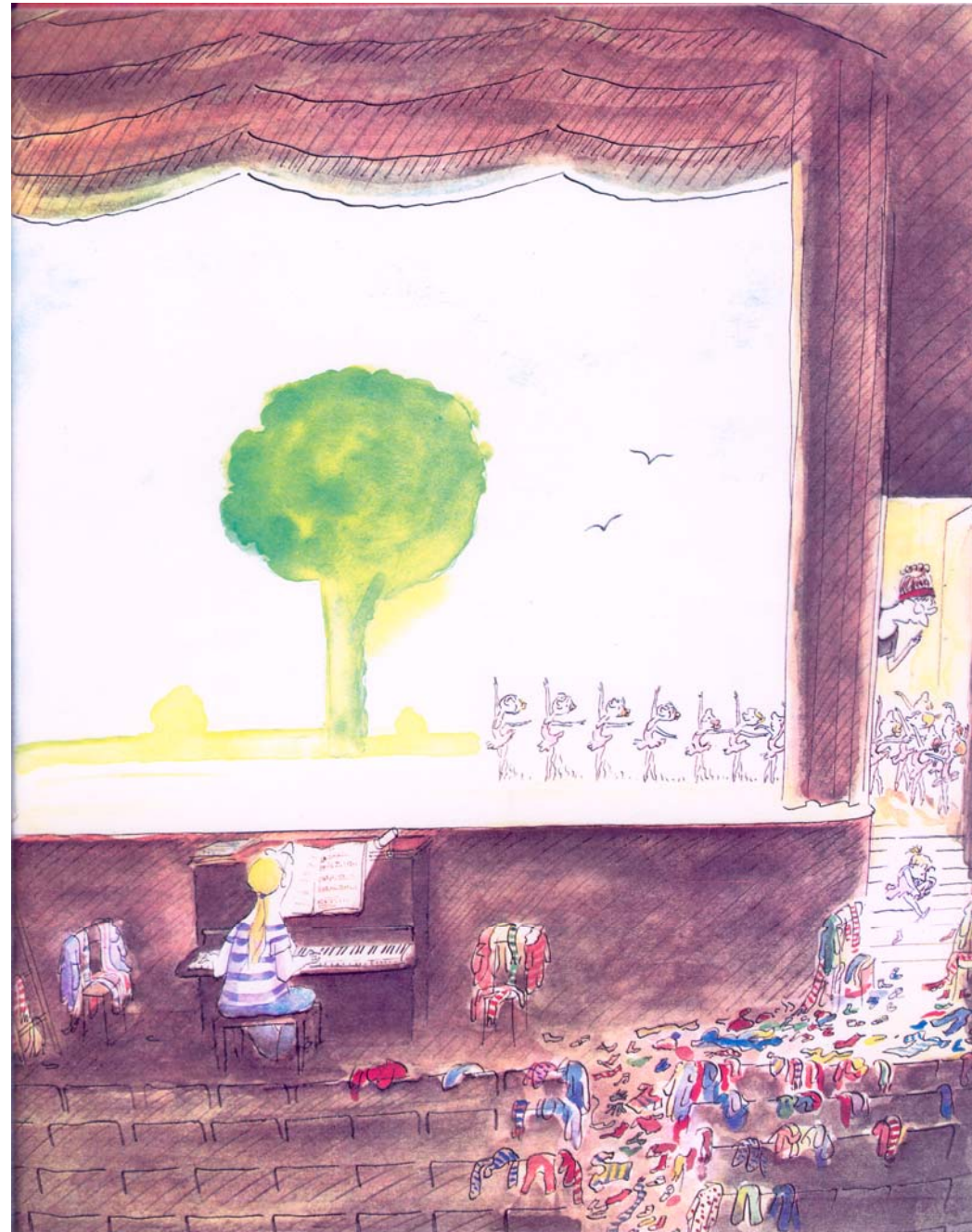
$$\langle \rho(\mathbf{r})\rho(\mathbf{r}') \rangle \neq \langle \rho(\mathbf{r}) \rangle \langle \rho(\mathbf{r}') \rangle$$

Temporal/spatial correlations in everyday life



Time/space average
insufficient

Correlations
vs.
long-range order



Sempe, THE NEW YORKER

3.
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 65.38 | 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 88.90585 | 40 Zr 91.224 | 41 Nb 92.90638 | 42 Mo 95.94 | 43 Tc 98 | 44 Ru 101.07 | 45 Rh 102.90550 | 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 | 57-71 Lanthanide series | 72 Hf 178.49 | 73 Ta 180.9479 | 74 W 183.84 | 75 Re 186.207 | 76 Os 190.23 | 77 Ir 192.217 | 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) | 89-103 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) |

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

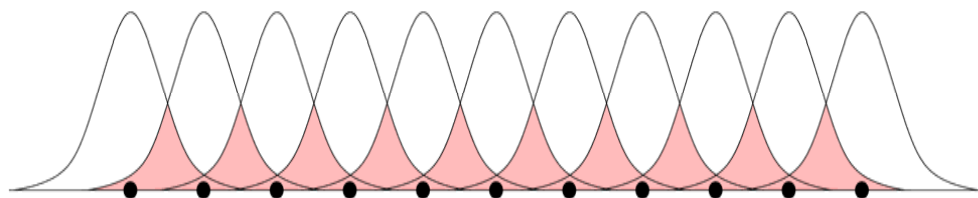
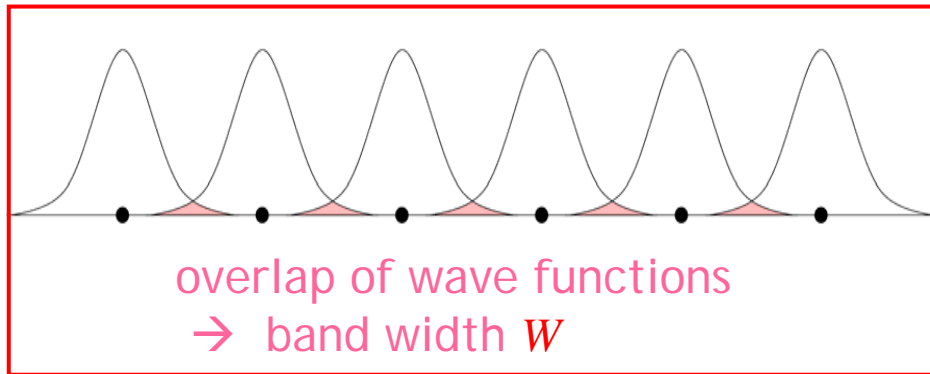
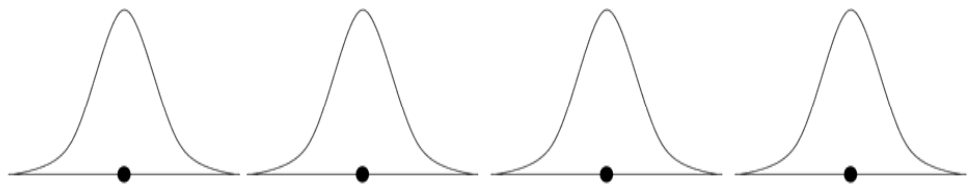
Partially filled d-orbitals

Partially filled f-orbitals

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.

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

Electronic Bands in Solids



| Property | Energy levels | Representation | Example |
|------------------|---------------|---|---|
| Insulator | Atomic levels | Localized electrons $n_{i\sigma}$ | Solid Ne NaCl |
| Correlated metal | Narrow bands | $n_{i\sigma} \leftrightarrow n_{k\sigma}$ | Transition + rare earth metals/oxides (Ni, V_2O_3 , Ce) |
| Simple metal | Broad bands | Extended waves $n_{k\sigma}$ | Na, Al |

Average time spent on atom $\tau \sim \frac{\hbar}{W}$

Narrow band \rightarrow small W : Strong electronic correlations

Consequences?

Correlated electron materials

Fascinating topics for fundamental research

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

} Large susceptibilities

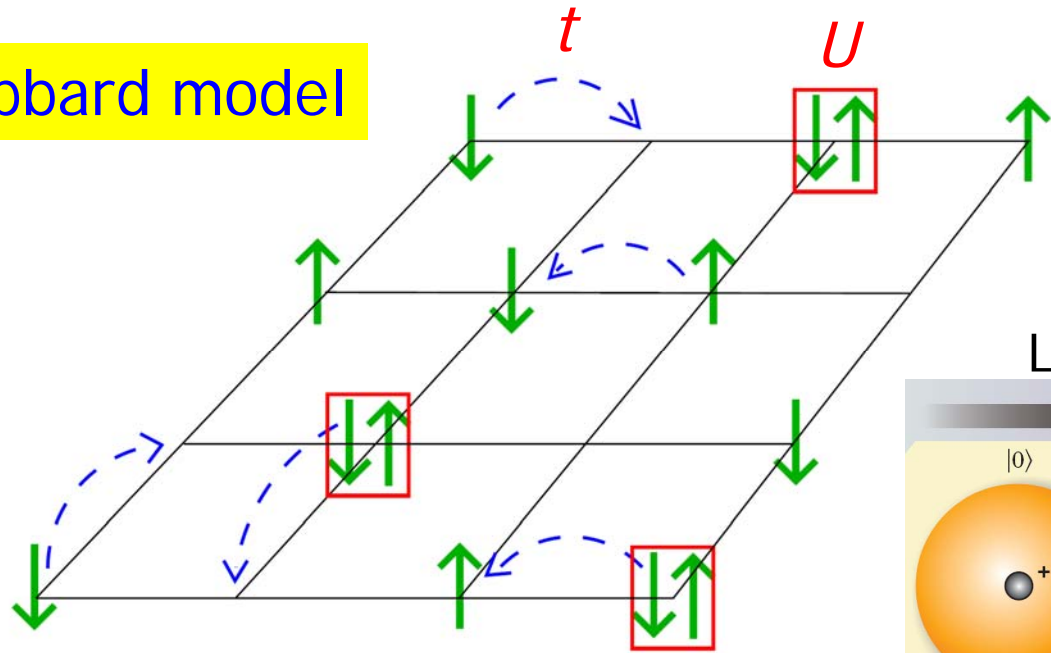
with

Technological applications:

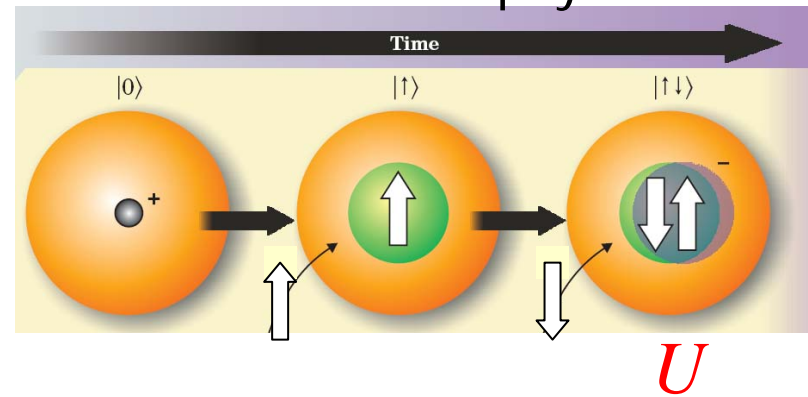
- sensors, switches
- magnetic storage
- refrigerators
- functional materials, ...

