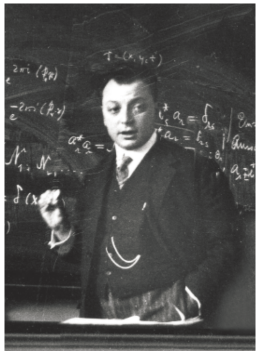
Center for Electronic Correlations and Magnetism
University of Augsburg

Surprising effects of the interaction between electrons in solids

Dieter Vollhardt



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

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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 (Fe_3O_4)

Macroscopic view:

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

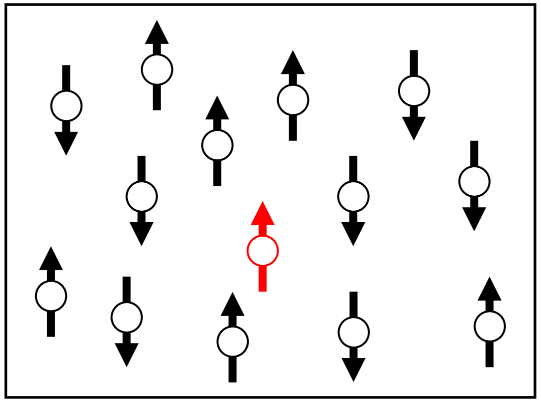
→ quantum many-particle problem

Fe_3O_4

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

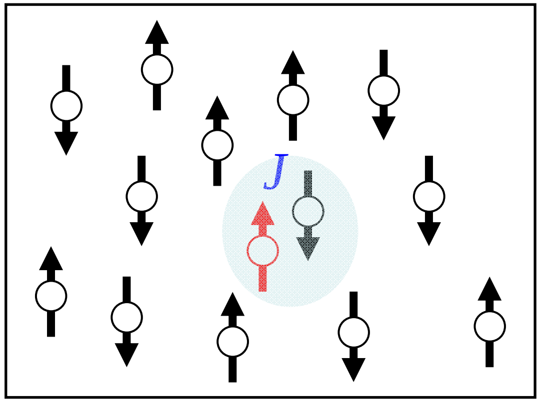
... but "dirt physics" can be fundamental and universal

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



$T>T_K$ (high energies)

Asymptotically free local moment



$T<T_K$ (low energies)

Screening of moment (confinement)

"Kondo effect"

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

Prototypical 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

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

effective $\boxed{\text{("quasi") particles}}$ + effective interactions

Non-interacting electrons

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

$N \to \infty$ $\Downarrow$

Pauli exclusion principle
(Hamburg, 1925)

