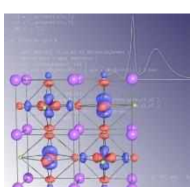
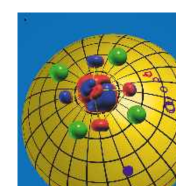
Center for Electronic Correlations and Magnetism
University of Augsburg

Why calculate in infinite dimensions?

Dieter Vollhardt



Autumn School on Correlated Electrons:
Dynamical Mean-Field Theory of Correlated Electrons
Forschungszentrum Jülich; October 4, 2022



Outline

- Spatial dimensions: From zero to infinity
- Classical many-body systems in infinite dimensions
- Correlated electrons in infinite dimensions
- Dynamical mean-field theory (DMFT)
- Application of DMFT to correlated electron materials
- Beyond mean-field theory

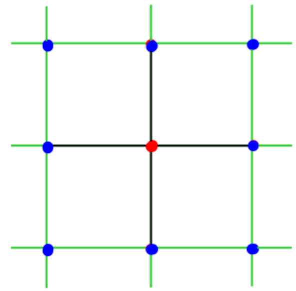
Spatial dimensions:
From zero to infinity


V
W
U
d=3

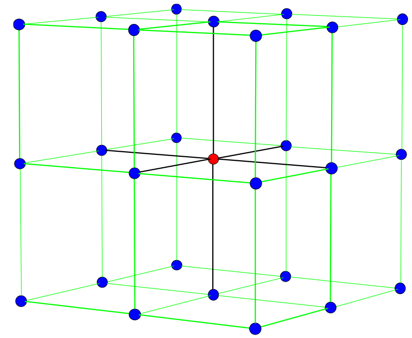
Integer dimensions

d=0

d=1



d=2



d=3

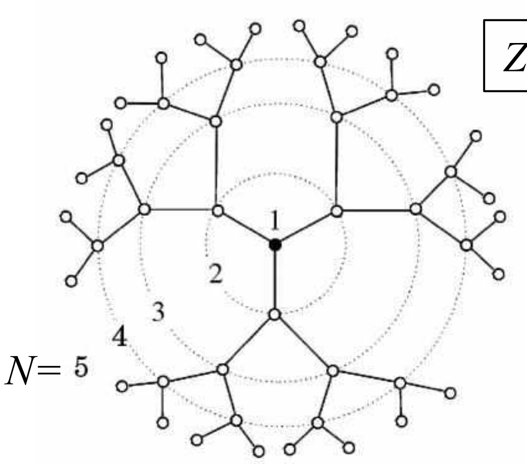
...

d>3

Coordination number Z = # nearest neighbors
Hypercubic lattices: $Z=2d$

Bethe “lattice”/Cayley tree:
connected cycle-free graph

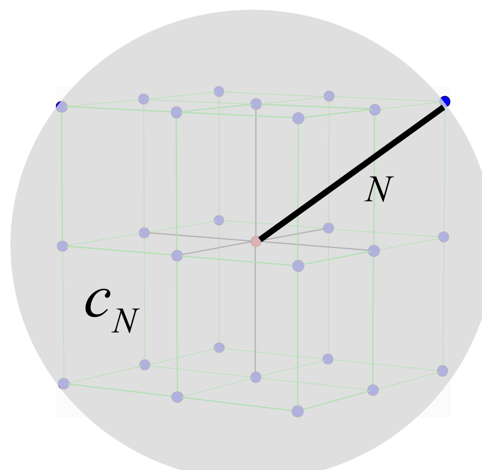
$Z=3$



$$c_N \sim Z^N \xrightarrow{N\to\infty} \infty$$

Bethe lattice is “infinite dimensional”

How to define “dimensionality of lattice“ ?