Electronic Correlations: Models

Hubbard model



Local Hubbard physics:

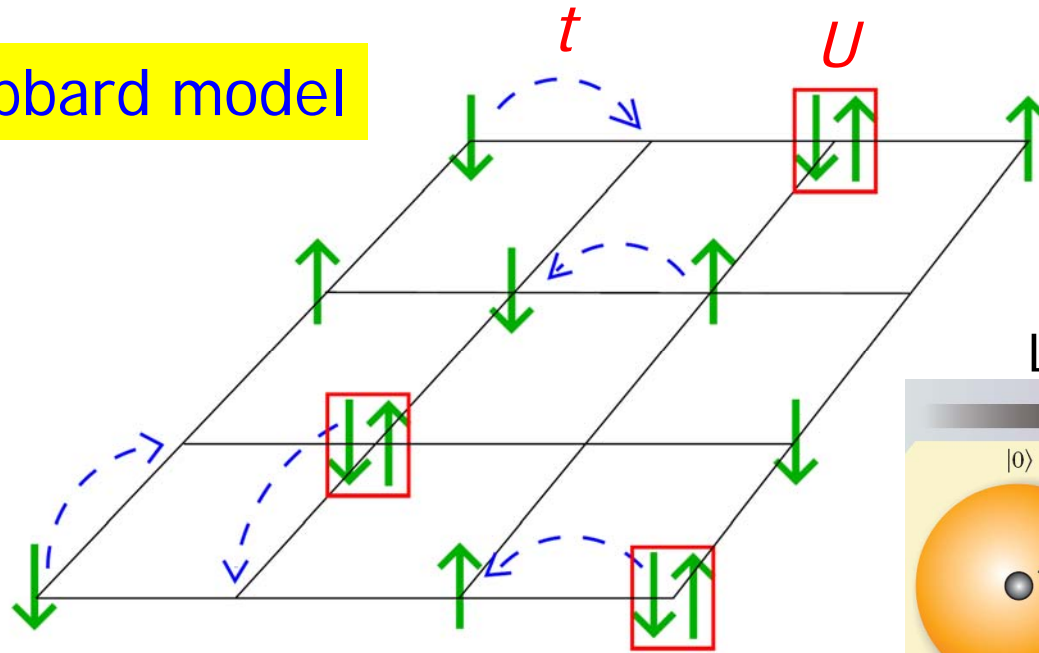


$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

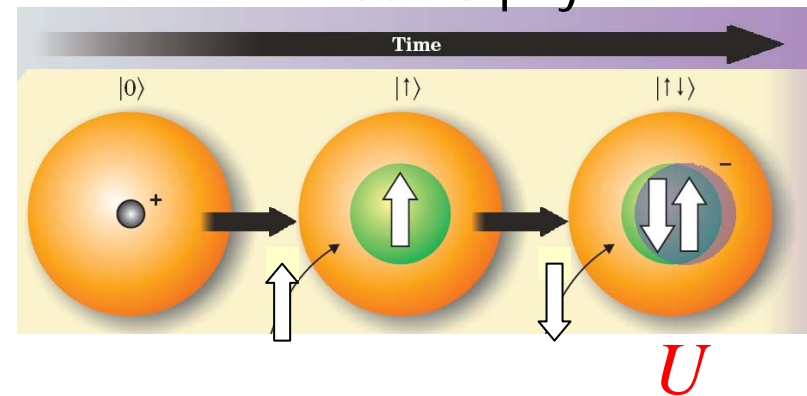


time

Hubbard model



Local Hubbard physics:



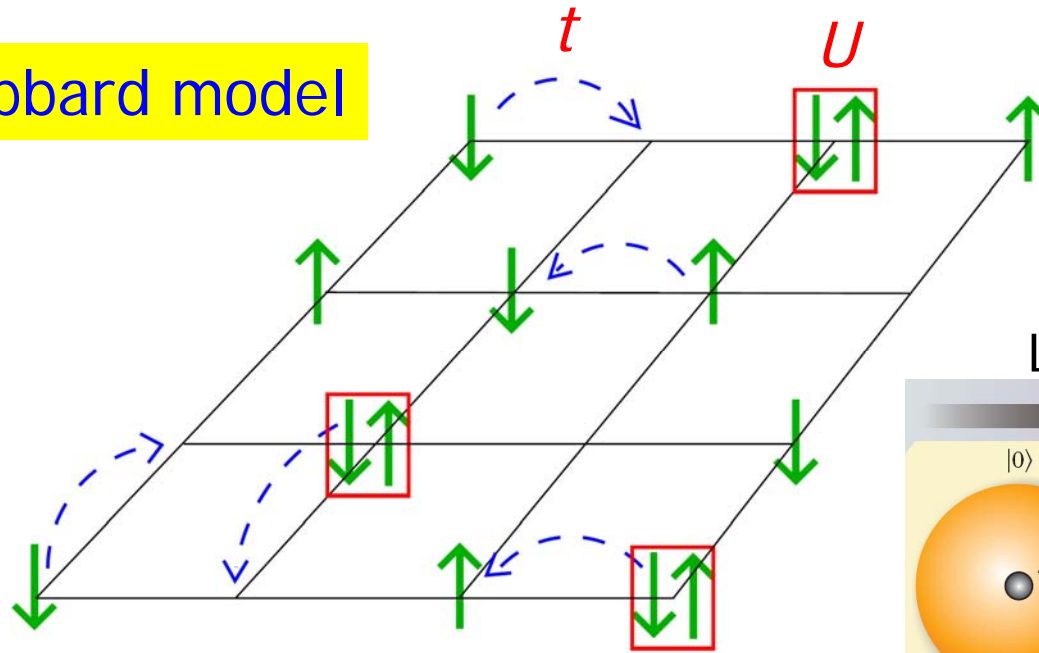
$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

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

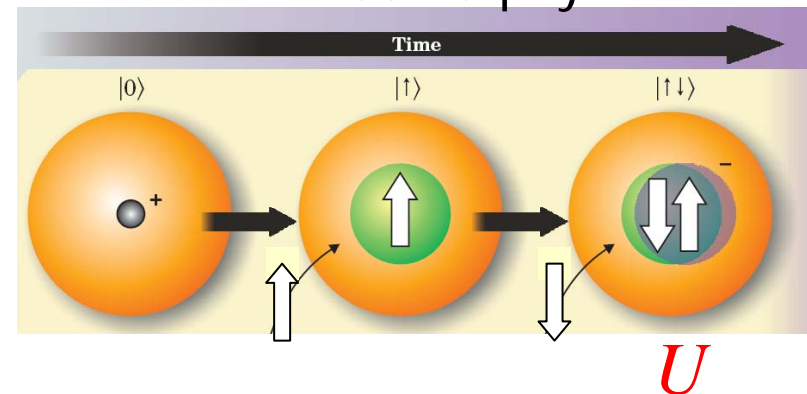
Correlation phenomena:
Metal-insulator transition, ...

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

Hubbard model



Local Hubbard physics:



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

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

Main theoretical challenge:
Construct reliable, comprehensive approximation schemes

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

4.