Fermi-Dirac statistics

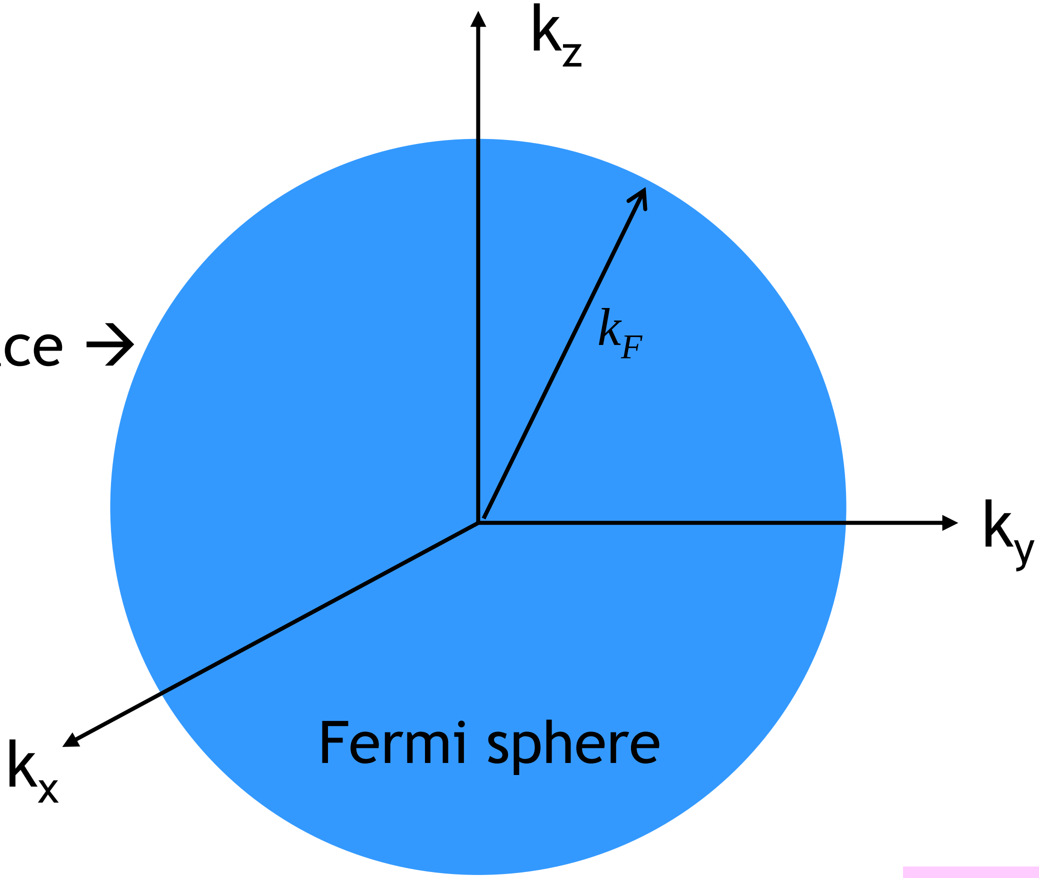
$\Downarrow$

Ground state: $\boxed{\text{Fermi body/surface}}$

Fermi gas: **Ground state**

Fermi surface →

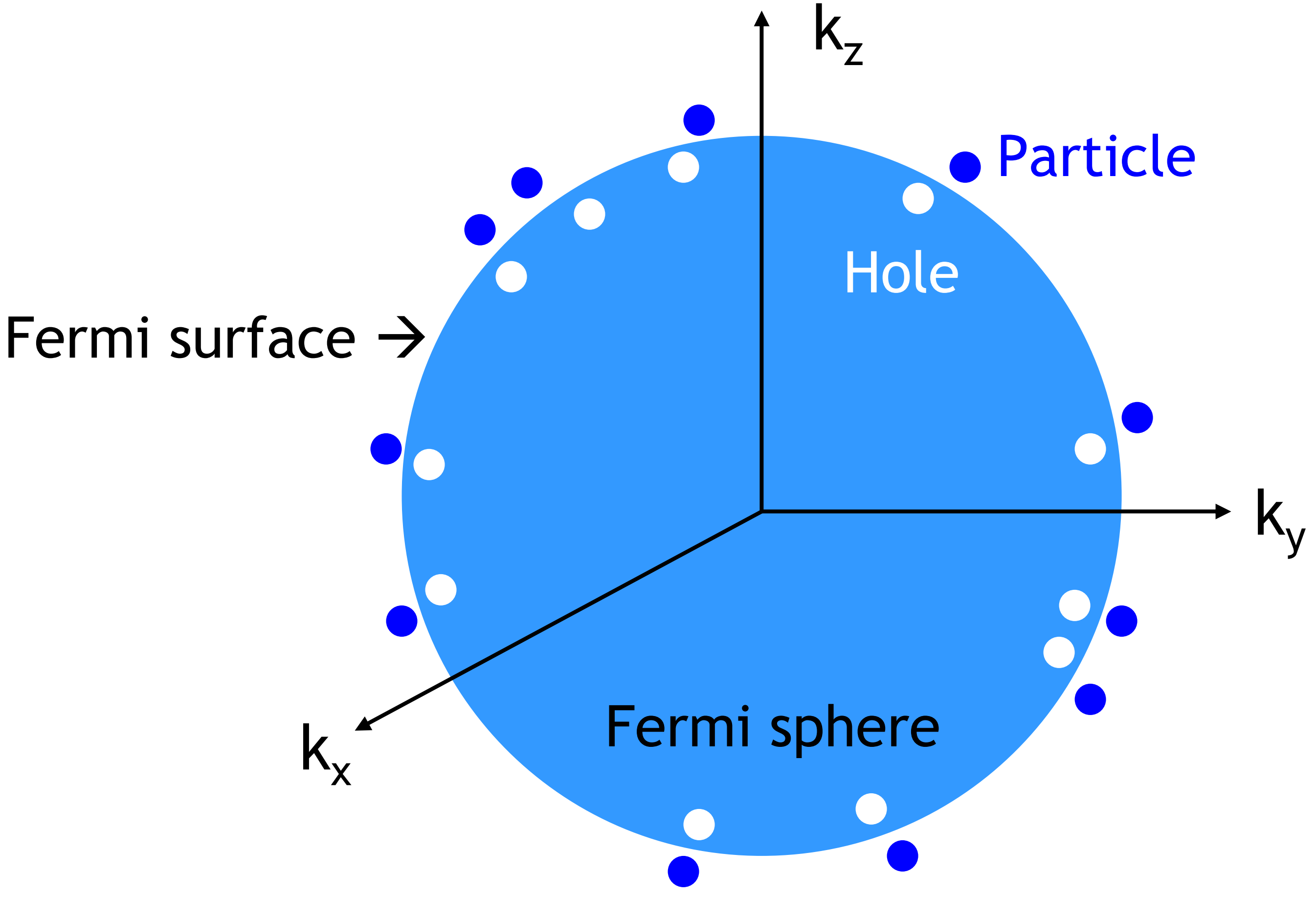
$$E_F = \frac{\hbar^2}{2m} k_F^2$$



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

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

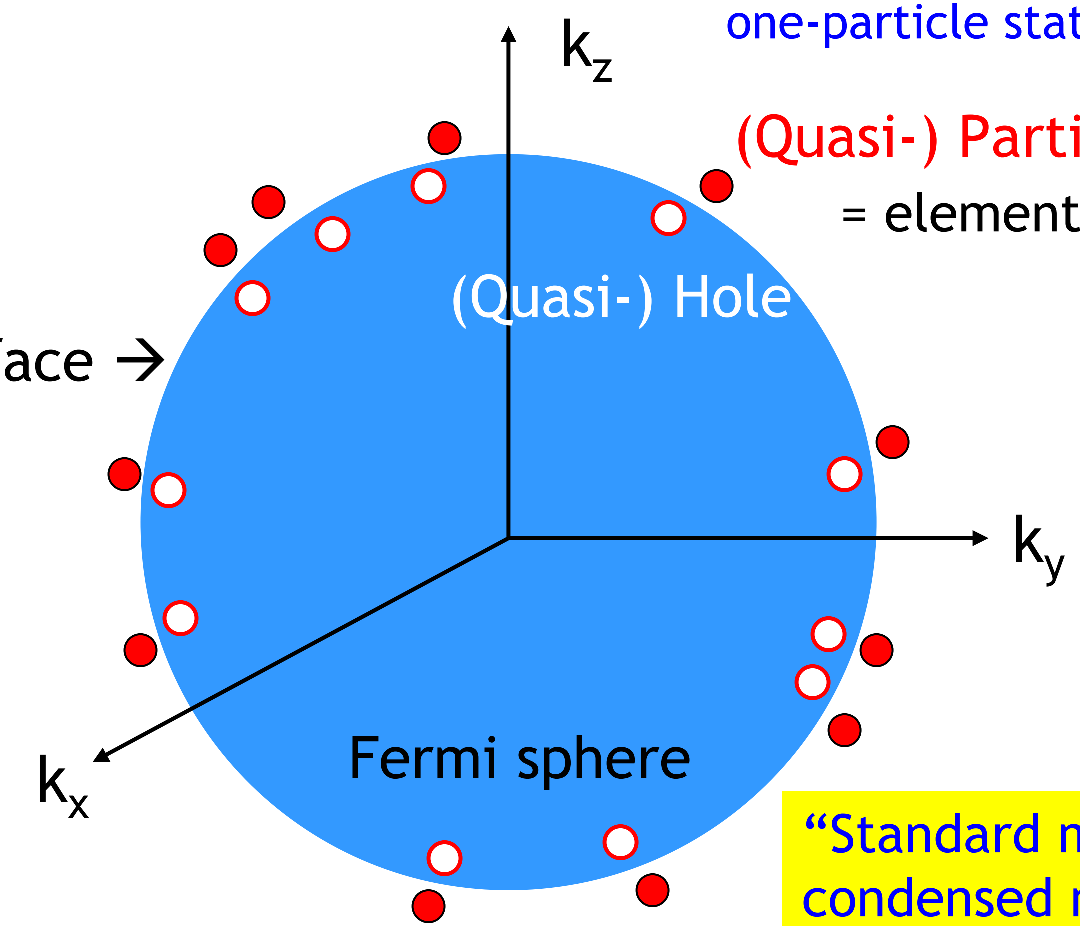
Landau (1956/58)

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

(Quasi-) Particle

= elementary excitation

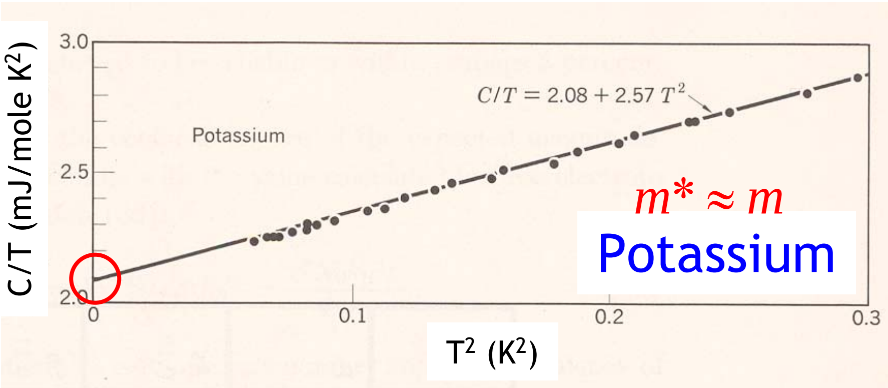
Fermi surface →



"Standard model of
condensed matter physics"

Well-defined **k**-states ("quasiparticles") with
- finite life time
- effective mass
- effective interaction

Simple metals

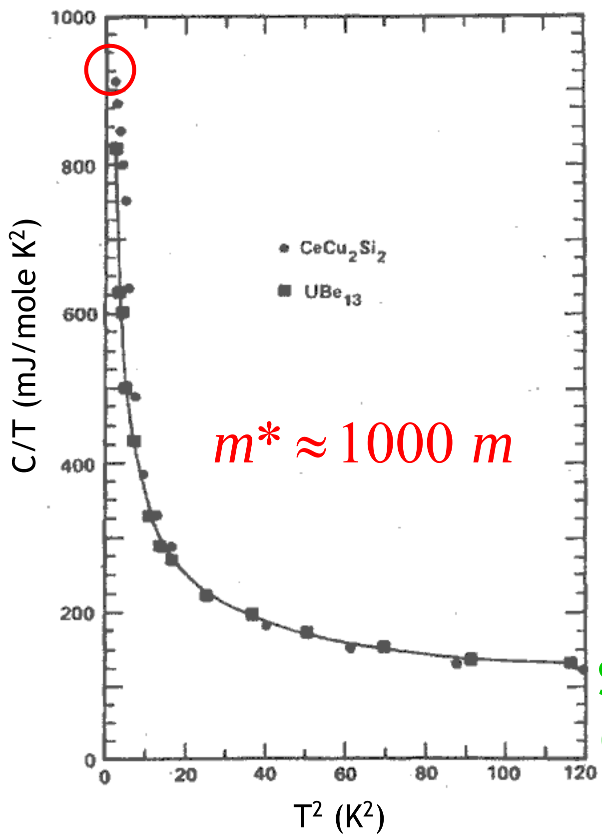


$$\lim_{T\to 0}\frac{c_V}{T} = \gamma \propto \frac{m^*}{m}$$

Result of
elementary excitations
(quasiparticles)

"Heavy Fermions"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

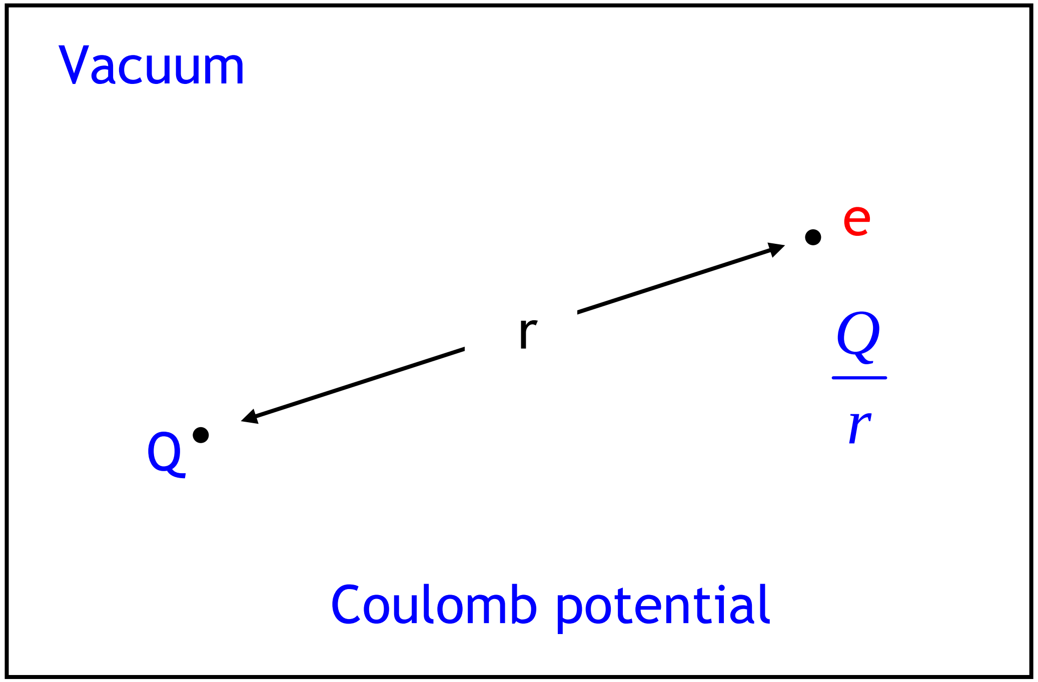
$CeCu_2Si_2$, UBe_{13}:
very heavy quasiparticles:
Kondo impurity physics

