

Solving correlated electron problems in infinite dimensions

Dieter Vollhardt

International Conference on Recent Progress in Many-Body Theories XXI
Feenberg Medal Award Session

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Outline

- Correlations in many-electron systems
- Brief history of the Hubbard model,
lattice fermions in $d \rightarrow \infty$,
dynamical mean-field theory
- Application to correlated electron materials
- Current status

Correlations in Many-Electron Systems

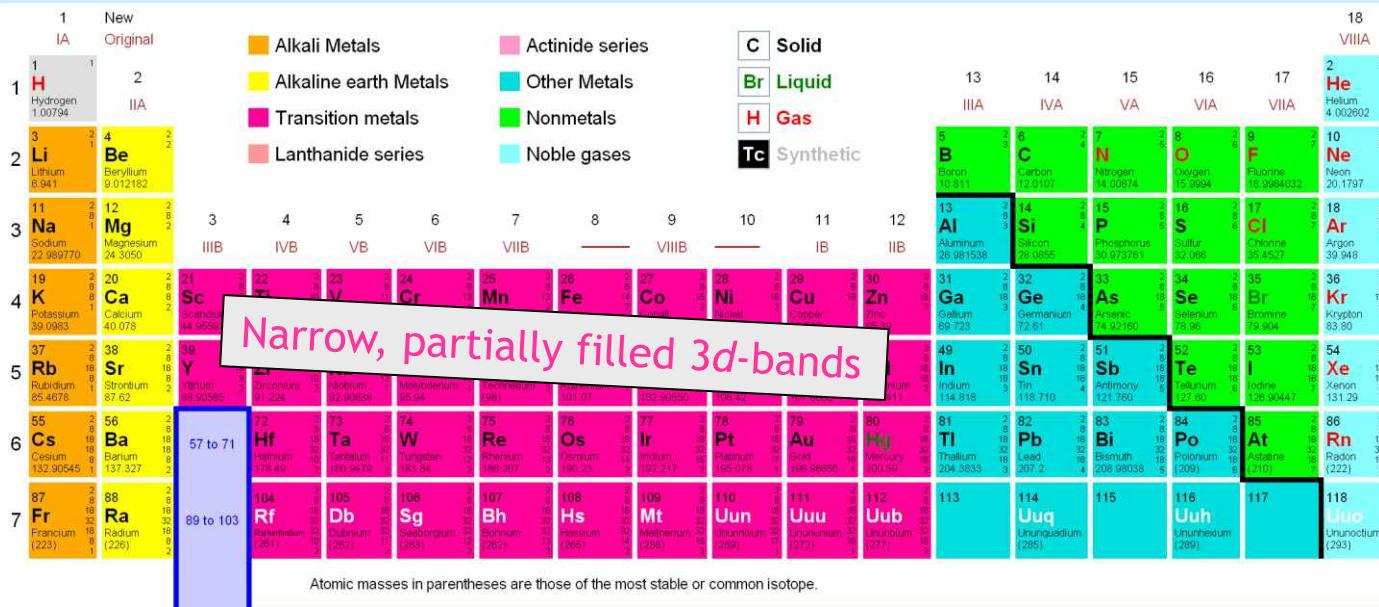
Electronic correlations (I):

Effects beyond factorization of the interaction (Hartree-Fock)

Wigner (1934)

$$\underbrace{\langle AB \rangle - \langle A \rangle \langle B \rangle}_{\text{quantifies correlations}}$$

Electronic correlations in the periodic table of elements



Early 1960s

Two fundamental, unsolved intermediate-coupling problems in solid state physics:

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

Minimal many-body model of correlated electrons ?

Related questions:

Magnetism and localized magnetic states in metals

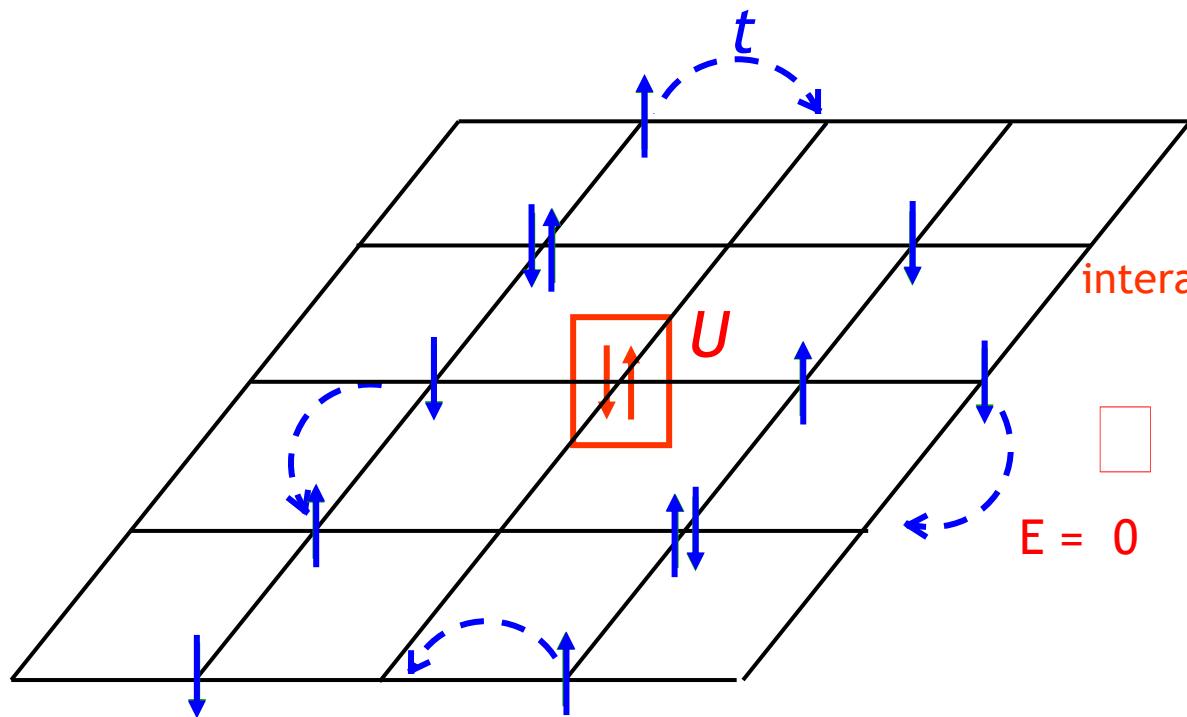
Anderson impurity model (“single-impurity Anderson model”):

local interaction between d -electrons $U n_{\uparrow}^d n_{\downarrow}^d$

Anderson (1961)
Wolff (1961)

Single-impurity Anderson model

Anderson (1961)



Non-interacting
conduction (*s*-) electrons
+
Immobile *d*-electrons with
interaction U on a single site ("impurity")