Dynamical Mean-Field Theory (DMFT)
of Correlated Electrons

Theory of strongly correlated electrons

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

Hypercubic lattices: Coordination number $Z=2d$

Dimension $d=1$



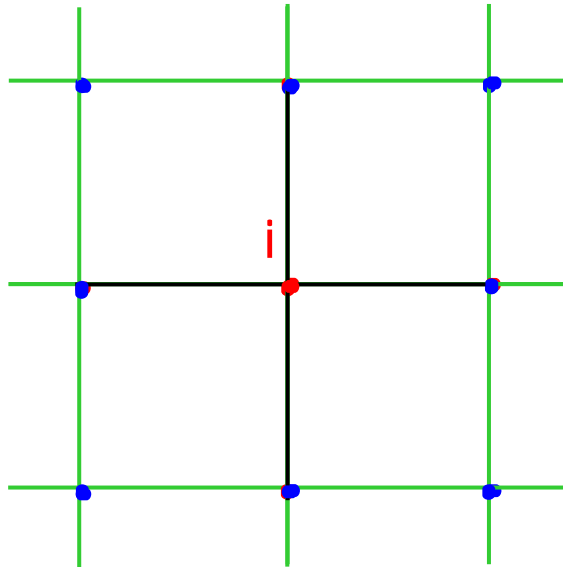
$$Z=2$$

Theory of strongly correlated electrons

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

Hypercubic lattices: Coordination number $Z=2d$

Dimension $d=2$



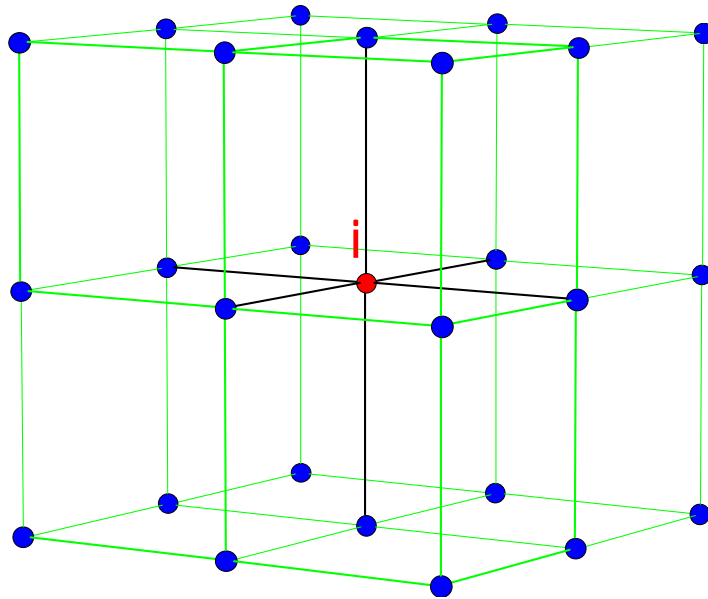
$Z=4$

Theory of strongly correlated electrons

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

Hypercubic lattices: Coordination number $Z=2d$

Dimension $d=3$



$Z=6$

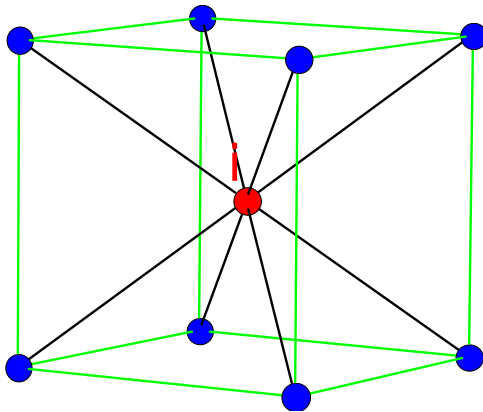
Theory of strongly correlated electrons

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

Hubbard model

Body-centered cubic lattice

Dimension $d=3$



$$Z=8$$

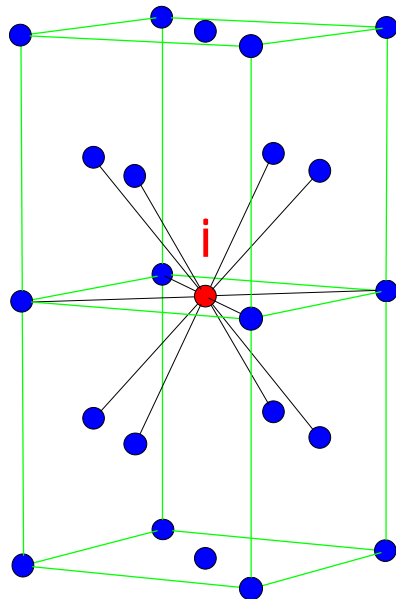
Theory of strongly correlated electrons

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

Hubbard model

Face-centered cubic lattice

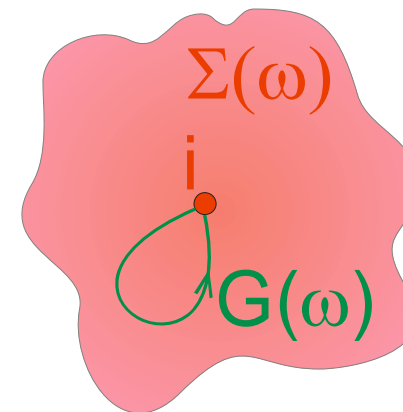
Dimension $d=3$



$Z=12$

Metzner, DV (1989)

$d \rightarrow \infty$
 $Z \rightarrow \infty$

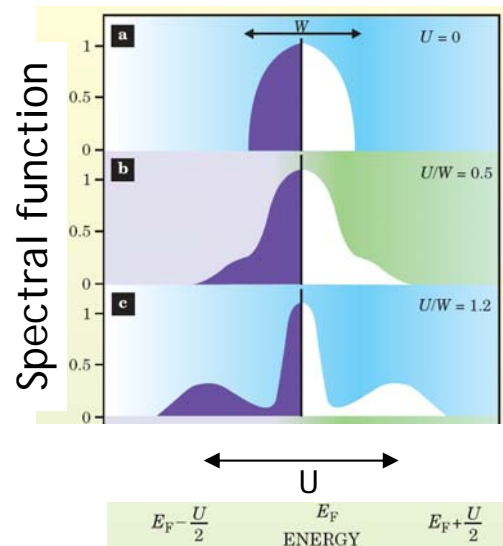
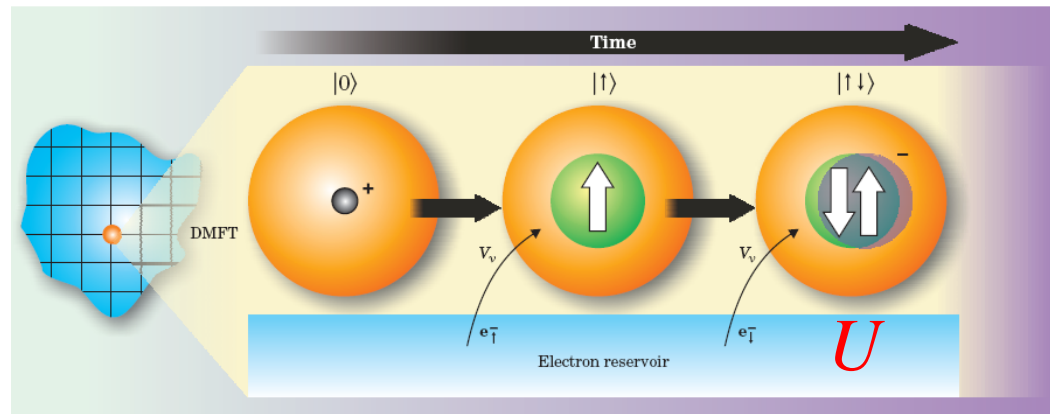


“Dynamical mean-field theory”

Müller-Hartmann (1989), Janis (1991)
Georges and Kotliar (1992)

Dynamical mean-field theory of correlated electrons

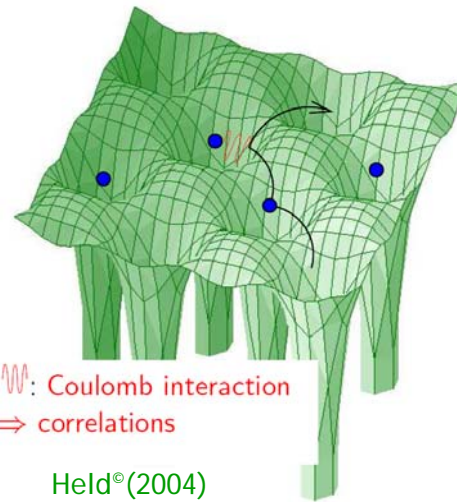
Proper **time** resolved treatment of **local** electronic interactions:



Physics Today
Kotliar, DV (2004)

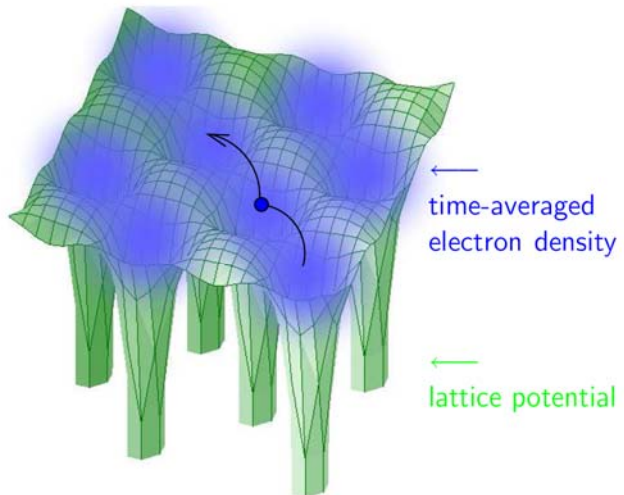
Experimentally
measurable ?

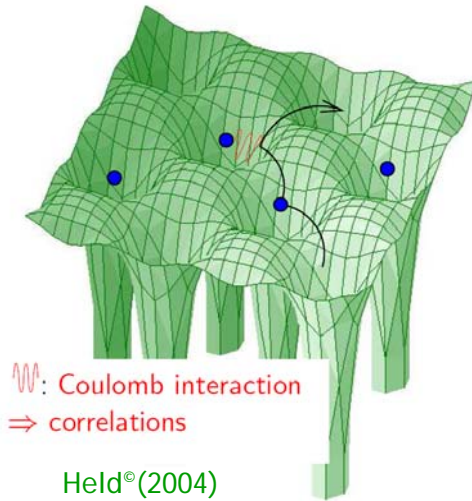
Correlated Electron: Materials



DFT/LDA

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



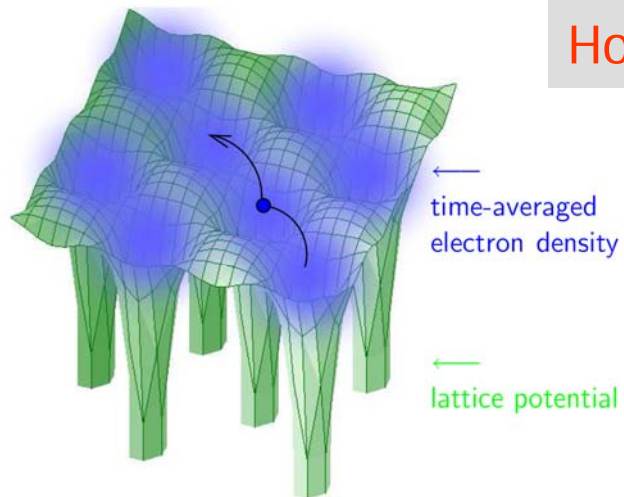


DFT/LDA

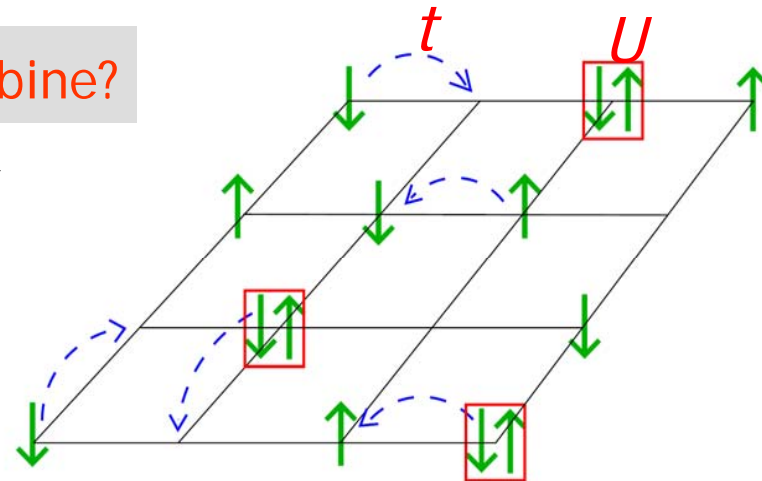
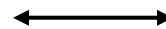
Model Hamiltonians

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

- 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, KKR, ...)