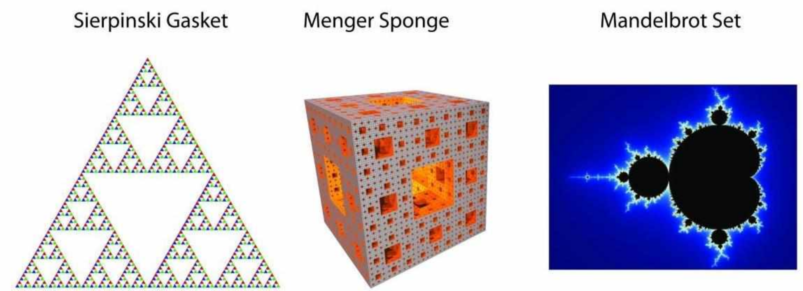
c_N = # sites N steps away from given site

Regular d-dimensional lattices $c_N \sim N^d$

$$\Rightarrow \boxed{\lim_{N\to\infty} \frac{\ln c_N}{\ln N} = d}$$

Non-integer dimensions

Fractal dimensions



Fractal objects with non-integer fractal dimension

Continuous dimensions

Analytic continuation of d to continuous values, e.g.,
in RG theory: ε-expansion with $\varepsilon = d_{\mathrm{crit}} - d << 1$, e.g., $d_{\mathrm{crit}}=4$

$$\boxed{\int d^d k_1 d^d k_2 \cdots f(k_1, k_2, \cdots)}$$

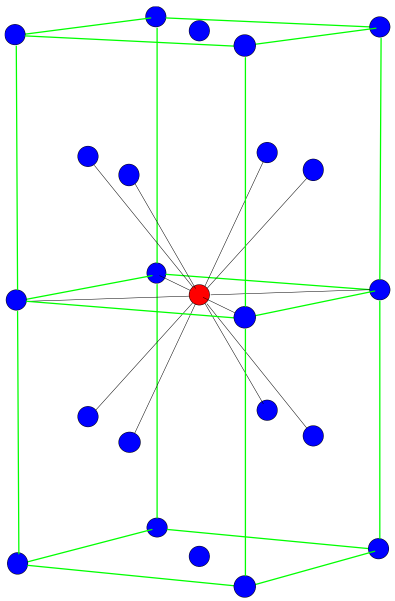
VOLUME 28, NUMBER 4 | PHYSICAL REVIEW LETTERS | 24 JANUARY 1972

Critical Exponents in 3.99 Dimensions*

Kenneth G. Wilson and Michael E. Fisher
Laboratory of Nuclear Studies and Baker Laboratory, Cornell University, Ithaca, New York 14850

The limit $d, Z \to \infty$

$d=3$ (face-centered cubic)



$Z=12$

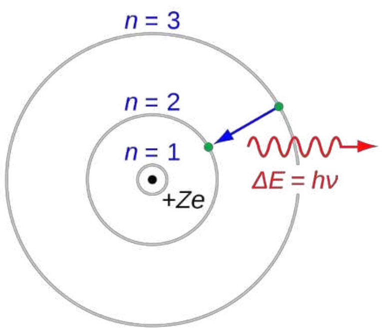
$\xrightarrow{d, Z \to \infty}$ what happens ?

- Mathematical expressions simplify (if scaled properly)
- Fluctuations decrease
- "Mean-field" solution of many-body problems

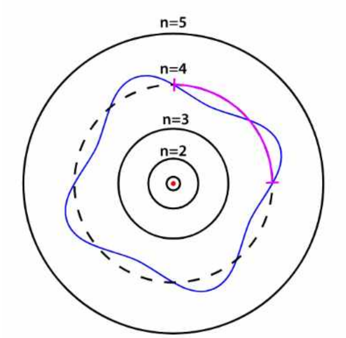
Illustration: Derivation of Bohr's atomic model from the Schrödinger equation

Bohr model of the atom

Bohr (1913)