\uparrow or \downarrow

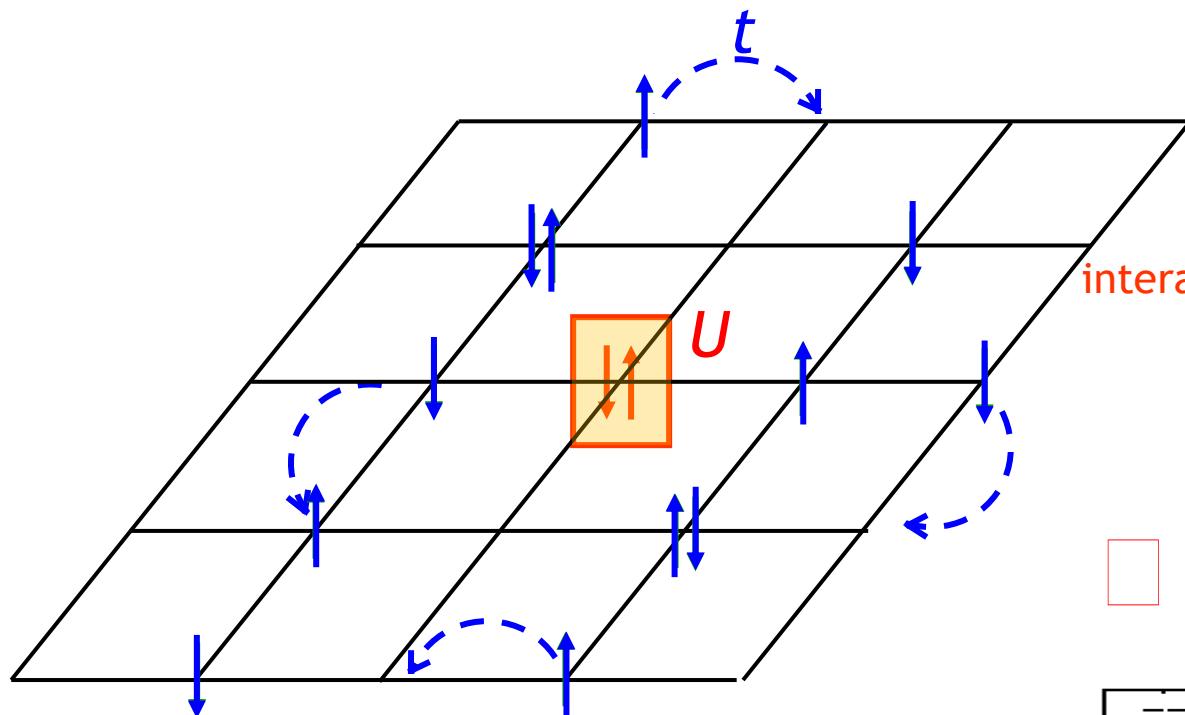
$\uparrow\downarrow$

ε_d
local moment

trivial eigenstates

Single-impurity Anderson model

Anderson (1961)



Non-interacting
conduction (s -) electrons
+
Immobile d -electrons with
interaction U on a single site ("impurity")
+

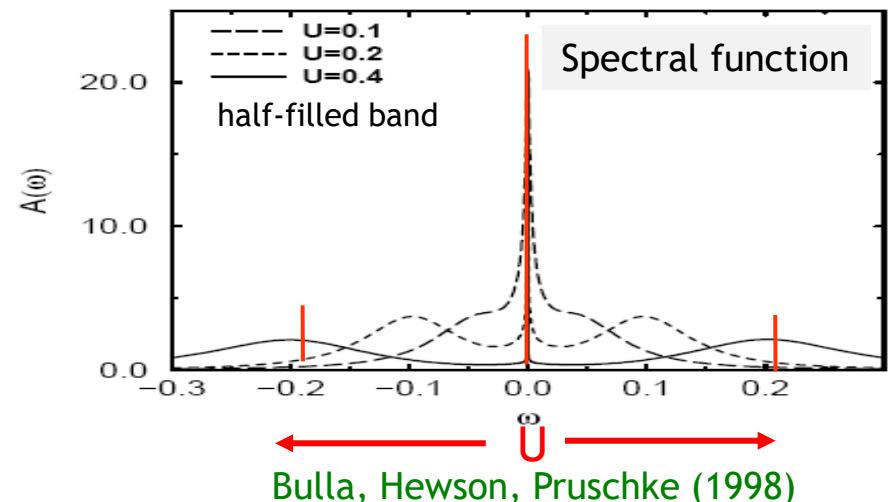
s,d -hybridization

Time



"Abrikosov-Suhl/Kondo resonance" at E_F
due to spin-flip scattering:
non-perturbatively narrow energy scale

→ characteristic 3-peak structure



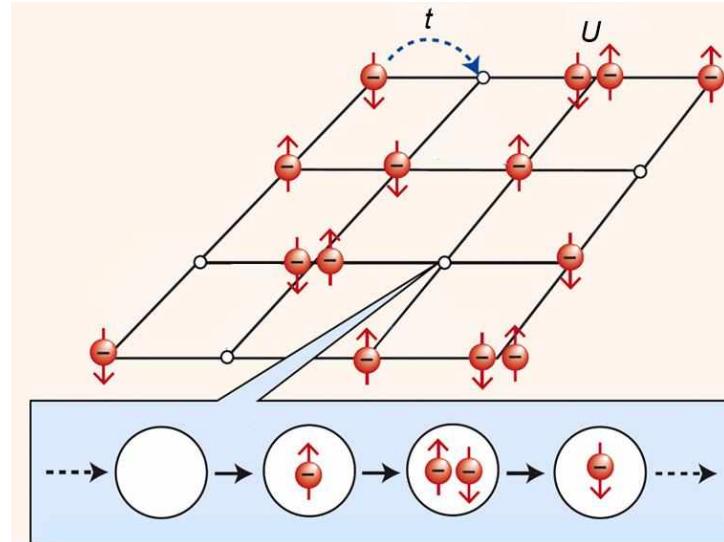
Bulla, Hewson, Pruschke (1998)

Minimal lattice model of correlated electrons

(for ferromagnetism of transition metals ?)

Hubbard model

- tight binding
 - extreme screening assumed:
only local interaction
→ in ferromagnetic phase $\langle H_{\text{int}} \rangle = 0$
- no classical analogue



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

Single-band model: $H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} D_{\mathbf{i}}, \quad D_{\mathbf{i}} = n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$

Diagonal in
momentum space
(waves)

Diagonal in
position space
(particles)

- How to solve ?
 - No fully numerical solution possible even today
- Find good approximations

Gutzwiller variational approach

$$H = \sum_{i,j,\sigma} \color{red} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \color{red} U \underbrace{\sum_i n_{i\uparrow} n_{i\downarrow}}_D$$

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

- Gutzwiller variational wave function $|\psi_G\rangle = e^{-\lambda D} |\psi_0\rangle$

$$E_G(\lambda) = \frac{\langle \psi_G | H | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$$

↑
One-particle wave function

- Gutzwiller approximation (GA):

Gutzwiller (1963/65)

Semi-classical evaluation of expectation values
by counting classical spin configurations

General framework:

Variational Wave Functions

$$|\Psi_{\text{var}}\rangle = \hat{C}|\Psi_0\rangle$$

$$|\Psi_0\rangle$$

$$\hat{C}(\lambda_1, \dots, \lambda_n)$$

$$\lambda_i$$

Applications, e.g.:

- Quantum liquids ^3He , ^4He
- Nuclear physics
- Correlated electrons
- Heavy fermions
- FQHE
- High- T_c superconductivity