+

Local electronic correlations
(Many-body theory: DMFT)



LDA+DMFT

Anisimov *et al.* (1997)
Lichtenstein, Katsnelson (1998)
Nekrasov *et al.* (2000)

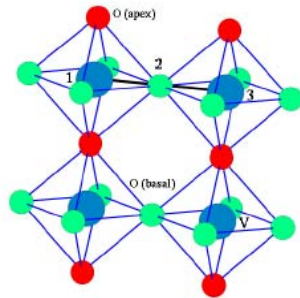
Kotliar, DV (Physics Today, March 2004)
Kotliar *et al.* (RMP, 2006)

Application of LDA+DMFT:
(Sr,Ca)VO₃

Electronic structure

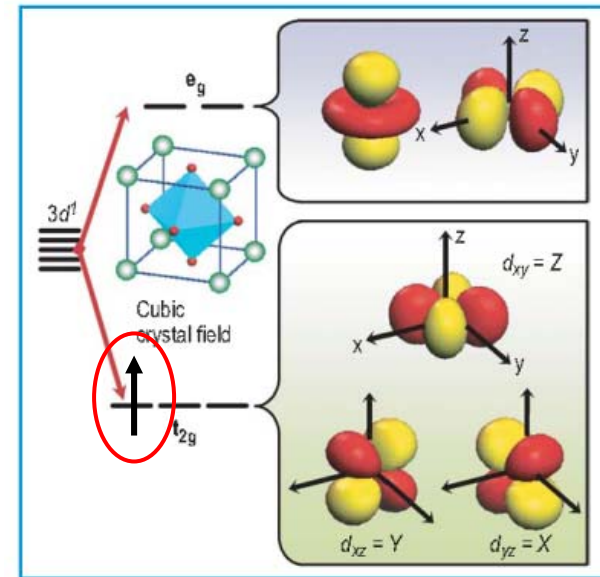
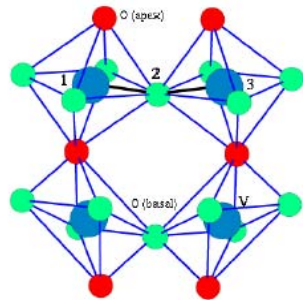
Crystal structure

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

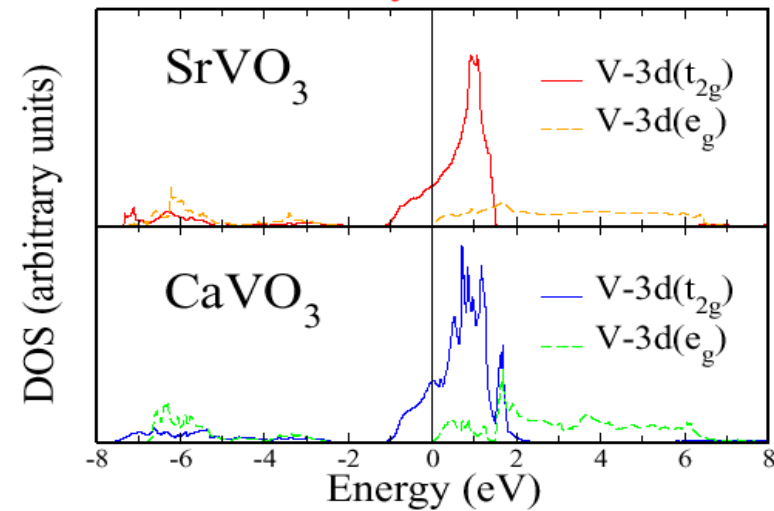


orthorhombic distortion

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

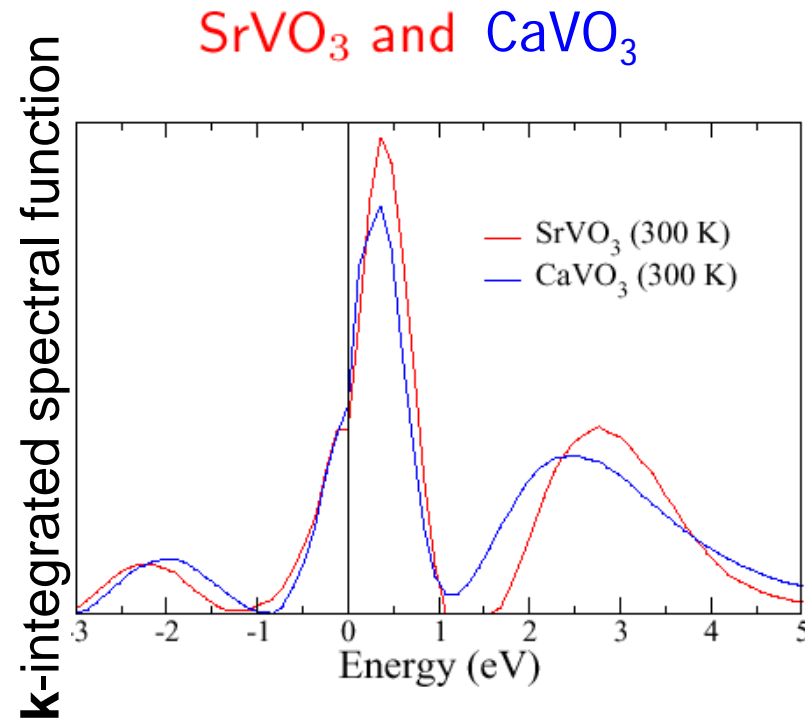


LDA density of states



No correlation effects/spectral transfer

LDA+DMFT results



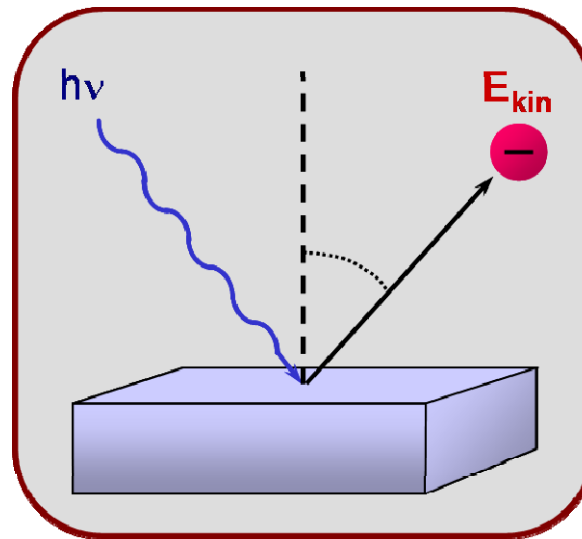
constrained LDA:
U=5.55 eV, J=1.0 eV

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

How to measure ?

Excursion: Spectroscopy

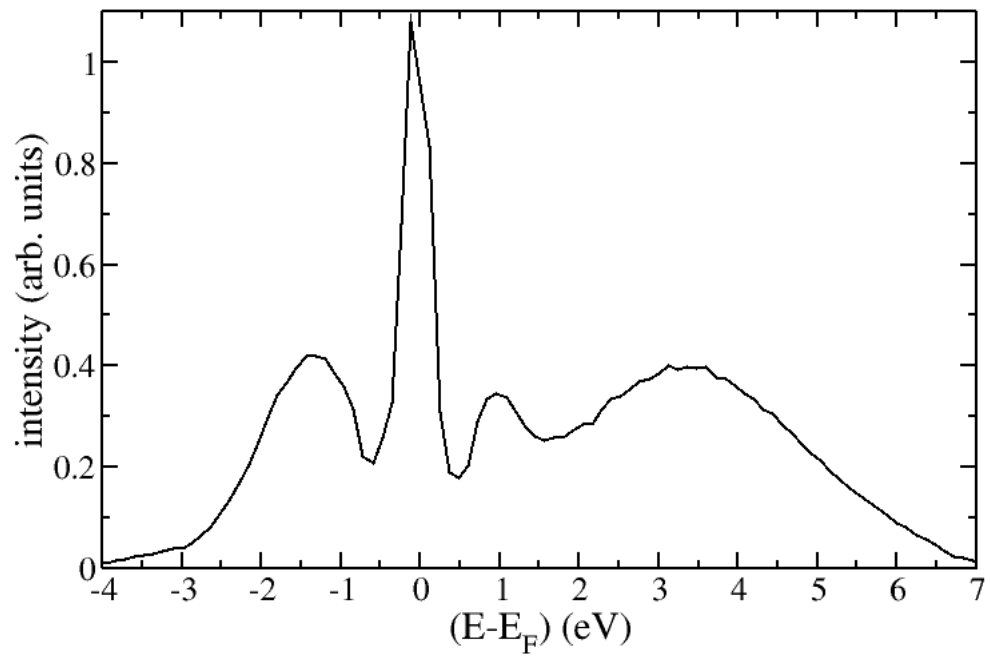
1. Photoemission Spectroscopy (PES)