Interacting many-particle systems

Elementary (“bare”) particles + fundamental interactions

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

effective (“quasi”) particles + $\boxed{\text{effective interactions}}$



Interacting many-particle systems

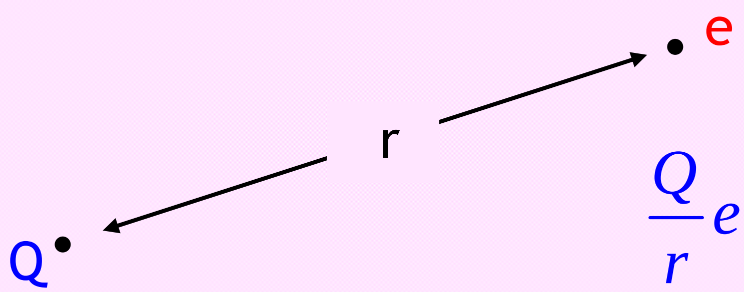
Elementary ("bare") particles + fundamental interactions

$$\Big\downarrow \ \text{\# particles } N \to \infty$$

effective ("quasi") particles + $\boxed{\text{effective interactions}}$

Electron gas: Screening

Simplest approximation: Thomas-Fermi



$$\frac{Q}{r} e^{-r/\xi}$$

Effective Yukawa potential

Interacting many-particle systems

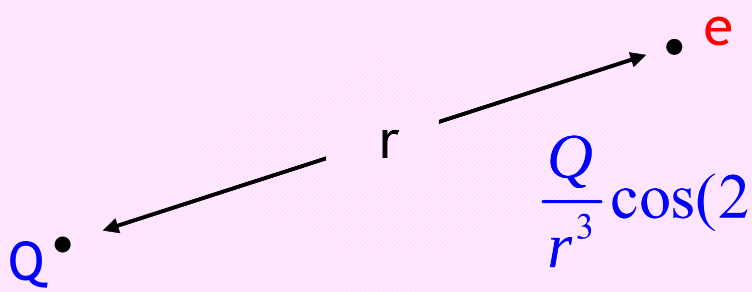
Elementary ("bare") particles + fundamental interactions

$$\Big\downarrow \ \text{\# particles } N \to \infty$$

effective ("quasi") particles + $\boxed{\text{effective interactions}}$

Electron gas: Screening

Better approximation: Lindhard



$$\frac{Q}{r^3}\cos(2k_F r)$$

Friedel oscillations

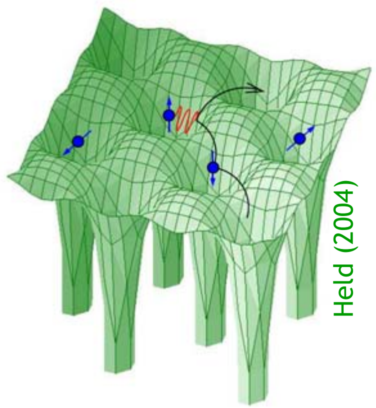
Interacting many-particle systems

Elementary (“bare”) particles + fundamental interactions

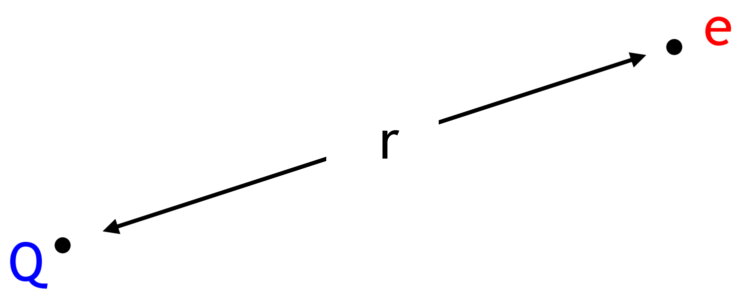
$\downarrow$ # particles $N \to \infty$

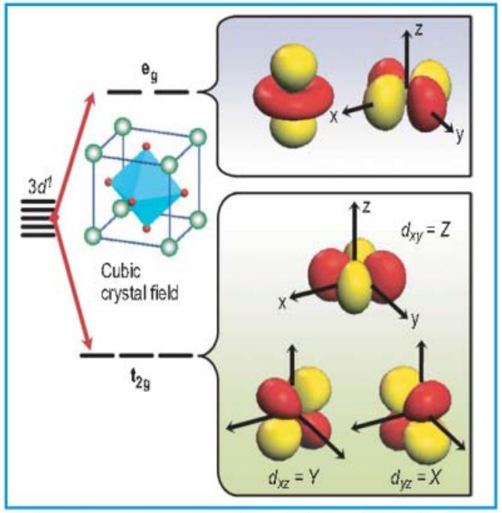
effective (“quasi”) particles + $\boxed{\text{effective interactions}}$

Electrons in real solids



Held (2004)





“Strong effective interaction”
of electrons in localized orbitals

Interacting many-particle systems

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

Entirely new phenomena, e.g., phase transitions

$\downarrow$

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

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

Entirely new phenomena, e.g., phase transitions

$\downarrow$

Unpredicted behavior "emerges"

Examples:

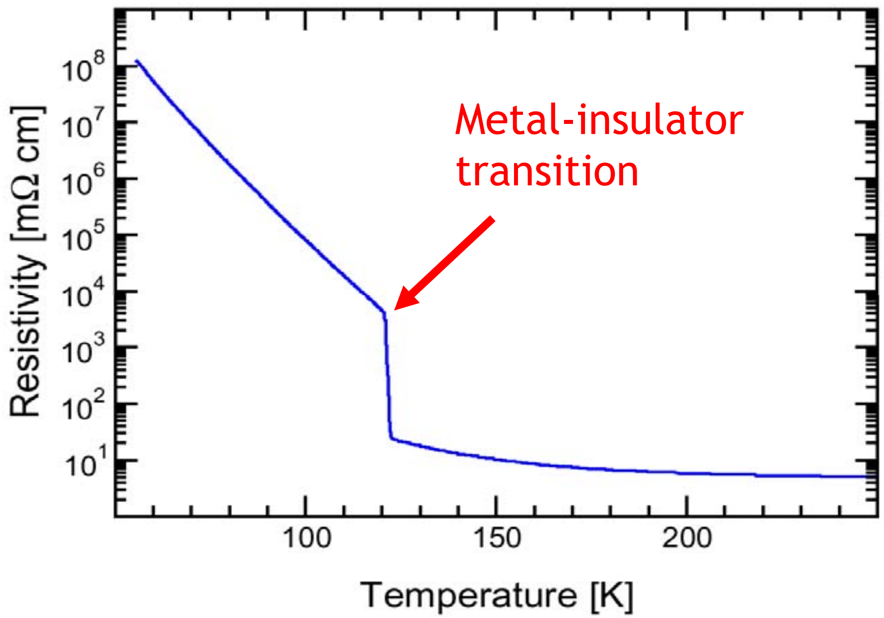
Superconductivity	Traffic
Magnetism	Weather
Metal-insulator transition	Stock market

Interacting many-particle systems

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

Entirely new phenomena, e.g., phase transitions

Fe_3O_4



Why?