One-particle wave function

Correlation operator
reduces energetically unfavorable
configurations in $|\Psi_0\rangle$

Variational parameters

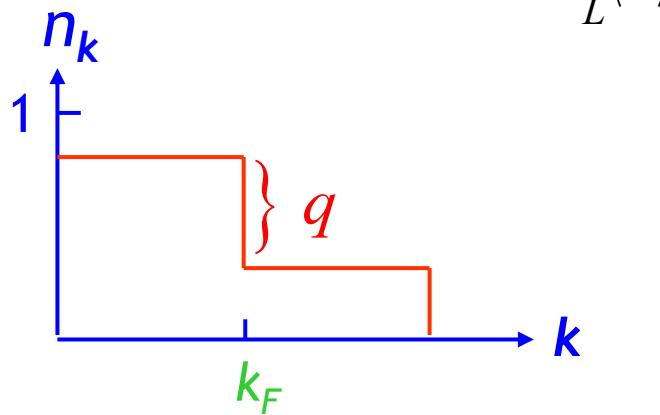
Example: Correlated basis function theory
E. Feenberg, *Theory of Quantum Fluids* (1969)



Gutzwiller variational approach

Gutzwiller (1963/65)

$$\frac{E_G(\lambda)}{L} = q(d) \varepsilon_0 + U d , \quad d \equiv d(\lambda)$$



$$\frac{\partial E_G}{\partial d} = 0$$

Conditions for ferromagnetic ground state?

Brinkman, Rice (1970)

$$d = \frac{1}{4} \left(1 - \frac{U}{U_c} \right)$$

$$U_c = 8\varepsilon_0$$

$$q = 1 - \left(\frac{U}{U_c} \right)^2$$

$$E_G = -L\varepsilon_0 \left(1 - \frac{U}{U_c} \right)^2$$

$$\frac{m^*}{m} = q^{-1} \xrightarrow{U \rightarrow U_c} \infty$$

describes
metal-insulator
("Mott") transition
 $\rightarrow V_2O_3$

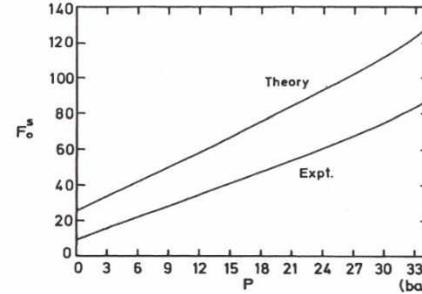
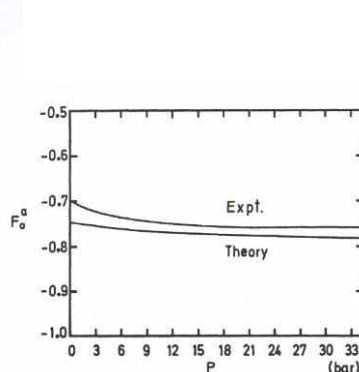
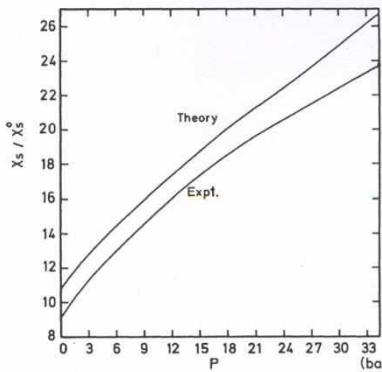
Application of Gutzwiller-Brinkman-Rice theory

$$\frac{E_G(\lambda)^{GA}}{L} = q(d)\epsilon_0 + Ud$$

Normal liquid ^3He : “almost localized Fermi liquid“ ?

Anderson, Brinkman (1975)

Gutzwiller approximation \leftrightarrow Landau Fermi liquid theory DV (1984)



Reviews of Modern Physics, Vol. 56, No. 1, January 1984

Normal ^3He : an almost localized Fermi liquid

Dieter Vollhardt

Brown, 1973). In that respect the rather more numerical techniques of the correlated-basis-function approach (Feenberg, 1969; Krotscheck and Smith, 1983), a variational method for optimizing the wave function of the system, appear to be more promising. In view of these

Gutzwiller approximation:

- very “physical“ + gives remarkably good results
- mean-field-like
- how to improve?

Systematic derivation by quantum many-body methods?

- Slave boson mean-field theory (1986)
- Infinite dimensions (1986-1989)

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PHYSICAL REVIEW LETTERS

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New Functional Integral Approach to Strongly Correlated Fermi Systems: The Gutzwiller Approximation as a Saddle Point

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⁽²⁾Department of Physics, University of California at San Diego, La Jolla, California 92093

(Received 21 April 1986)

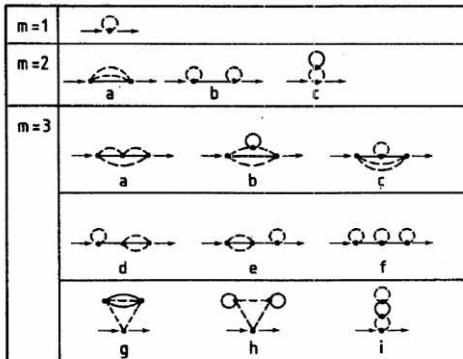
Gutzwiller wave function

Analytic evaluation of $E_G = \frac{\langle \psi_G | H | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$ in d=1

Metzner, DV (1987/1988)



Walter Metzner



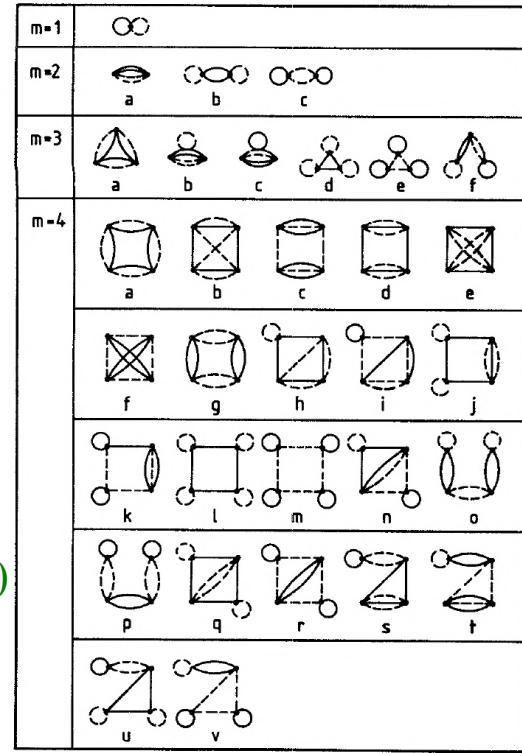
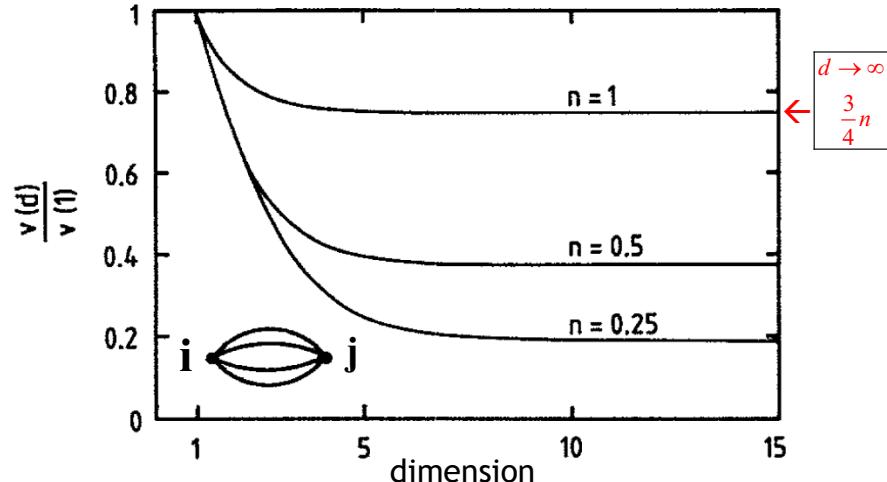
Diagrams (kinetic energy)