Angular Resolved PES = ARPES

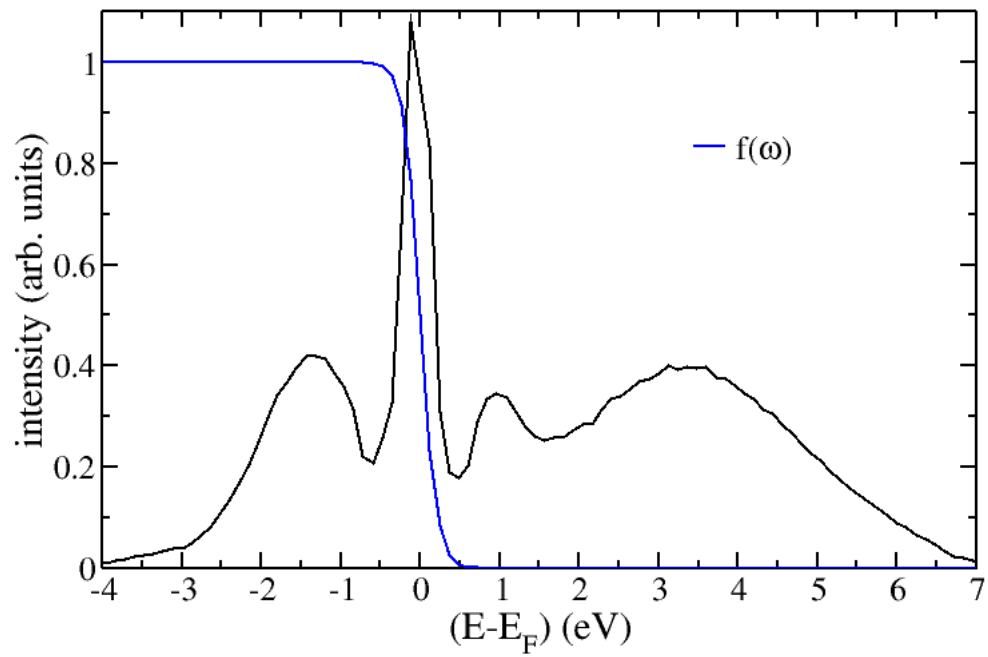
Measures **occupied** states of electronic spectral function

PES



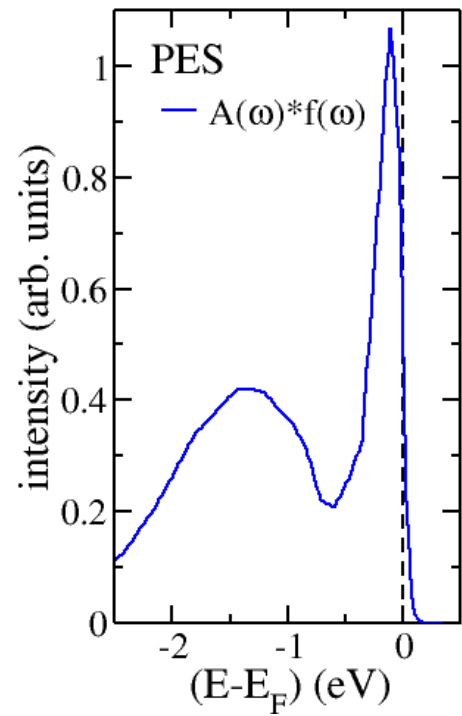
Ideal spectral function of a material

PES



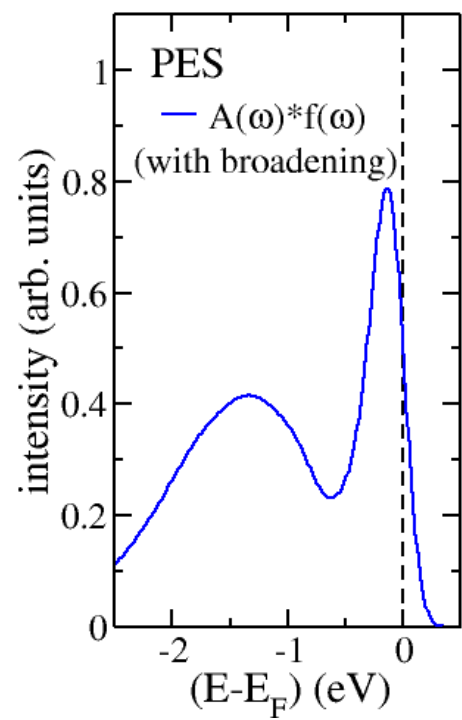
Ideal spectral function of a material

PES



Occupied states
(ideal)

PES



Occupied states
(experiment)

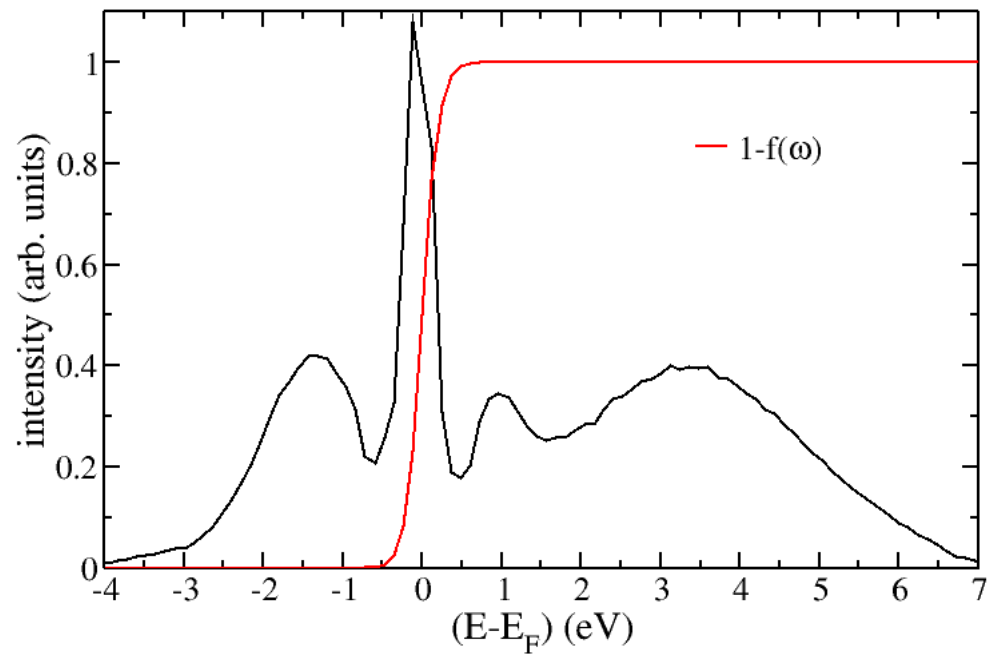
2. Inverse Photoemission Spectroscopy (IPES)

Measures **unoccupied** states of electronic spectral function

Information also available by:

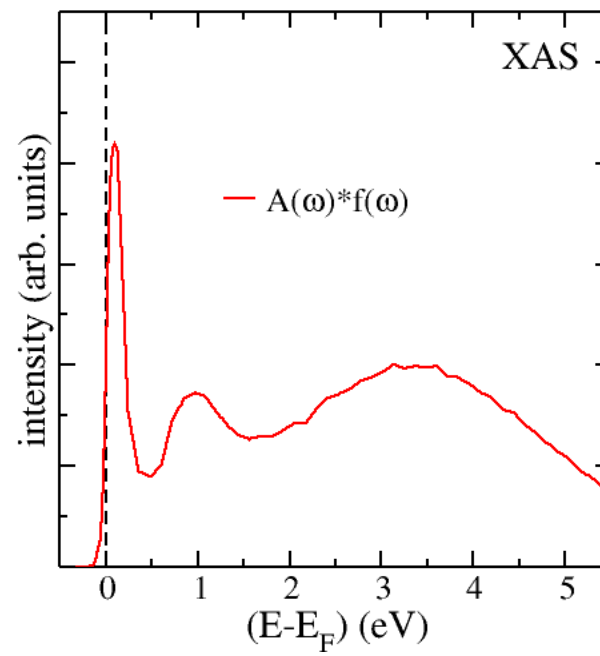
X-ray absorption spectroscopy (XAS)

IPES/XAS



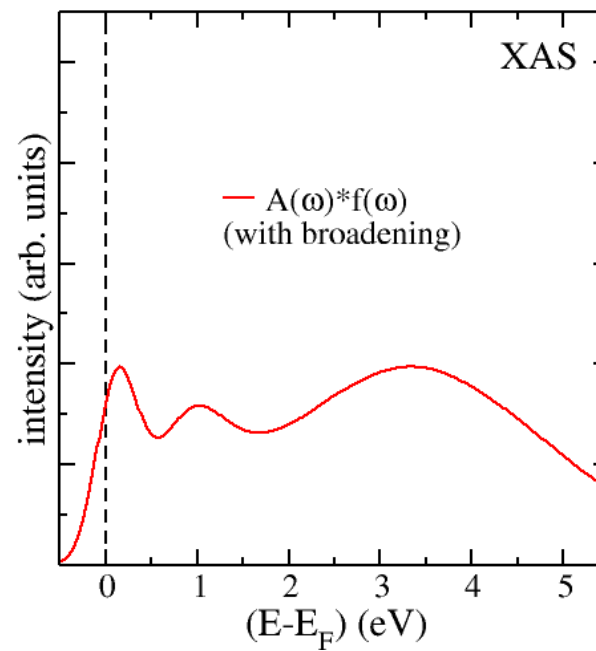
Ideal spectral function of a material

IPES/XAS



Unoccupied states
(ideal)