Electrons interact by strong effective repulsion

Correlations

Correlations in mathematics, natural sciences:

$$\boxed{\langle AB \rangle \neq \langle A \rangle \langle B \rangle}$$

e.g., densities:

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

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

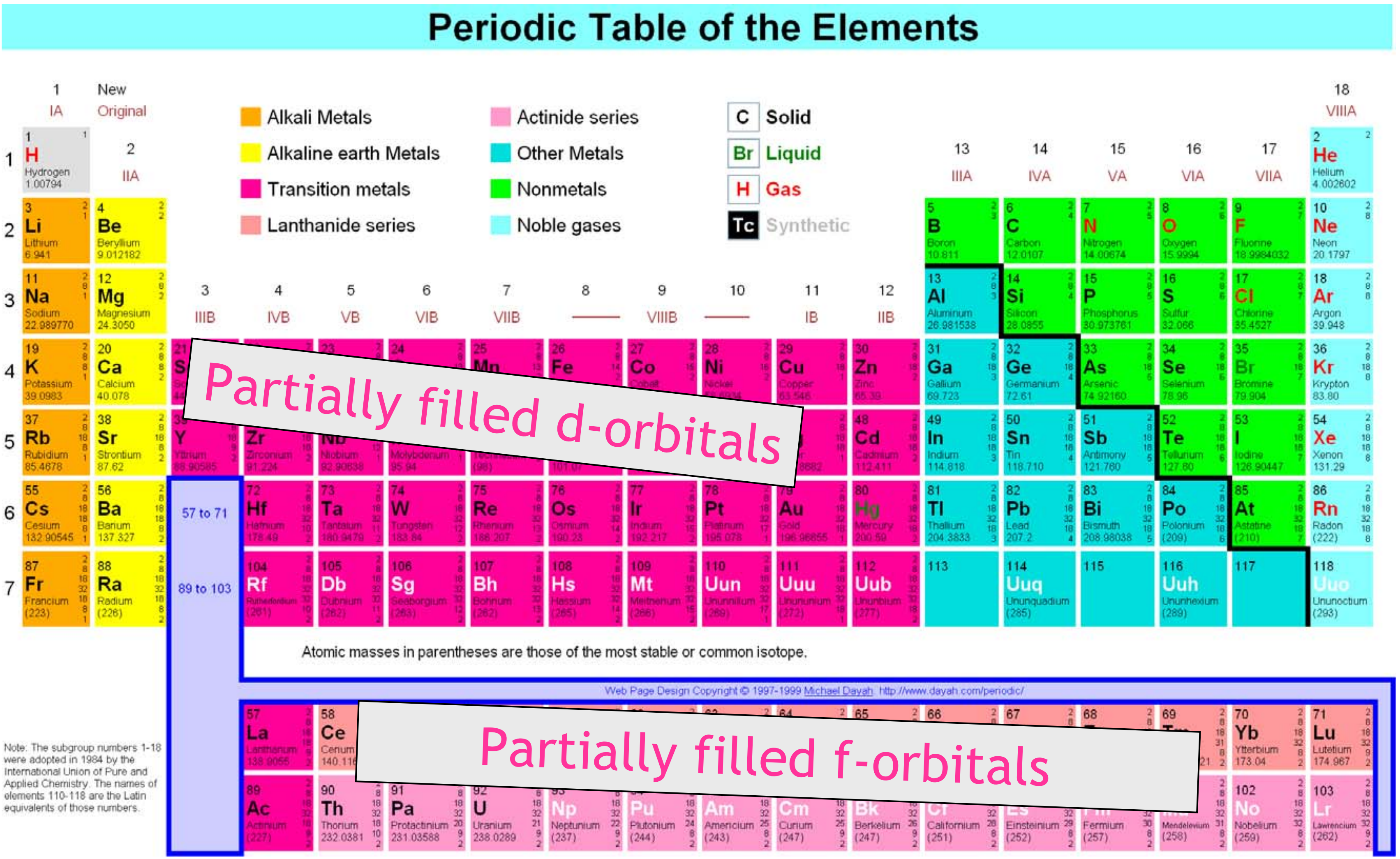
→ The Fermi gas $\psi(1,\ldots,N) = \mathcal{A} \prod_{i=1}^{N} \psi_{\nu_i}(i)$ is uncorrelated,

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



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:

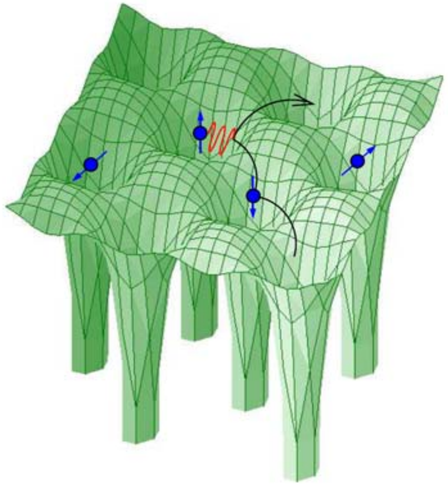
- sensors, switches, Mottronics
- spintronics
- thermoelectrics
- high-T_c superconductors
- functional materials:
  oxide heterostructures …

How to study correlated systems theoretically?

material

modeling $\Rightarrow$

realistic model

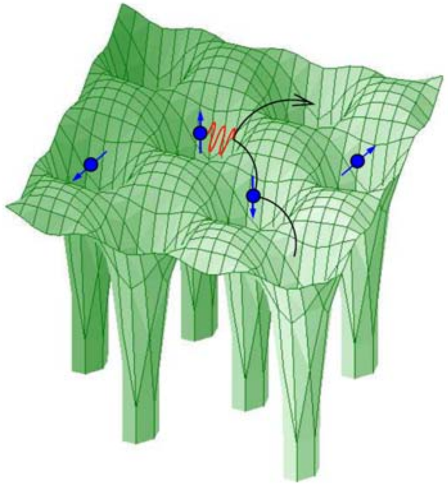


quantum many-particle problem

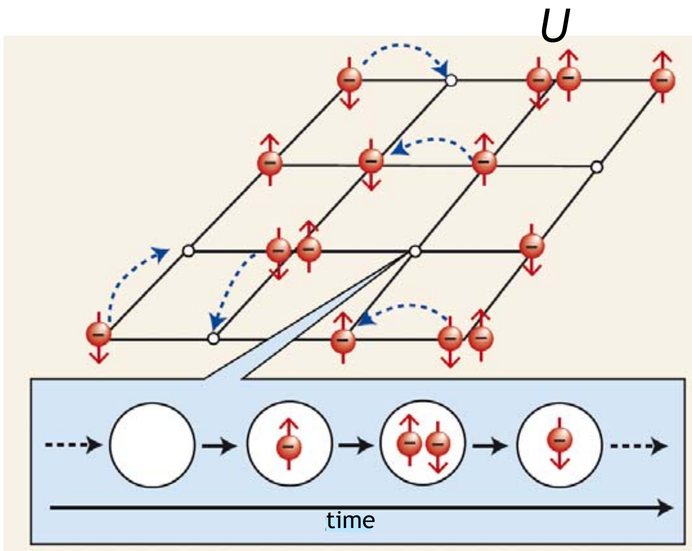
"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved."

Dirac (1929)

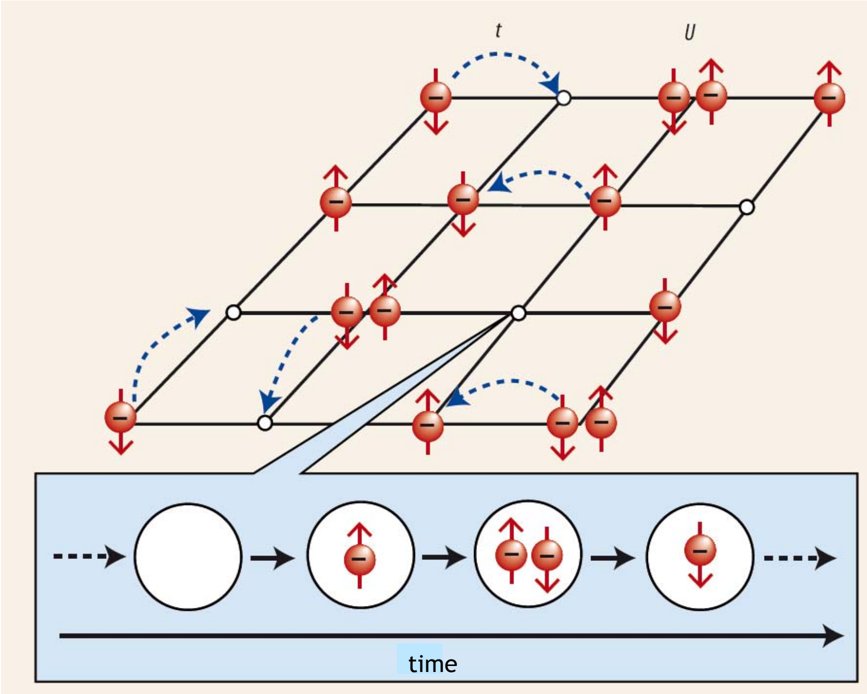
material $\overset{\text{modeling}}{\Longrightarrow}$ realistic model