Exact, analytic calculation of all diagrams possible

→ all correlation functions Gebhard, DV (1987/1988)

d>1

Numerical calculation by Monte-Carlo integration



Diagrams (Hubbard interaction)

Great simplifications for $d \rightarrow \infty$:

- internal momenta become independent
- again all diagrams can be calculated exactly
- results of GA recovered

→ fully diagrammatic derivation of the GA

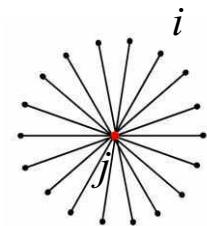
Correlated Lattice Fermions in $d = \infty$ Dimensions

Walter Metzner and Dieter Vollhardt

*Institut für Theoretische Physik C, Technische Hochschule Aachen, Sommerfeldstrasse 26/28,
D-5100 Aachen, Federal Republic of Germany*
(Received 28 September 1988)

$$\langle \hat{H}_{\text{kin}} \rangle_0 = -t \sum_{\mathbf{i}, \sigma} \underbrace{\sum_{\mathbf{j}(NN \mathbf{i})} \underbrace{\langle \hat{c}_{\mathbf{i}\sigma}^\dagger \hat{c}_{\mathbf{j}\sigma} \rangle_0}_{g_{ij,\sigma}^0}}_Z \quad \text{Probability amplitude for hopping } \mathbf{j} \rightarrow \text{NN } \mathbf{i}$$

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



$$\Rightarrow |\text{Amplitude for hopping } \mathbf{j} \rightarrow \text{NN } \mathbf{i}| = g_{ij,\sigma}^0 \propto \frac{1}{\sqrt{Z}} \text{ or } \frac{1}{\sqrt{d}}, \quad Z = 2d \text{ (hypercubic lattice)}$$

Correlated Lattice Fermions in $d = \infty$ Dimensions

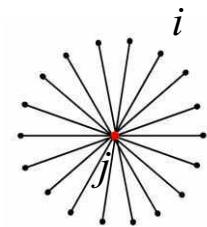
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$$\left\langle \hat{H}_{\text{kin}} \right\rangle_0 = - \frac{t}{\sqrt{Z}} \sum_{\mathbf{i}, \sigma} \sum_{\substack{\mathbf{j} (\text{NN } \mathbf{i}) \\ Z}} \underbrace{\left\langle \hat{c}_{\mathbf{i}\sigma}^\dagger \hat{c}_{\mathbf{j}\sigma} \right\rangle_0}_{g_{ij,\sigma}^0 \propto \frac{1}{\sqrt{Z}}}$$

Quantum scaling $t = \frac{t^*}{\sqrt{2d}}$

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



\Rightarrow Amplitude for hopping $\mathbf{j} \rightarrow \text{NN } \mathbf{i}$ $= g_{ij,\sigma}^0 \propto \frac{1}{\sqrt{Z}}$ or $\frac{1}{\sqrt{d}}$, $Z = 2d$ (hypercubic lattice)

Correlated Lattice Fermions in $d = \infty$ Dimensions

Walter Metzner and Dieter Vollhardt

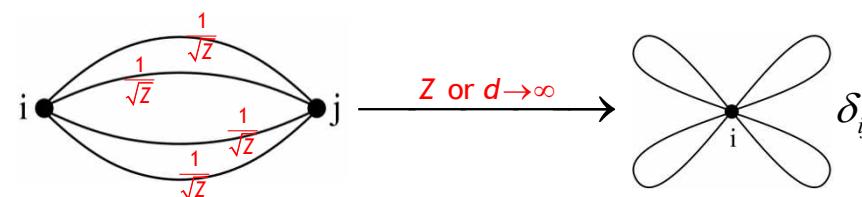
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Quantum scaling $t = \frac{t^*}{\sqrt{2d}}$

$\xrightarrow{Z \text{ or } d \rightarrow \infty}$ Collapse of all connected, irreducible diagrams in position space

Example:



→ Great simplification of many-body perturbation theory, e.g., self-energy diagram purely local

Holds also for time-dependent propagator, since $g_{ij,\sigma}^0 = \lim_{t \rightarrow 0^-} G_{ij,\sigma}^0(t)$

Correlated Lattice Fermions in $d = \infty$ Dimensions

Walter Metzner and Dieter Vollhardt

*Institut für Theoretische Physik C, Technische Hochschule Aachen, Sommerfeldstrasse 26/28,
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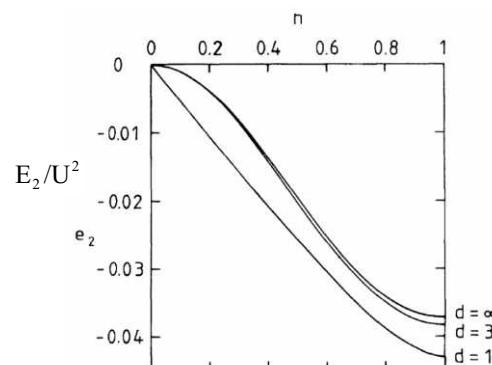
Quantum scaling $t = \frac{t^*}{\sqrt{2d}}$

Z or $d \rightarrow \infty$ →

Collapse of all connected, irreducible diagrams in position space

Correlations remain non-trivial even in infinite dimensions

Example: Correlation energy of Hubbard model



Excellent approximation for $d=3$

$d \rightarrow \infty$: new mean-field limit for fermions

Mean-field theory of the Hubbard model

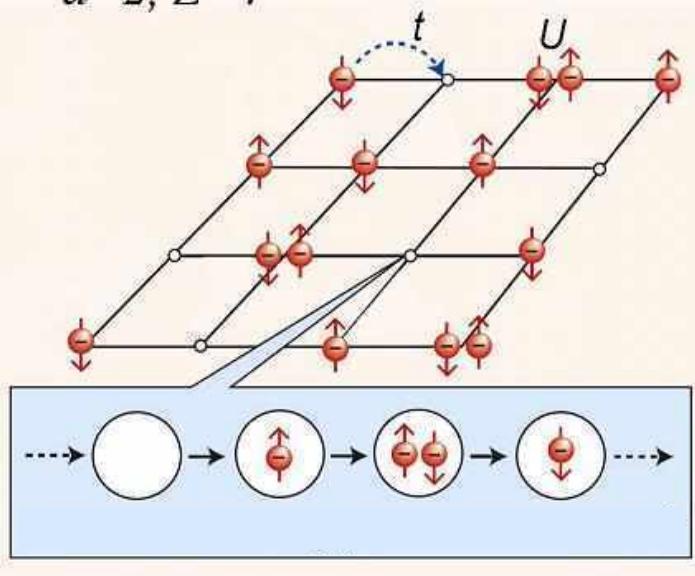
$$H = -\frac{t^*}{\sqrt{Z}} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Metzner, DV (1989)