IPES/XAS

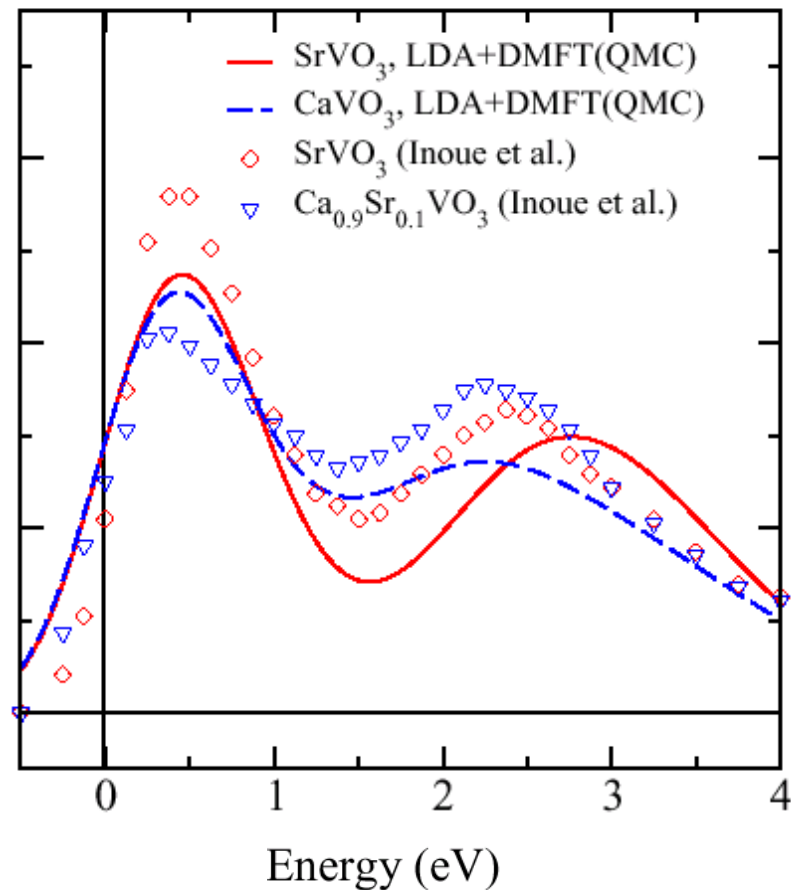
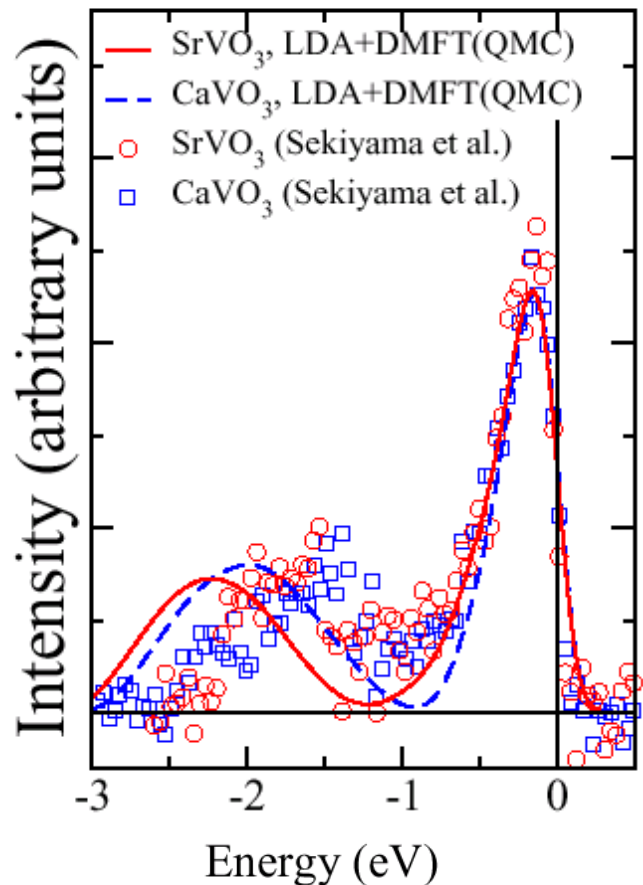


Unoccupied states
(measured)

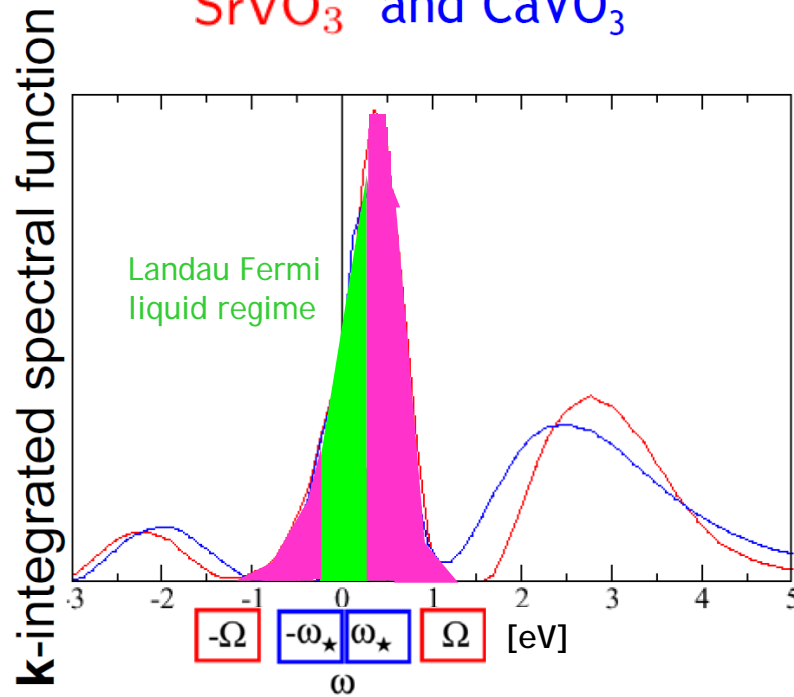
Comparison with experiment

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

- (i) bulk-sensitive high-resolution photoemission spectra (PES)
- (ii) $1s$ x-ray absorption spectra (XAS) → unoccupied states



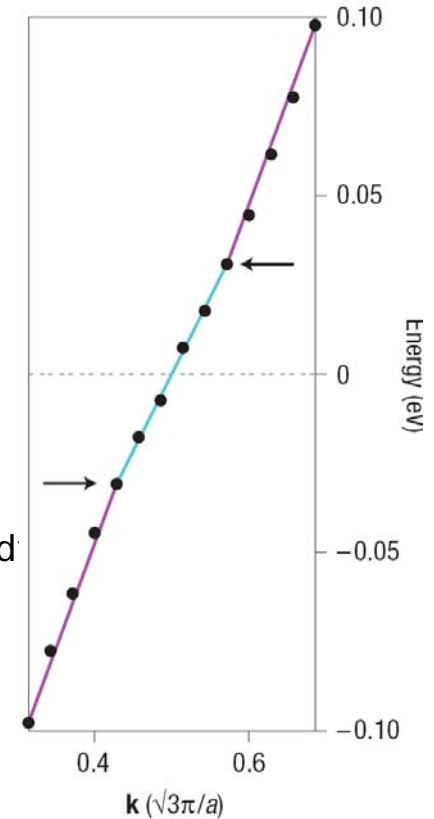
SrVO₃ and CaVO₃



Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV; Nature Phys. (2007)

$$\omega_* = Z_{FL} D_{LDA}$$

LDA bandwidth



“Kinks” in the quasiparticle dispersion E_k at $\pm\omega_*$

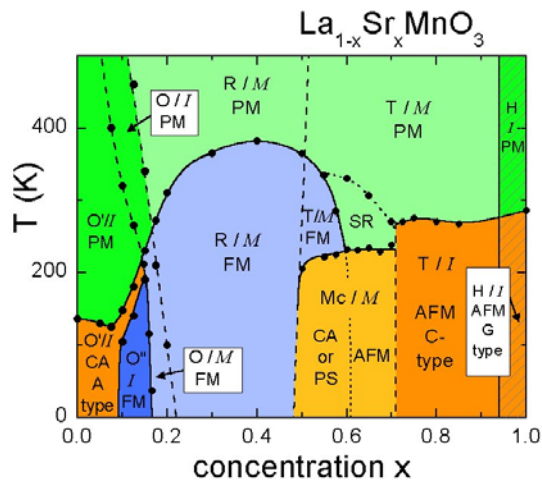
→ Kinks in high-resolution ARPES of Ni(110)

Hofmann, Cui, Schäfer, Meyer, Höpfner, Blumenstein, Paul, Patthey, Rotenberg, Bünemann, Gebhard, Ohm, Weber, Claessen; PRL (2009)

5. New Developments & Perspectives

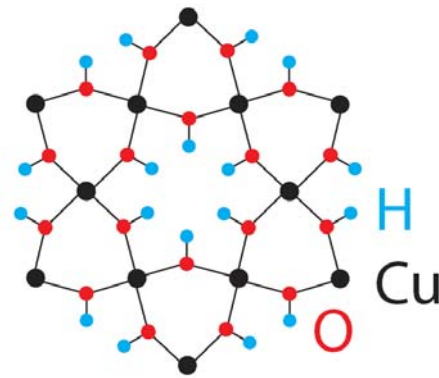
(i) Complex correlated electron materials

Explanation & prediction of properties of complex materials

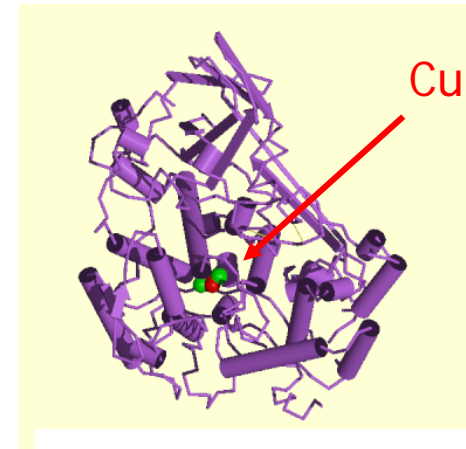


Phase diagram of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$

Hemberger *et al.* (2002)



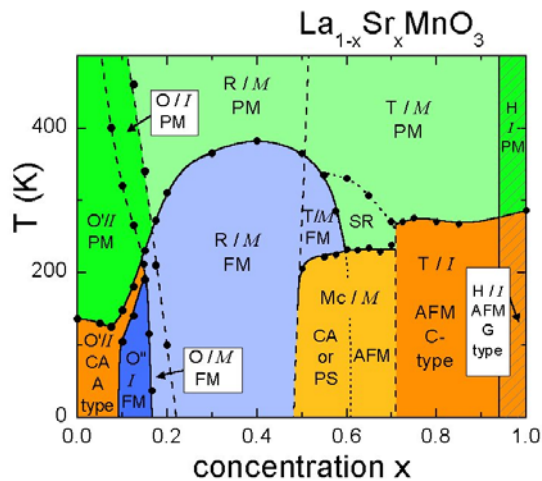
Kagome layer in $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ (herbertsmithite):
Spin liquid behavior