$\Longrightarrow$ maximal reduction: Hubbard model



Hubbard model



Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

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

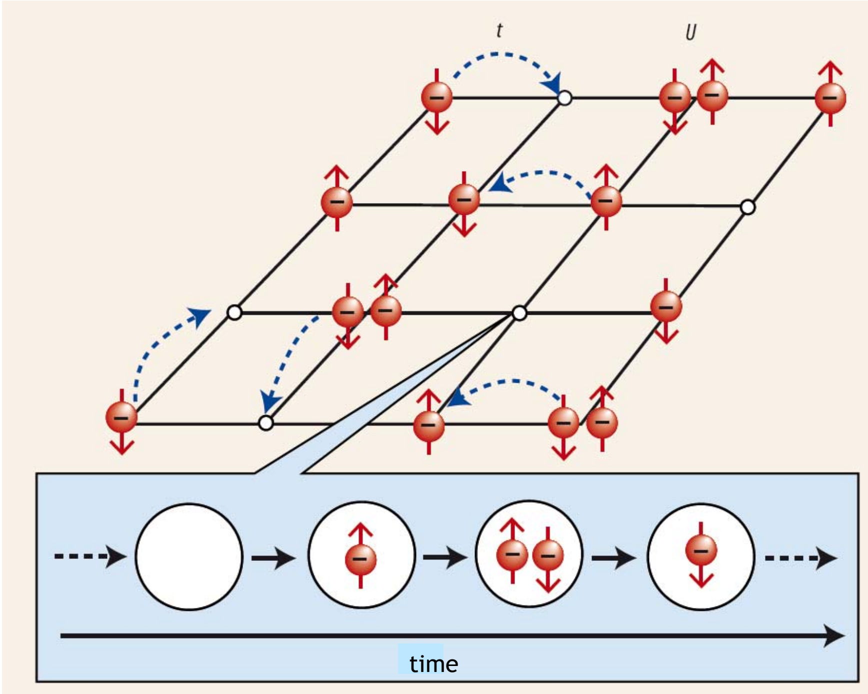
$$\boxed{\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \rangle \neq \langle n_{\mathbf{i}\uparrow} \rangle \langle n_{\mathbf{i}\downarrow} \rangle}$$

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



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

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

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

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

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

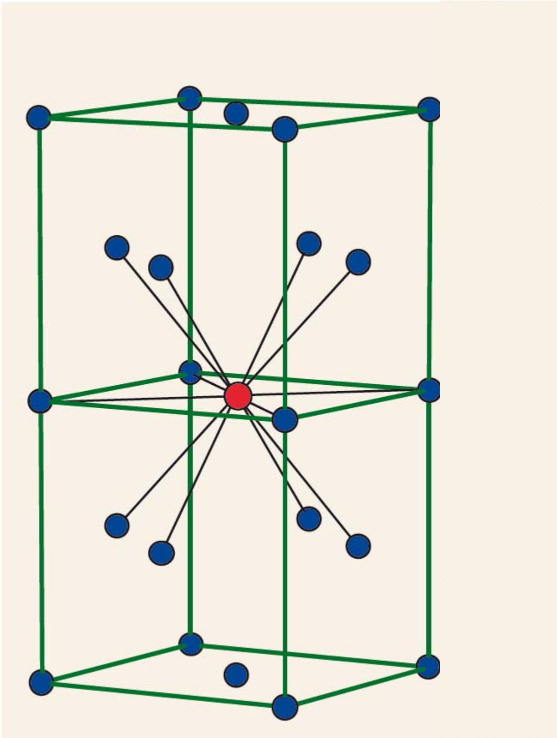
Dynamical Mean-Field Theory (DMFT) of Correlated Electrons

Theory of correlated electrons

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

Hubbard model

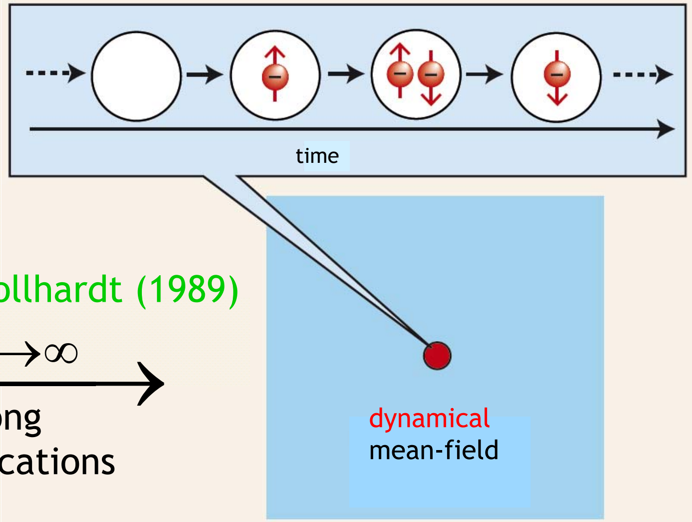
Face-centered cubic lattice (d=3)



Z=12

Metzner, Vollhardt (1989)

$$\xrightarrow[\text{Strong simplifications}]{d, Z \to \infty}$$

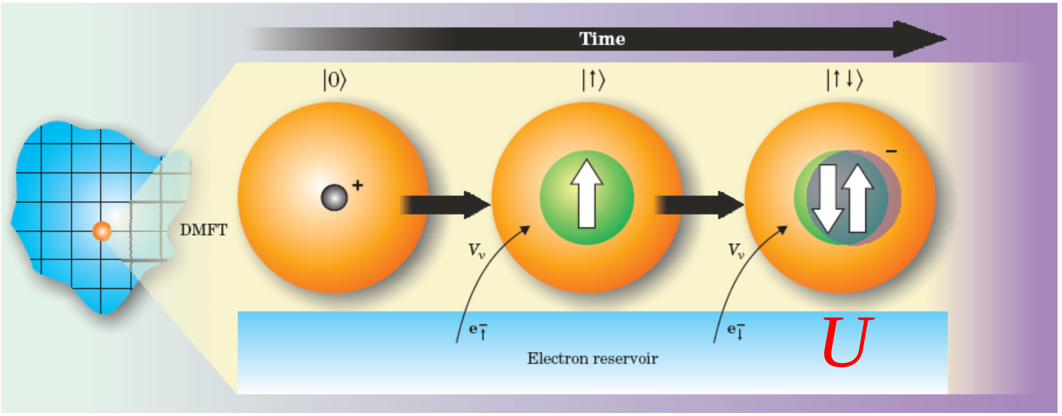


Self-consistent single-impurity Anderson model

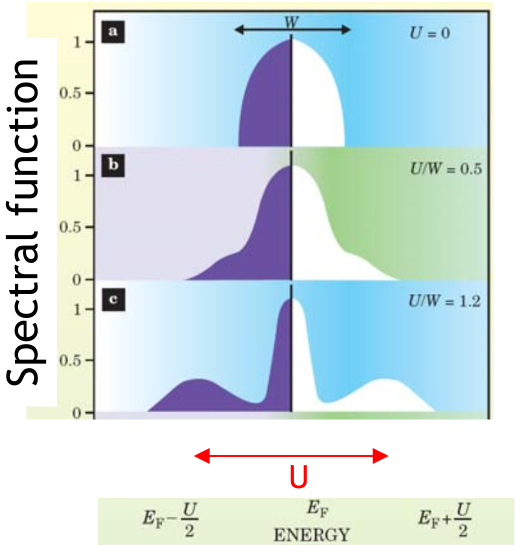
Georges, Kotliar (1992))

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

Dynamical mean-field theory (DMFT) of correlated electrons



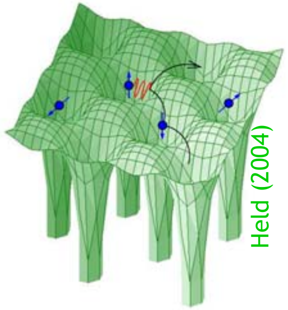
Exact time resolved treatment of local electronic interactions



Correlations (II):
Transfer of spectral weight

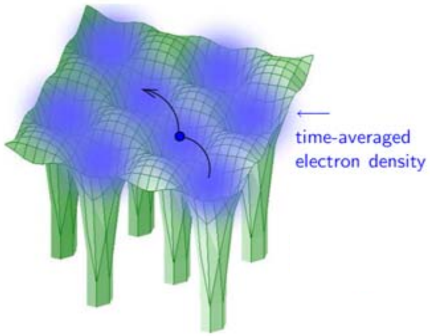
Experimentally detectable ?

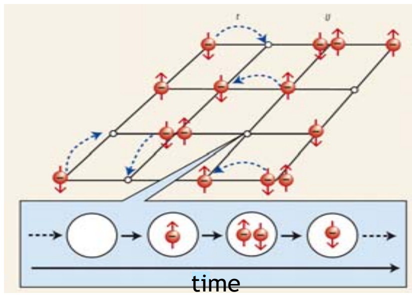
Correlated Electron Materials



Comprehensive, non-perturbative approximation scheme needed

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

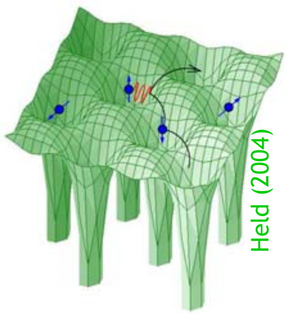




Material-specific input
Density functional theory
(LDA/GGA) or GW

?