Quantum scaling $t = \frac{t^*}{\sqrt{2d}}$

Purely local interaction:
independent of d, Z

$d=2, Z=4$



Thou shalt not factorize:

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

Local quantum fluctuations always present → dynamic

Quantum fluctuations neglected → static

Hartree(-Fock)

Mean-field theory of the Hubbard model

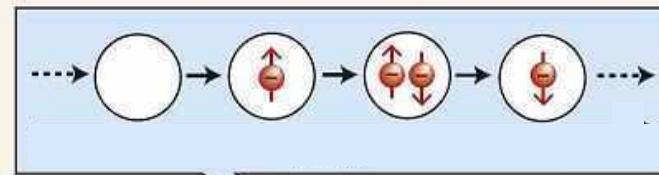
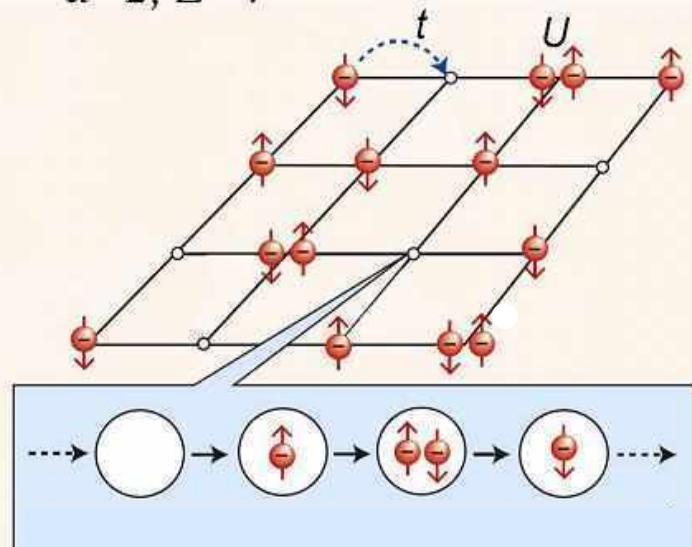
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Metzner, DV (1989)

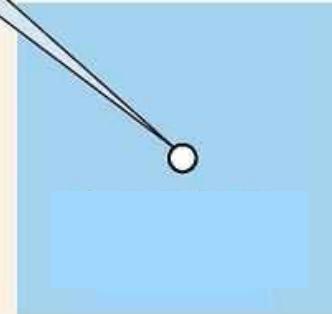
Quantum scaling

$$t = \frac{t^*}{\sqrt{2d}}$$

$d=2, Z=4$



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



becomes local
("single-site")

Müller-Hartmann (1989)

Mean-field theory of the Hubbard model

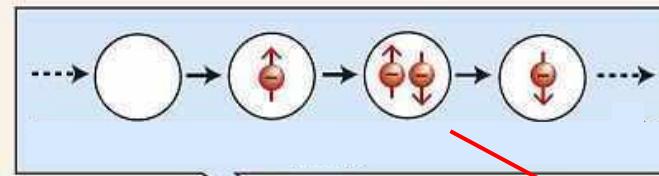
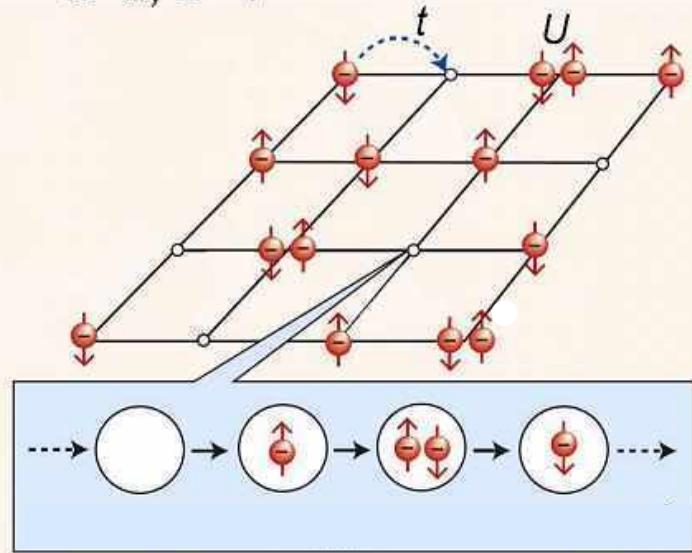
$$H = -\frac{t^*}{\sqrt{Z}} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Metzner, DV (1989)

Quantum scaling

$$t = \frac{t^*}{\sqrt{2d}}$$

$d=2, Z=4$



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

dynamical mean field

becomes local
("single-site")

mutually dependent

Müller-Hartmann (1989)

Self-consistent mean-field theory

Janiš (1991)

How to solve?

Mean-field theory of the Hubbard model

PHYSICAL REVIEW B

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Hubbard model in infinite dimensions

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Gabriel Kotliar

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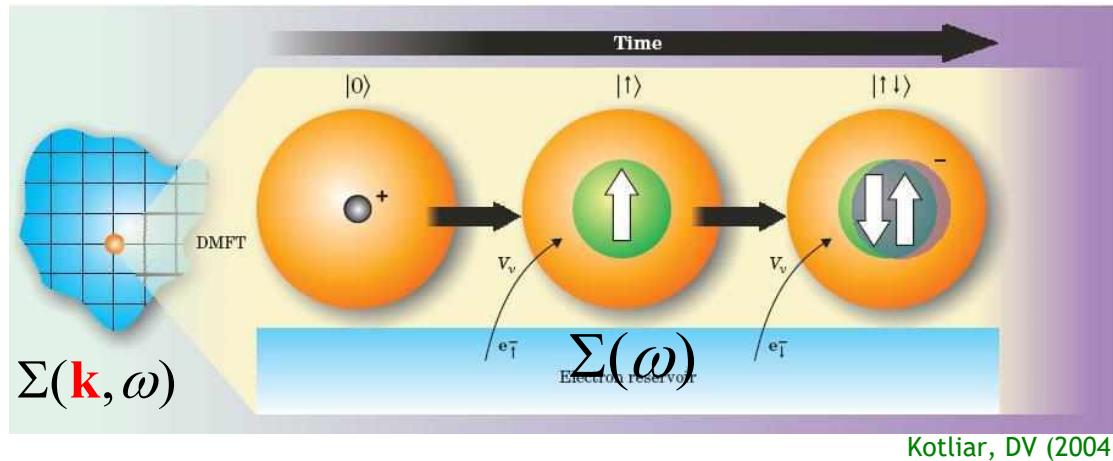
(Received 23 September 1991)