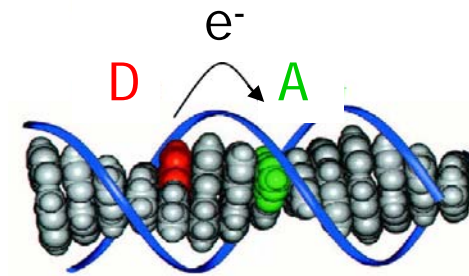
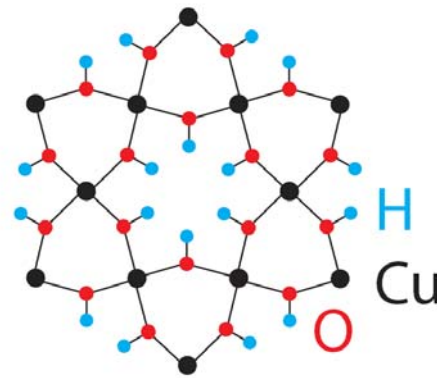
1, 2, ... multi-electron transfer in metalloprotein complexes
→ Photosynthesis

(i) Complex correlated electron materials

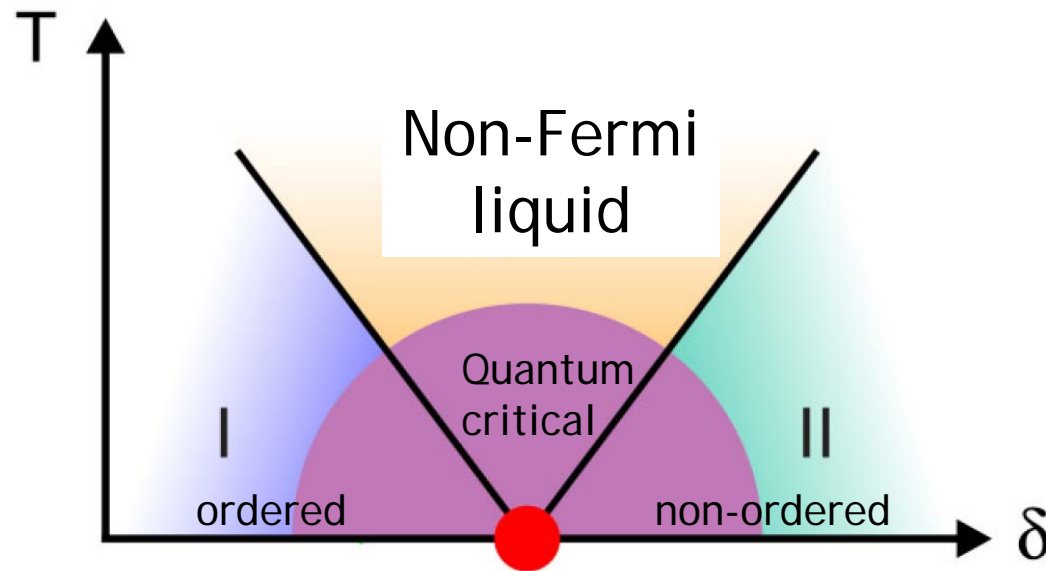
Explanation & prediction of properties of complex materials



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



(ii) Quantum phase transitions



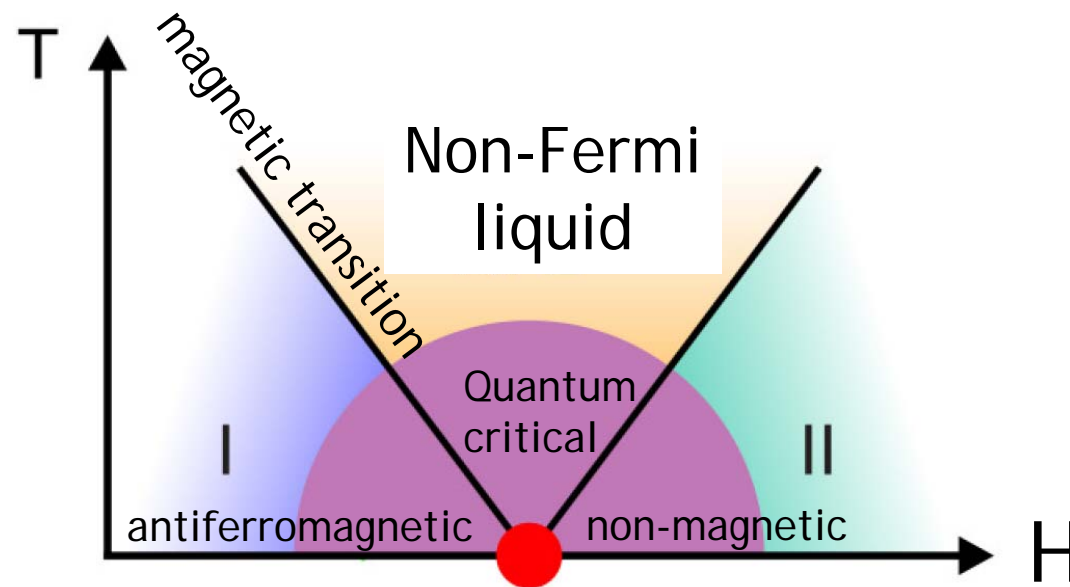
Quantum critical point

© DFG Research Unit
(Augsburg-Dresden-Göttingen-
Karlsruhe-Köln-München, 2007)

Driven by quantum fluctuations

- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

(ii) Quantum phase transitions



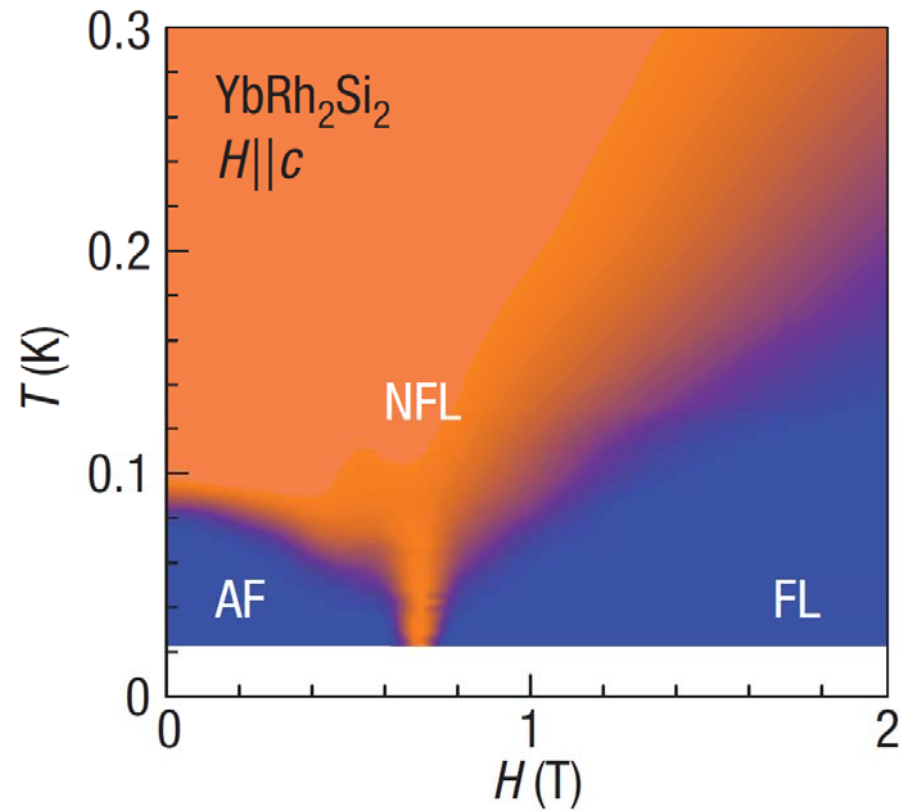
Quantum critical point

© DFG Research Unit
(Augsburg-Dresden-Göttingen-
Karlsruhe-Köln-München, 2007)

Driven by quantum fluctuations

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(ii) Quantum phase transitions



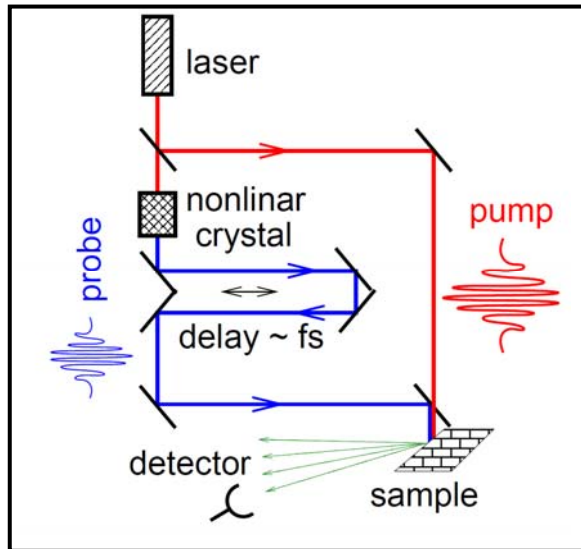
Custers *et al.* (2003)

Driven by quantum fluctuations

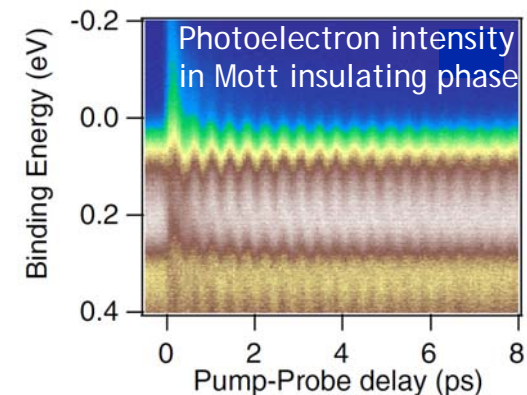
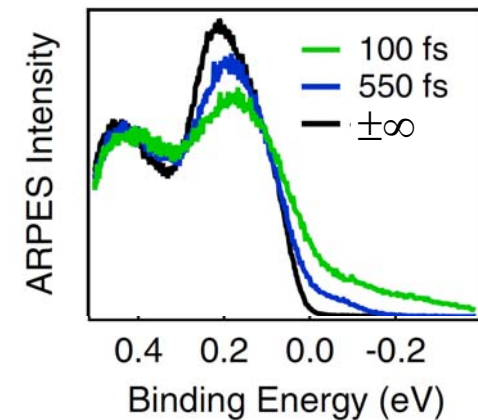
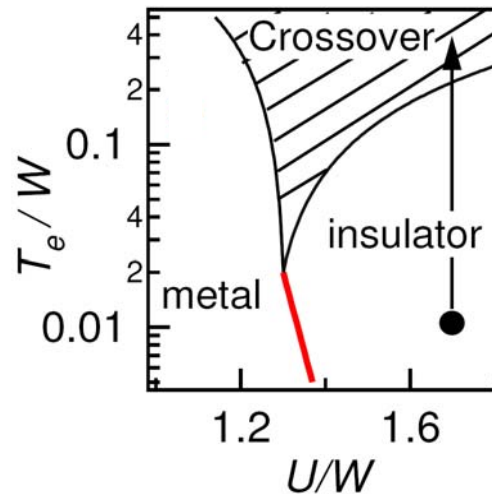
- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