Electronic correlations
Many-body theory



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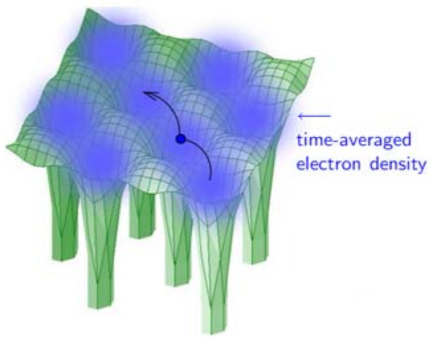
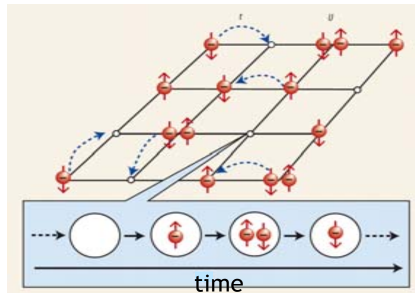




Material-specific input
Density functional theory
(LDA/GGA) or GW

+

Electronic correlations
Many-body theory
(DMFT)

⇓

LDA+DMFT

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

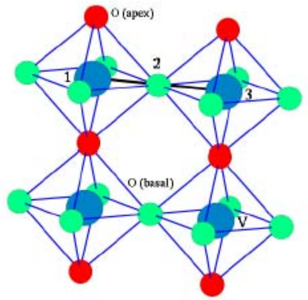
Application of LDA+DMFT

(Sr,Ca)VO_3: $3d^1$ system

Electronic structure

Crystal structure

SrVO$_3$: $\angle V - O - V = 180°$

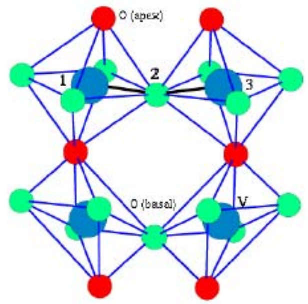


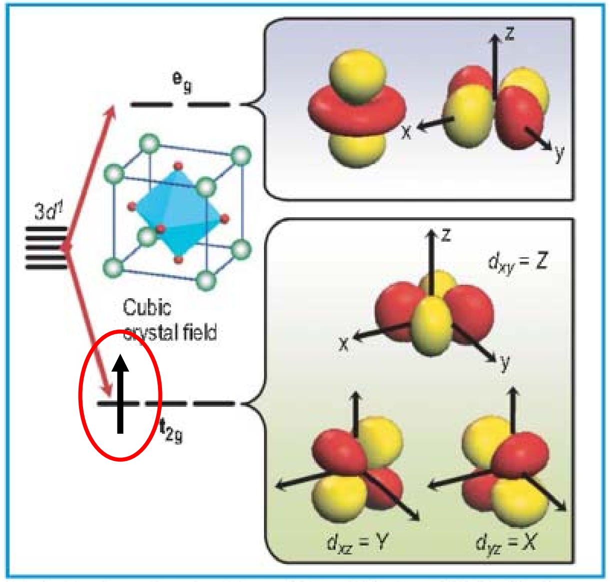
$\Downarrow$

orthorhombic distortion

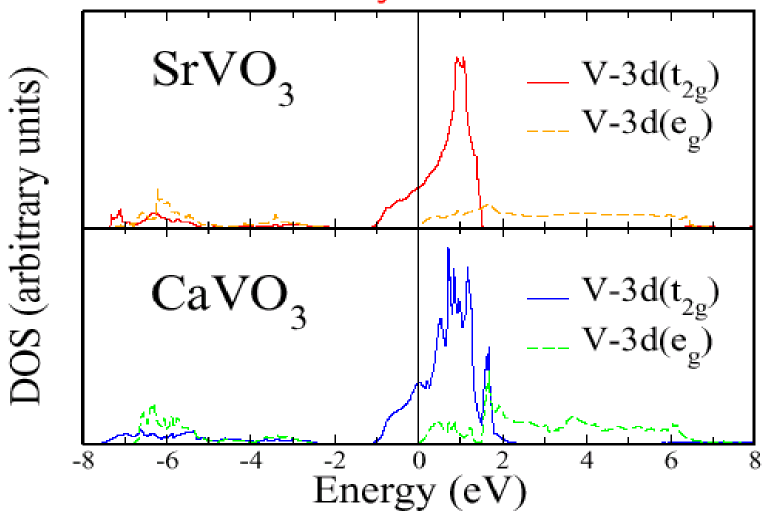
$\Downarrow$

CaVO$_3$: $\angle V - O - V \approx 162°$



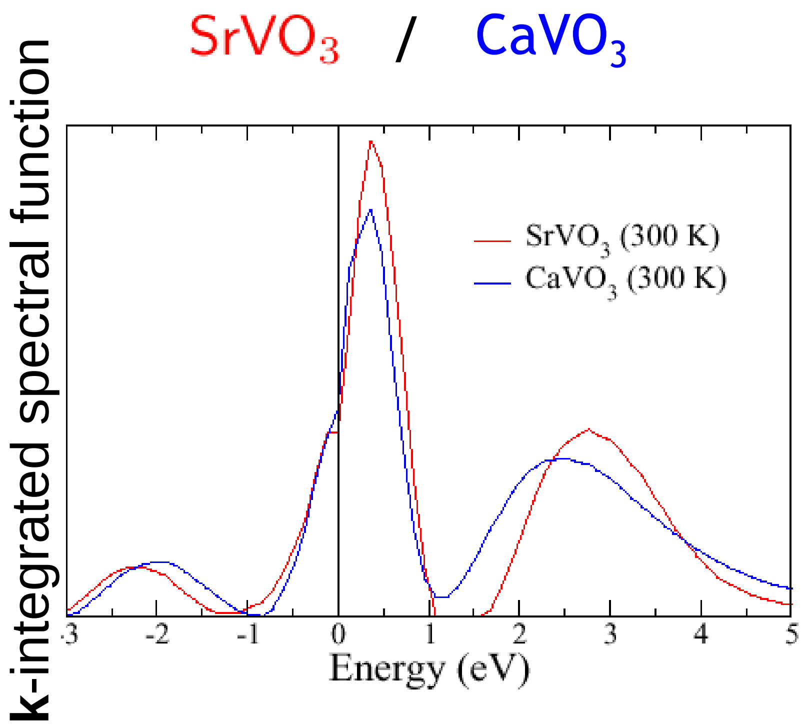


LDA density of states



No correlation effects/spectral transfer

LDA+DMFT results



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

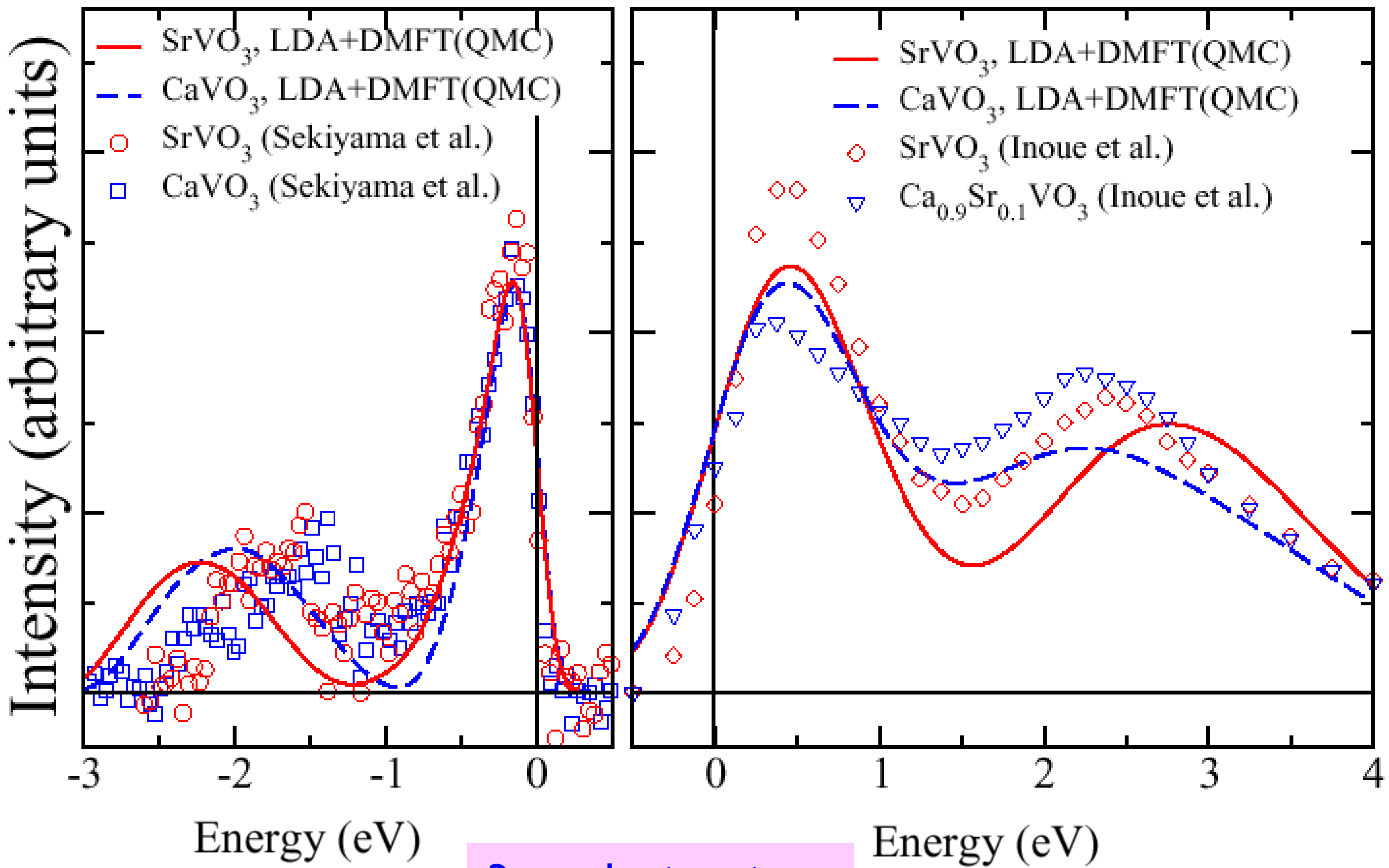
Osaka – Augsburg – Ekaterinburg collaboration: Sekiyama *et al.* (2004)