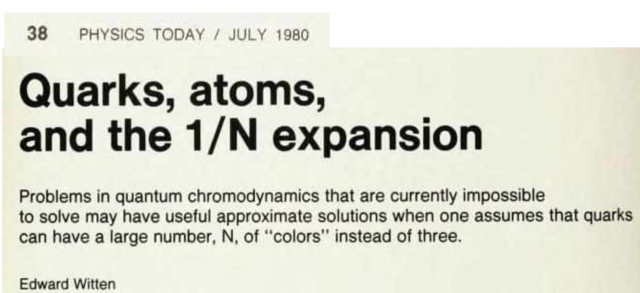
+ <u>Postulates:</u>
- discrete energies E_n , $n = 1, 2, 3, \ldots$
- frequency of emitted light $= E_n - E_m / h$
- quantization condition for circular orbits



Circumference $u_n = n\lambda_{\text{de Broglie}}$

Modern day applications:
highly excited Rydberg atoms, cavity QED, …

Can the Bohr model be derived from "proper" quantum mechanics? How?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Quarks, atoms, and the 1/N expansion

Problems in quantum chromodynamics that are currently impossible to solve may have useful approximate solutions when one assumes that quarks can have a large number, N, of "colors" instead of three.

Edward Witten

Simple example: Hydrogen atom with $N \equiv d \to \infty$

Illustration: Derivation of Bohr's atomic model from the Schrödinger equation

Svidzinsky, Scully, Herschbach (2014)

Hydrogen atom: radial Schrödinger equation for electron in d dimensions (atomic units)

$$\boxed{\left[-\frac{1}{2}\left(\frac{d^2}{d\rho^2}+\frac{d-1}{\rho}\frac{d}{d\rho}\right)+\frac{l(l+d-2)}{2\rho^2}-\frac{1}{\rho}\right]R(\rho)=\varepsilon R(\rho)}$$

$\rho = r/a_0$

$\varepsilon = E/(e^2/a_0)$

(i) Eliminate 1st order derivative by writing $R(\rho)=\dfrac{u(\rho)}{\rho^{(d-1)/2}}$

$d=3: \quad R(\rho)=\dfrac{u(\rho)}{\rho}$ ✓

$$\boxed{\left(-\frac{1}{2}\frac{d^2}{d\rho^2}+\frac{\Lambda(\Lambda+1)}{2\rho^2}-\frac{1}{\rho}\right)u(\rho)=\varepsilon u(\rho)}$$

$d \geq 3$

$\Lambda = l+(d-3)/2$ replaces l

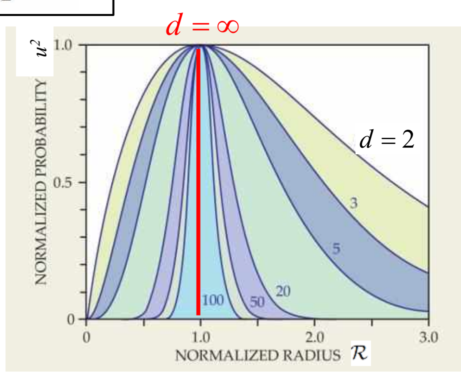
(ii) Keep centrifugal term finite for $d\to\infty$: dimensional rescaling

$\mathcal{R} := \left(\frac{d-1}{2}\right)^{-2}\varrho$

$\mathcal{E} := \left(\frac{d-1}{2}\right)^{2}\varepsilon$,

$$\boxed{\left(-\frac{2}{(d-1)^2}\frac{\mathrm{d}^2}{\mathrm{d}\mathcal{R}^2}+\frac{1}{2}\frac{d-3}{d-1}\frac{1}{\mathcal{R}^2}-\frac{1}{\mathcal{R}}\right)u=\mathcal{E}\,u}$$

$l=0$



$d \gg 3$

- Electron probab. distrib. → thin shell around nucleus with $\mathcal{R}\approx 1$
- Factor $(\sin\vartheta)^{d-2}$ in d-dim. vol. element → polar angle $\vartheta \to \pi/2$
  → planar, circular orbit (Bohr!)