(iii) Correlated electrons in non-equilibrium

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



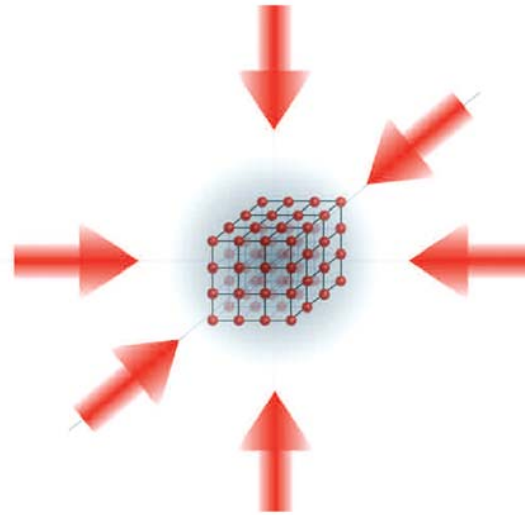
Pump-probe experiment



Perfetti *et al.* (2006)

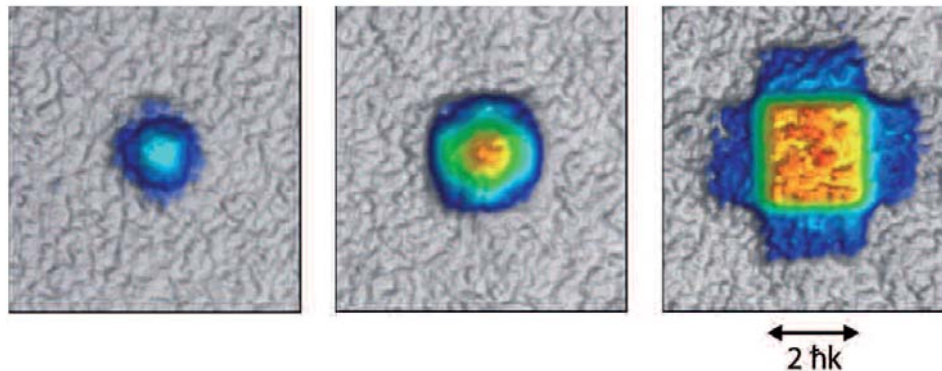
Required: Theory of non-equilibrium beyond
linear response in correlated **bulk** materials

(iv) Correlated fermionic/bosonic atoms in optical lattices



Modugno et al. (2003)

Bosonic/fermionic atoms in optical lattices

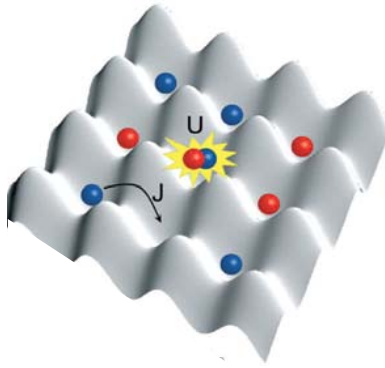


Köhl, Esslinger (2006)

Observation of Fermi surface (^{40}K atoms)

High degree of tunability: "Many-body tool box"

(iv) Correlated fermionic/bosonic atoms in optical lattices



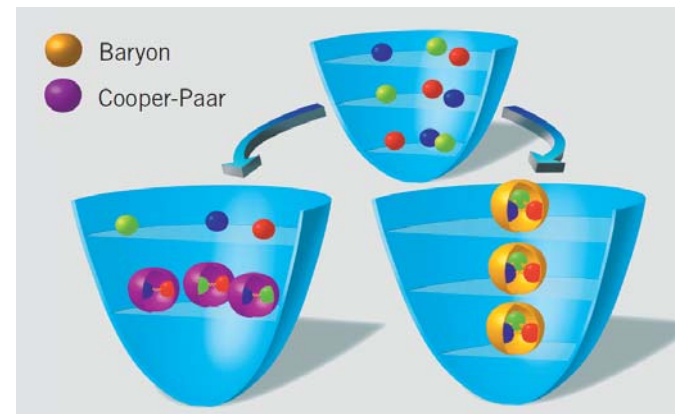
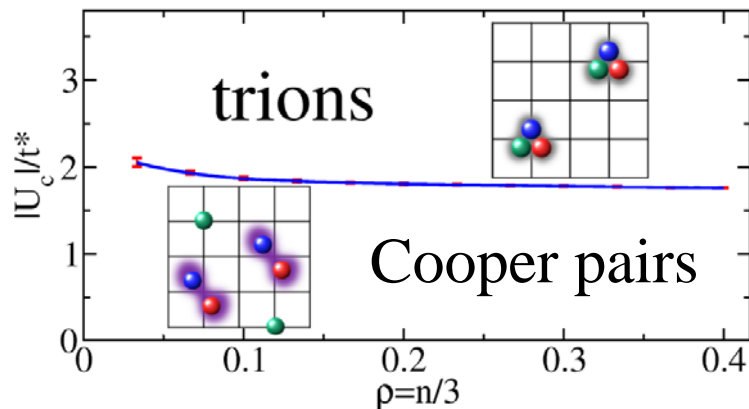
Hubbard model with ultracold atoms Jaksch *et al.* (1998)

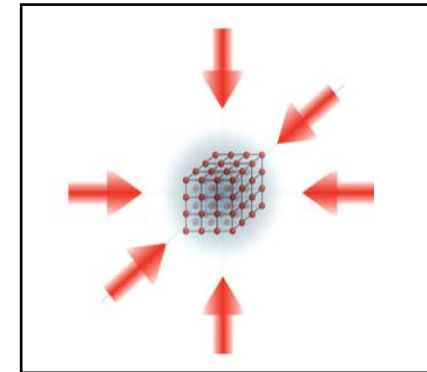
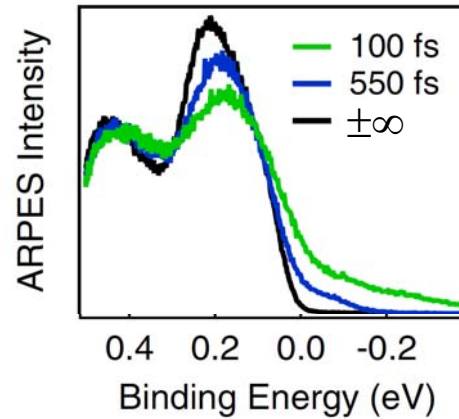
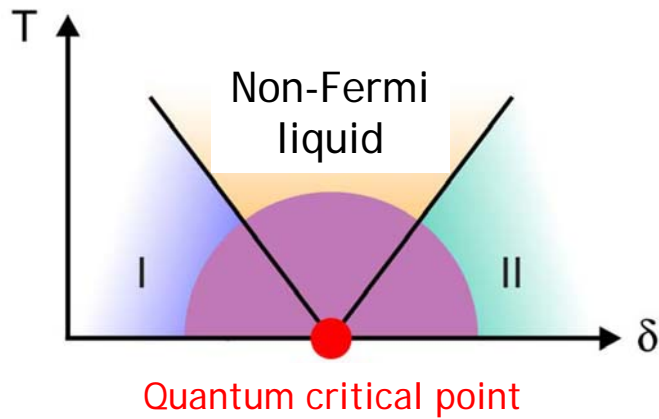
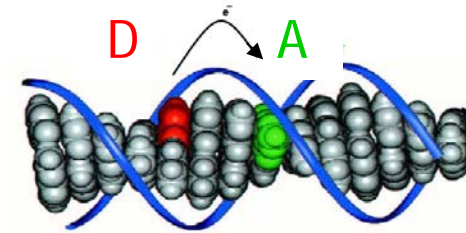
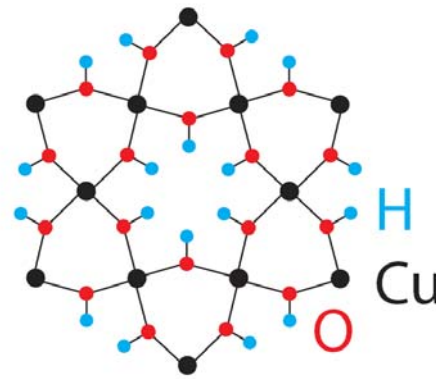
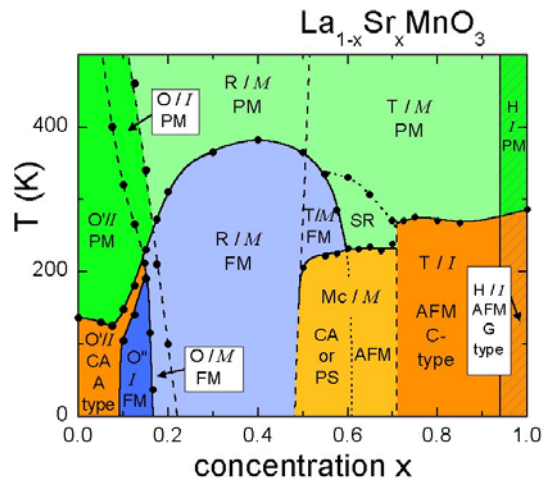
Angular momentum $L^{\text{tot}} = F \rightarrow N=2F+1$ hyperfine states

\rightarrow SU(N) Hubbard models

Honerkamp, Hofstetter (2004)

$N=3$, e.g. ${}^6\text{Li}$, $U < 0$: Color superconductivity, baryon formation (QCD)
Rapp *et al.* (2006)





Correlated many-particle systems:
More manifold and fascinating than ever