Comparison with experiment

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

Bulk sensitive photoemission spectroscopy → occupied states

X-ray absorption spectroscopy → unoccupied states

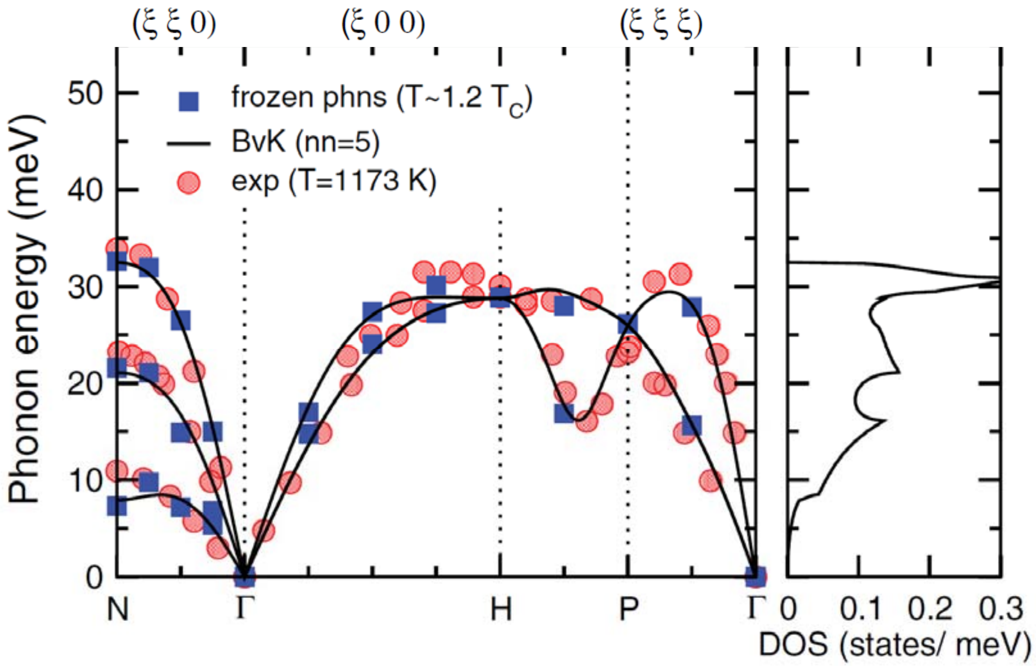


3-peak structure detected

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

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

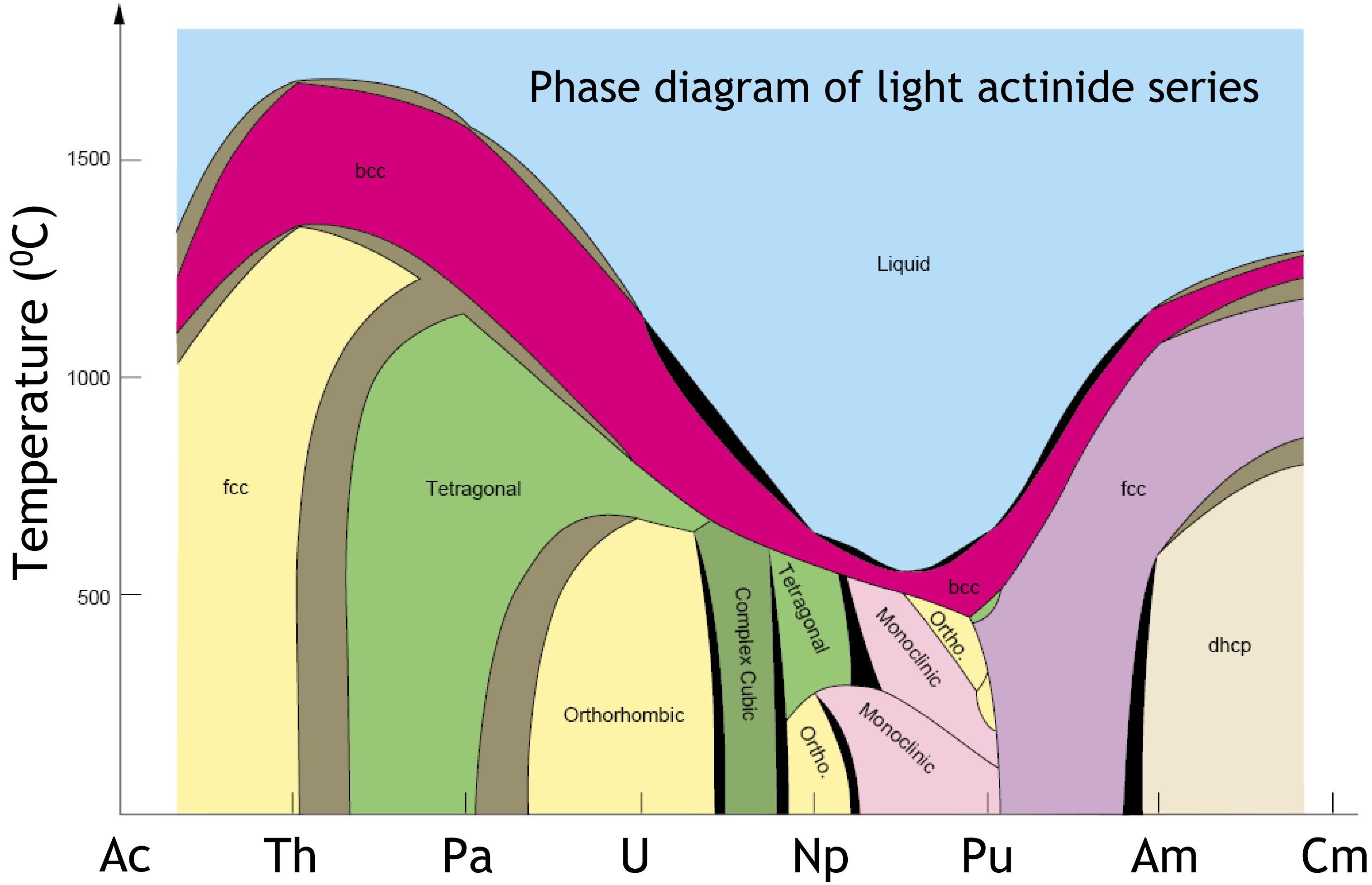
GGA+DMFT phonon dispersion at 1.2 T_C



Exp.: Neuhaus, Petry, Krimmel (1997)

Perspective of the LDA+DMFT approach

Explain and predict properties of complex correlated materials



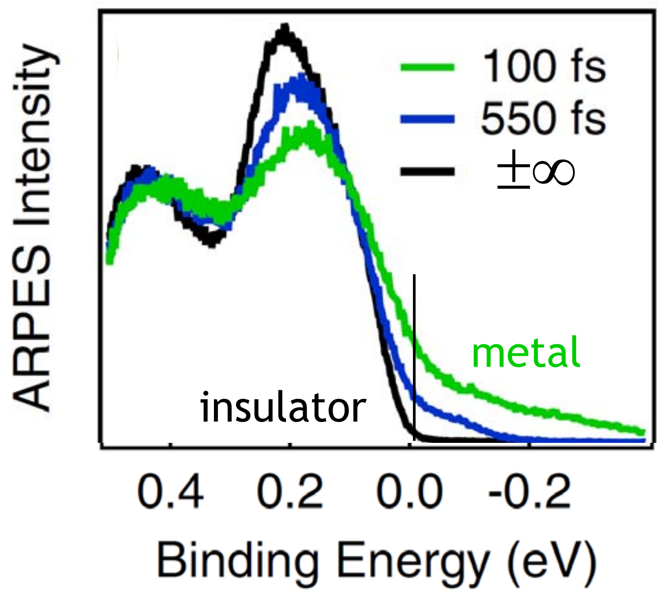
Phase diagram connecting individual binary alloy diagrams
Black: two-phase regions; Brown : details unknown