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

Jarrell (1992)

- physically appealing and powerful
- directly numerically accessible by quantum Monte Carlo for SIAM Hirsch, Fye (1986)

Mean-field theory of the Hubbard model



Fully dynamical, but mean-field in position space

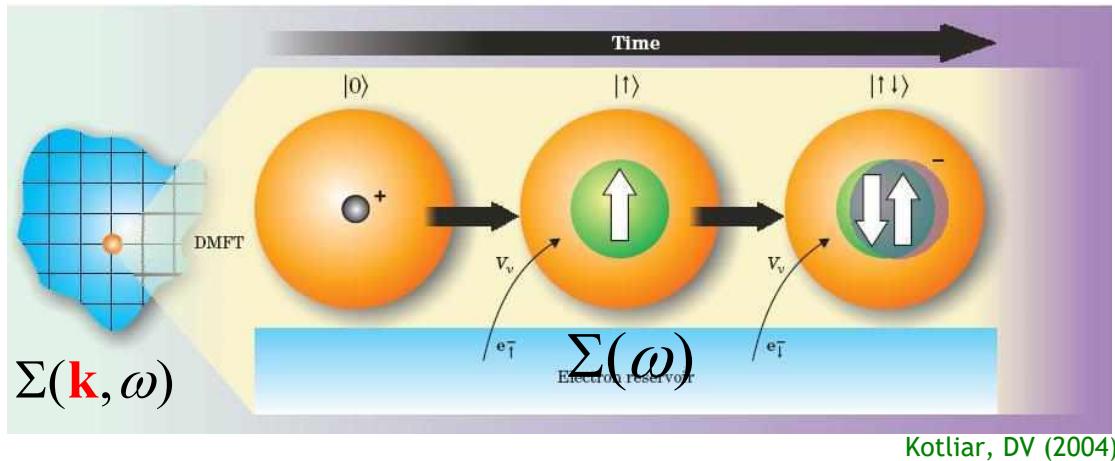
Dynamical Mean-Field Theory (DMFT)

Exact in $d, Z \rightarrow \infty$

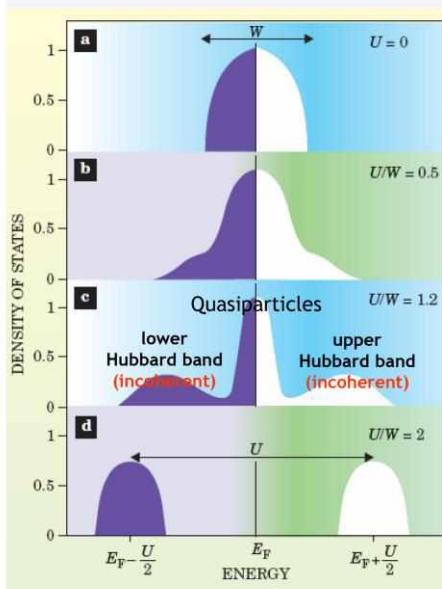
New type of MFT for quantum particles

Self-consistency equations → talks by A. Georges, G. Kotliar

Characteristic features of DMFT



Spectral function



Better definition of electronic correlations:

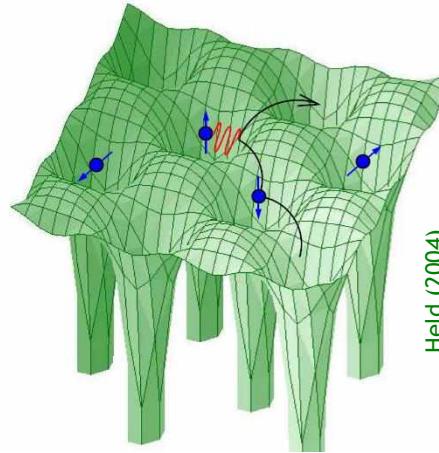
- transfer of spectral weight
- finite lifetime of excitations

Experimentally detectable
(PES, ARPES, ...)

→ DMFT describes Mott-Hubbard metal-insulator transition

Application of DMFT to correlated electron materials

Non-perturbative approaches for real materials

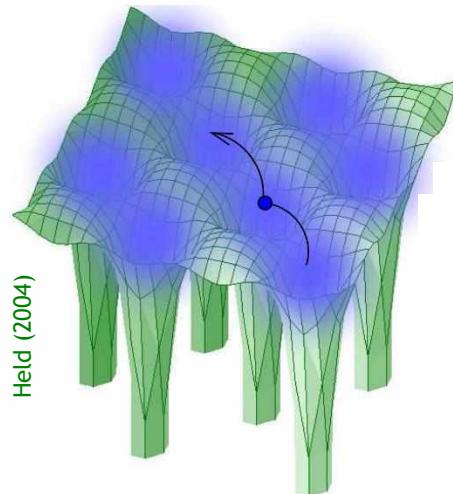


DFT/LDA, GGA

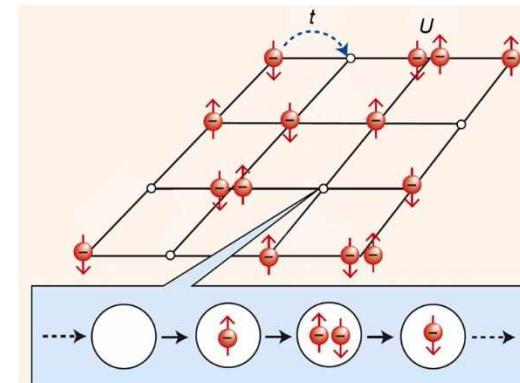
- + material specific
- + fast code packages
- fails for strong correlations

Model Hamiltonians

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



How to combine ?



Computational scheme for correlated electron materials

Initially:

LDA+DMFT

Anisimov, Poteryaev, Korotin, Anokhin, Kotliar (1997)
Lichtenstein, Katsnelson (1998)

=

Material specific electronic structure
(Density functional theory: LDA)

+

Local electronic correlations

-

Double counting correction

(Many-body theory: DMFT)

Computational scheme for correlated electron materials

More general:

X+DMFT

X= DFT (LDA, GGA)

GW

Biermann, Aryasetiawan, Georges (2003)

=

Material specific electronic structure

(Density functional theory: LDA, GGA, ...) or **GW**

+

Local electronic correlations

-

Double counting correction (LDA, GGA)

(Many-body theory: **DMFT**)