$d=\infty$

Kinetic energy = 0; classical energy $\mathcal{E}(\mathcal{R})=\dfrac{1}{2\mathcal{R}^2}-\dfrac{1}{\mathcal{R}}$

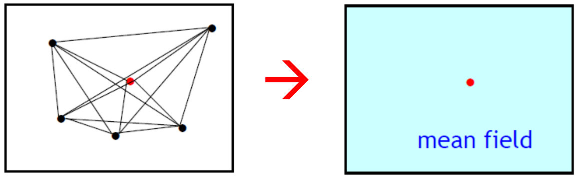
minimal at $\mathcal{R}=1,\ \mathcal{E}=-1/2$

- No quantum fluctuations
- Bohr's model justified in $d=\infty$

Application to He atom and H_2 molecule with $1/d$ corrections → excellent results

Classical many-body systems in infinite dimensions

Mean-Field Theories (MFT)



1. Construction by factorization

- Spin models (finite range interaction), e.g., Ising

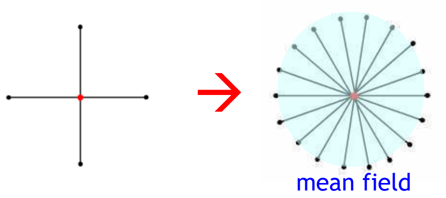
Factorization $JS_iS_j \rightarrow \underbrace{J\langle S_i \rangle}_{\text{mean field}} S_j$ (Weiss MFT)

- Electronic models (local interaction), e.g., Hubbard

Factorization $Un_{i\uparrow}n_{i\downarrow} \rightarrow \underbrace{U\langle n_{i\uparrow} \rangle}_{\text{mean field}} n_{i\downarrow}$ (Hartree MFT)

2. Construction by enhancement

$$\left.\begin{array}{l}\text{Spin } S \\ \text{Degeneracy } N \\ \text{Range of interaction, density} \quad \text{Brout (1960)} \\ \text{Spatial dimension } d \text{ or coordination number } Z \\ \qquad\qquad \text{Fisher, Gaunt (1964)}\end{array}\right\} \rightarrow \infty$$



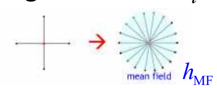
Ising Model in $d = \infty$

Ising model

$$H = -\frac{1}{2} J \sum_{\langle i,j \rangle} S_i S_j = \sum_i h_i S_i$$

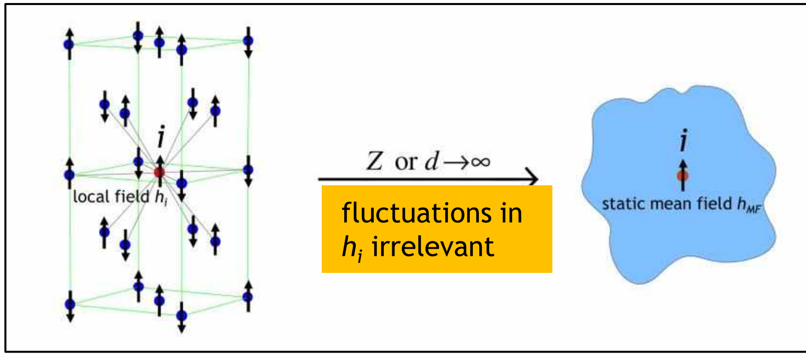
$$h_i = -J \sum_{j \in \text{ all NN of } i} S_j \xrightarrow[\text{law of large numbers: } S_i \to S]{Z \to \infty} -\underbrace{JZ}_{J^*} S \equiv h_{\text{MF}}$$

local (fluctuating) field



global ("molecular/Weiss") static field

$d \to \infty$



$$J \to \frac{J^*}{Z}, \quad J^* = \text{const}$$

"Classical scaling"