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

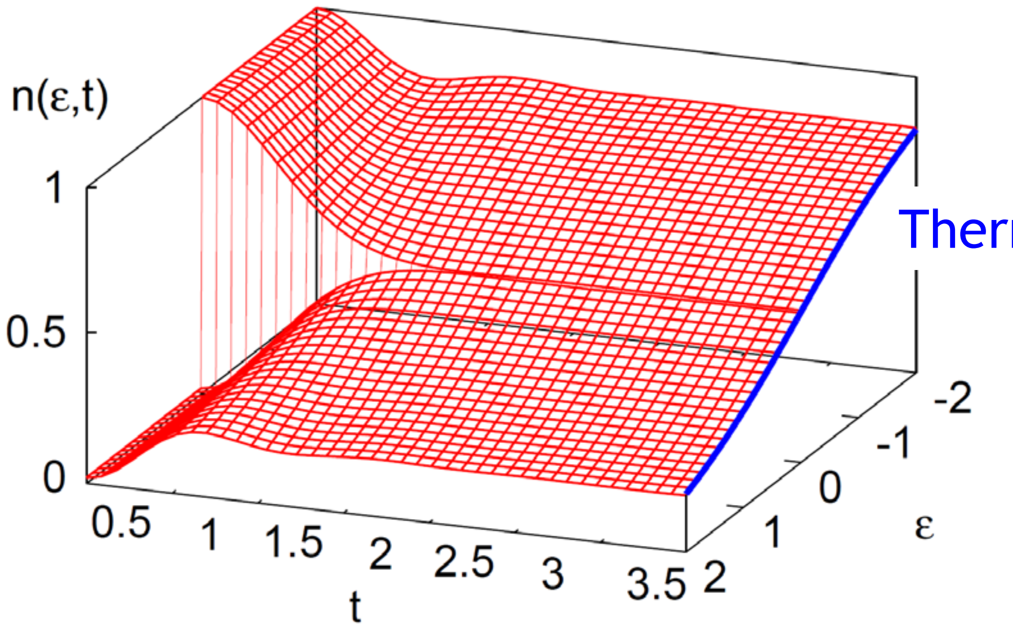
Freericks, Turkowski (2006)

Eckstein (2009)

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

Eckstein, Kollar, Werner (2009)

Momentum distribution (U=3.3)

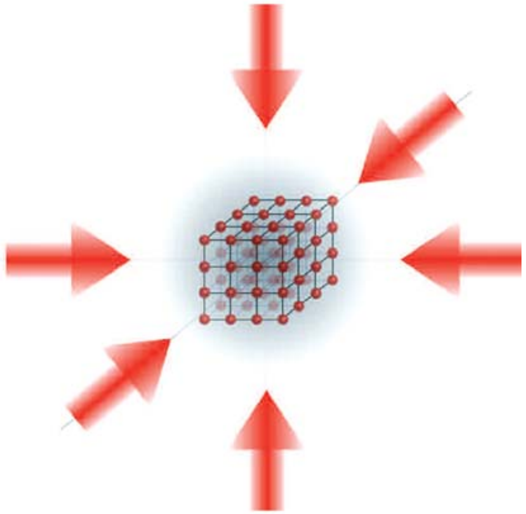


time after quench

Extension, e.g.

- time resolved PES
- pump-probe experiments

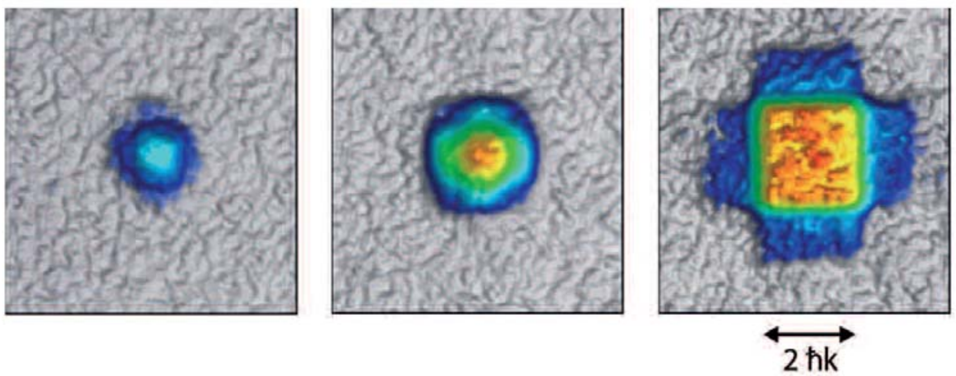
2. Correlated cold atoms in optical lattices



Greiner *et al.* (2002)

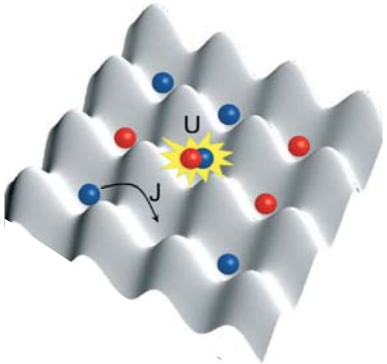
Bosonic/fermionic atoms in optical lattices: Exp. realization of models

High degree of tunability: “quantum simulator”



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

2. Correlated cold atoms in optical lattices



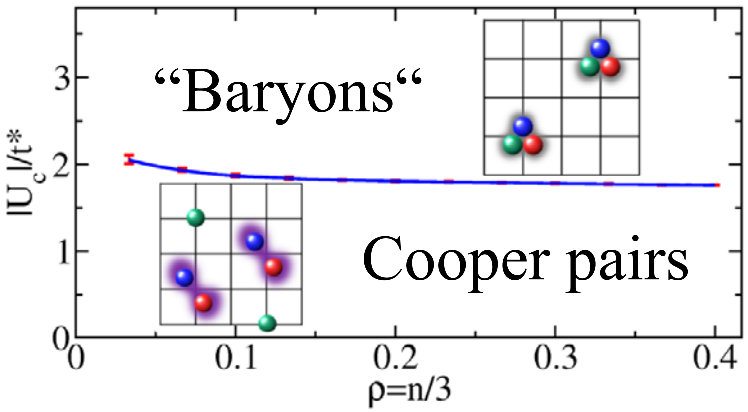
Hubbard model with ultracold atoms   Jaksch *et al.* (1998)

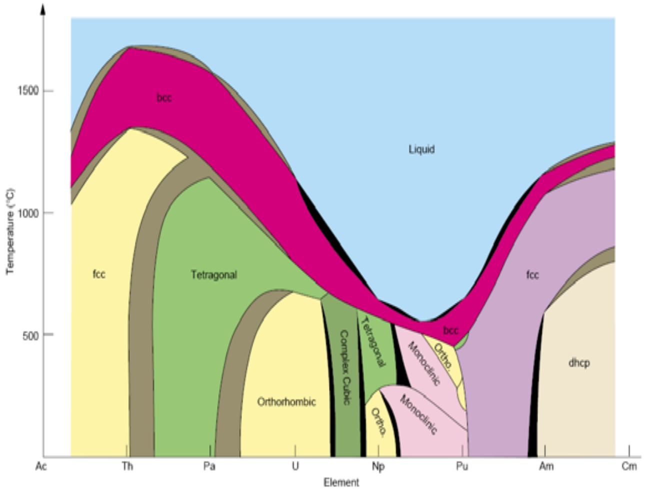
Atomic total angular momentum $L^{tot} = F$ → N=2F+1 hyperfine states

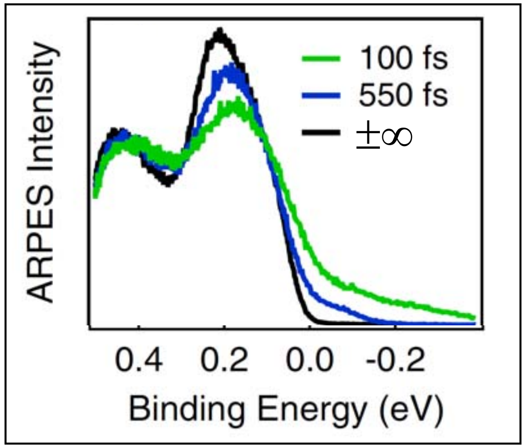
→ SU(N) Hubbard models

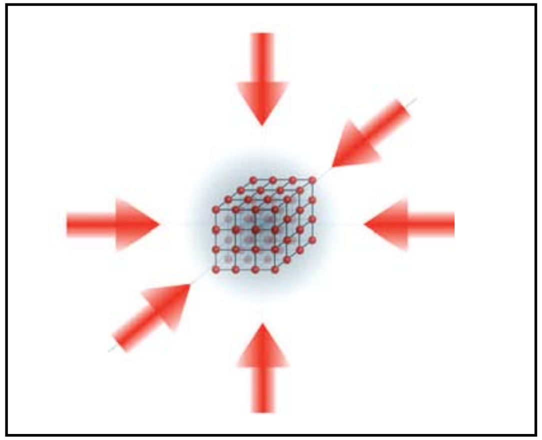
N=3, e.g. ^{6}Li, U<0: Color superconductivity, “baryon formation (QCD)”

Rapp *et al.* (2006)









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