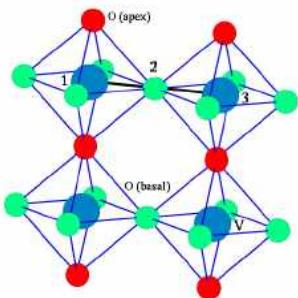
Early results of DFT+DMFT

(Sr,Ca)VO₃: 3d¹ test system

Electronic structure

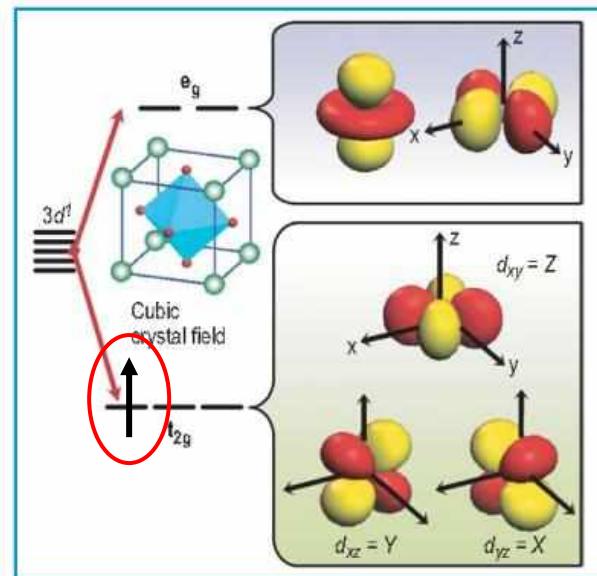
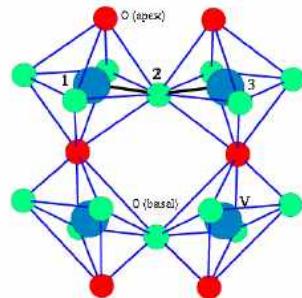
Crystal structure

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

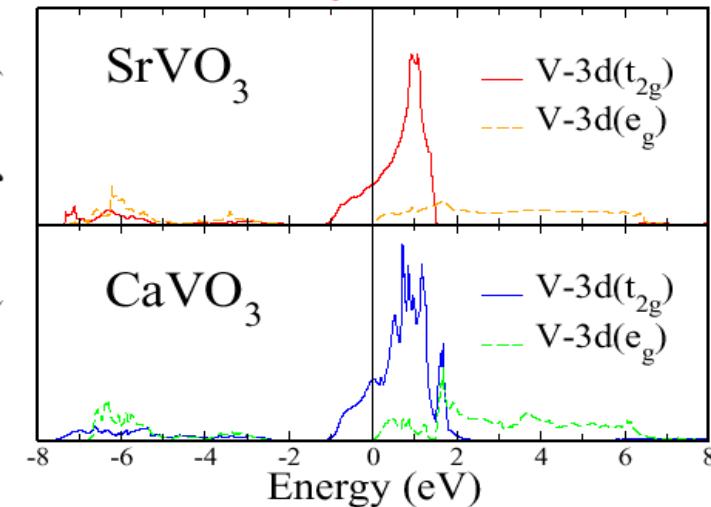


↓
orthorhombic distortion

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

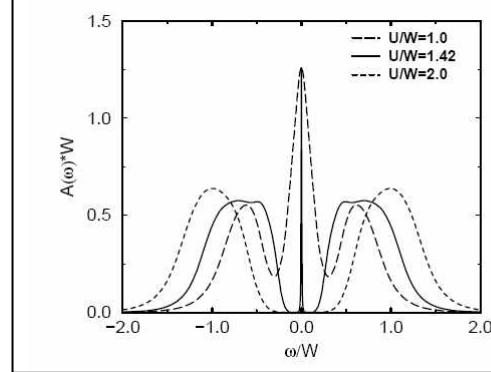
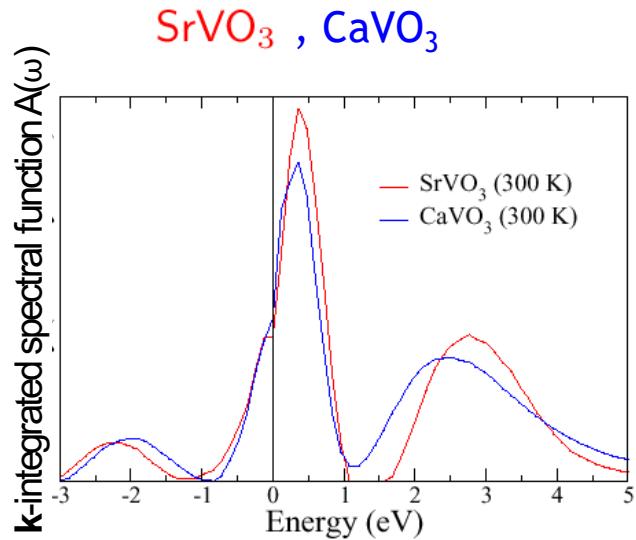


LDA density of states



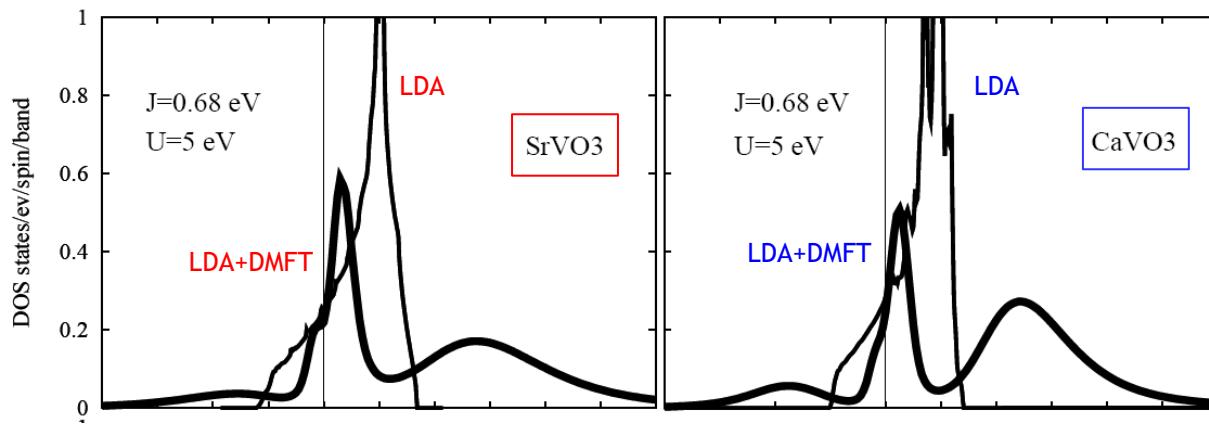
No correlation effects/spectral transfer

LDA+DMFT results



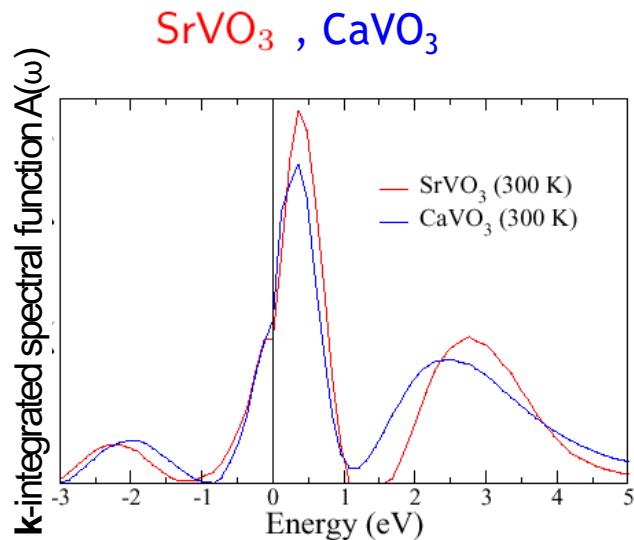
Single-band Hubbard model (DMFT)
Bulla (1999)