$$H \to H^{\text{MF}} = h_{\text{MF}} \sum_i S_i + E_{\text{shift}}$$

Effective static single-site problem

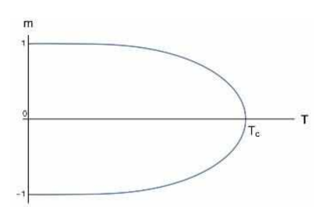
$$\Rightarrow m = \tanh(\beta h_{\text{MF}}) \equiv S$$

magnetization

+ self-consistency condition

$$h_{\text{MF}} = J^* m$$

$$\Rightarrow m = \tanh(J^* m / k_B T)$$

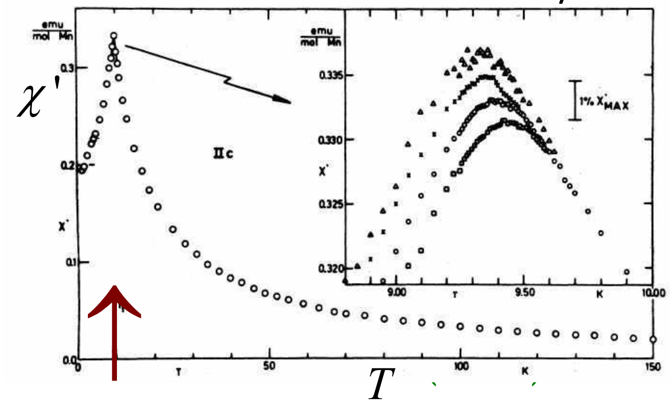


Weiss MFT

Ising model with random coupling in $d = \infty$: The spin glass problem

~ 1970: investigation of magnetic systems with static ("quenched") disorder, e.g. Cu/Mn, Au/Fe, …

Cu/Mn



"Spin glass freezing transition" to disordered configuration of magnetic moments

Edwards-Anderson model (1975)

$$H = -\sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j$$

Heisenberg model

J_{ij} : random, short-range couplings , $\langle J_{ij} \rangle = 0, \ \langle J_{ij}^2 \rangle = 1$

Investigate properties and construct order parameter of spin glass state by "replica trick": introduce n copies

$$\boxed{\ln \mathcal{Z} = \lim_{n \to 0} \frac{\mathcal{Z}^n - 1}{n} \rightarrow F_{\text{av}} = -k_B T \langle \ln \mathcal{Z} \rangle_{\text{av}}}$$

Ising model with random coupling in $d = \infty$: The spin glass problem

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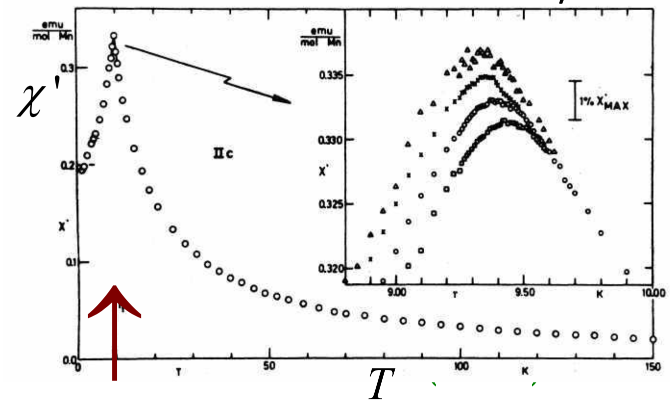
Cu/Mn



"Spin glass freezing transition" to disordered configuration of magnetic moments

Sherrington-Kirkpatrick (1975) : mean-field treatment

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j$$ Ising model

J_{ij} : random, infinite-range couplings, $\langle J_{ij}\rangle = 0,\ \langle J_{ij}^2\rangle = 1$