Constrained LDA: $U=5.55$ eV, $J=1.0$ eV
Osaka - Augsburg - Ekaterinburg collaboration: Sekiyama *et al.* (2004)



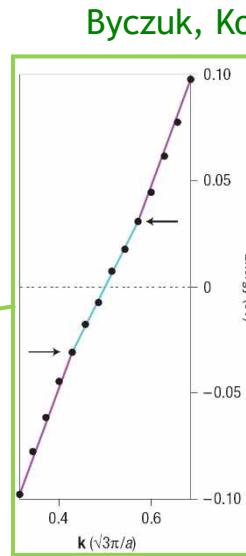
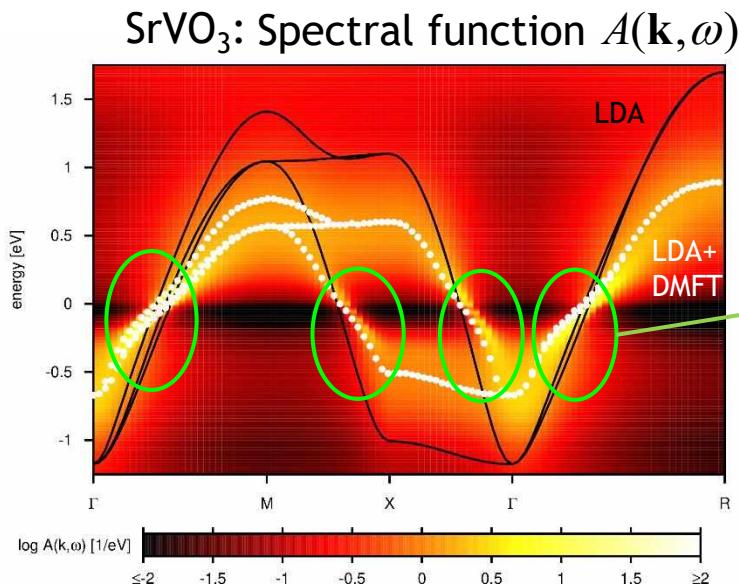
Pavarini, Biermann, Poteryaev, Lichtenstein, Georges, Andersen (2004)

LDA+DMFT results



Constrained LDA: $U=5.55 \text{ eV}$, $J=1.0 \text{ eV}$

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



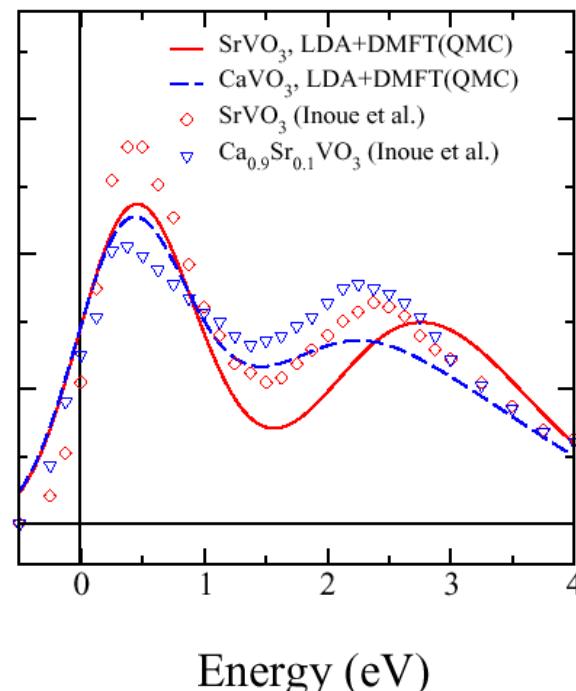
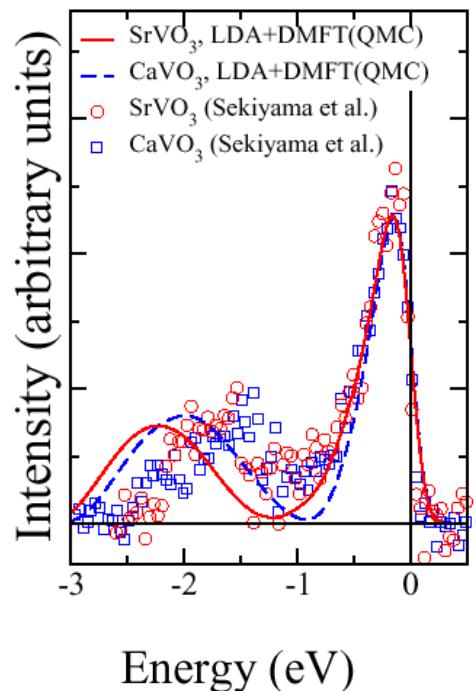
Electronic correlations →

- quasiparticle damping
- band narrowing
- “kinks”
 - at energy $\omega_* = Z_{FL} \times (\text{bare energy scale})$
 - sharpen with increasing interaction $\propto (Z_{FL})^{-2}$
 - Fermi liquid regime terminates at ω_*

LDA+DMFT for (Sr,Ca)VO₃: Comparison with experiment (Spring-8 beamline)

Sekiyama *et al.* (2004, 2005) [Osaka - Augsburg - Ekaterinburg collaboration]

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

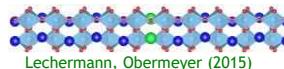


Correlation-induced
3-peak structure
confirmed

Applications of DMFT during 1997-2022: Current status

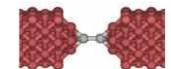
DMFT used to describe electronic correlations in:

- Bulk materials



Lechermann, Obermeyer (2015)

- Heterostructures, interlayers, surfaces



Jacob, Haule, Kotliar (2010)



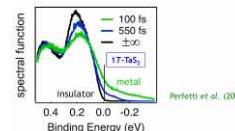
al-Badri et al. (2020)

- Molecular electronics, quantum chemistry, ligand binding



Markov, Rohringer, Rubtsov (2019)

- Topological materials



Perfetti et al. (2006)

- Nonequilibrium

DV (2020): SCES 2019

Non-local effects: Beyond single-site DMFT

→ talk by H. Terletska

- E-DMFT: Si, Smith (1996)
- DCA: Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy (1998)
- CDMFT: Lichtenstein, Katsnelson (2000)
Kotliar, Savrasov, Pálsson, Biroli (2001)
- DΓA: Toschi, Katanin, Held (2007)
- DF: Rubtsov, Katsnelson, Lichtenstein (2008)
- fRG+DMFT: Taranto *et al.* (2014)

Conclusion

- Hubbard model in infinite dimensions
≡
Dynamical mean-field theory (DMFT)
- DMFT is the **generic** mean-field theory
of correlated lattice fermions

I am grateful to my collaborators on infinite dimensions/DMFT, in particular:



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Krzysztof Byczuk



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Liviu Chioncel



Ivan Leonov



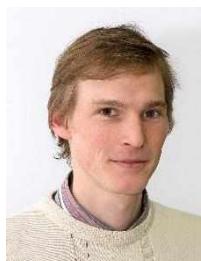
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Xinguo Ren



Florian Gebhard



Peter van Dongen



Ruud Vlaming



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