→ Scale $J_{ij} \to \dfrac{J_{ij}^*}{\sqrt{L}}$

L: # lattice sites

Alternative: finite-range J_{ij} and infinite d or Z

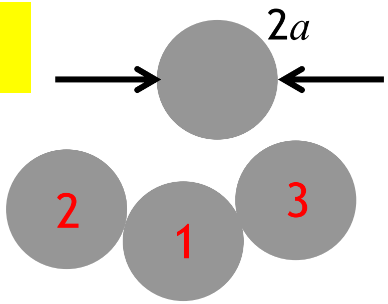
→ Scale $J_{ij} \to \dfrac{J_{ij}^*}{\sqrt{Z}}$

Problem: negative entropy for T → 0
Origin: "replica symmetry" assumed
Almeida, Thouless (1978)

Solution in $d \to \infty$: "Replica symmetry breaking" / multiple equilibria / infinite # order parameters in spin glass phase
Parisi (1979)

Nobel Prize in Physics 2021 "for groundbreaking contributions to our understanding of complex systems".

Hard-sphere fluid in $d=\infty$



Frisch, Rivier, Wyler (1985)
Wyler, Rivier, Frisch (1987)

Interaction of hard-core spheres

Continuum system

1,2 close and
1,3 close
→ 2,3 in general infinitely distant in $d=\infty$

Goal: equation of state by virial expansion

$$\boxed{\underbrace{\frac{PV}{k_B T}}_{\ln \mathcal{Z}} = N \sum_{l=0}^{\infty} B_{l+1} n^l}$$

N: # hard spheres, $n=\dfrac{N}{V}$

$B_1 = 1$ classical ideal gas

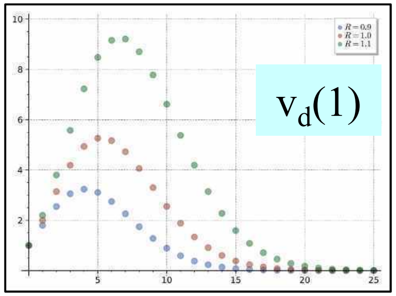
Partition function: $\mathcal{Z} = e^{\mathcal{Z}_c - 1}$, $\mathcal{Z}_c$: sum of connected graphs

$$\mathcal{Z}_c = \sum_{l=0}^{\infty} b_l \left(\frac{z}{\lambda^d}\right)^l, \quad z = e^{\mu/k_B T} \text{ fugacity}$$

$\lambda = \hbar\sqrt{2\pi / m k_B T}$ thermal wave length

Typical scale of volume: volume of hard sphere

$$\boxed{\mathrm{v}_d(a) = \underbrace{\mathrm{v}_d(1)}_{\frac{\pi^{d/2}}{\Gamma(1+d/2)}} a^d}$$



$\Rightarrow B_2 = \frac{1}{2}\mathrm{v}_d(a),\ B_{l>2} = 0$

Scale:
$$\boxed{\begin{array}{l} a = d^{\nu} a^*,\ \text{with } \mathrm{v}_d(a) \equiv \mathrm{v}(a^*) = \text{const} \\ \Rightarrow \nu = 1/2 \Rightarrow a = \sqrt{d}\, a^*,\ a^* = \text{const} \end{array}}$$

$$\boxed{\frac{PV}{k_B T} = N\left(1 + \frac{1}{2}\mathrm{v}(a^*) n\right)}$$

Conclusion: only 2-particle interaction important in $d=\infty$

Hard-sphere fluid in $d=\infty$

Frisch, Rivier, Wyler (1985)
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Interaction of hard-core spheres

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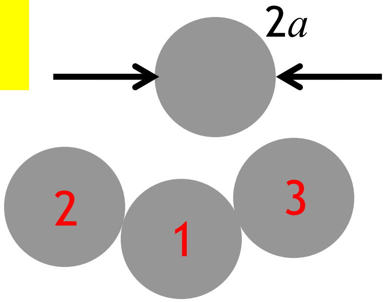

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$B_1 = 1$ classical

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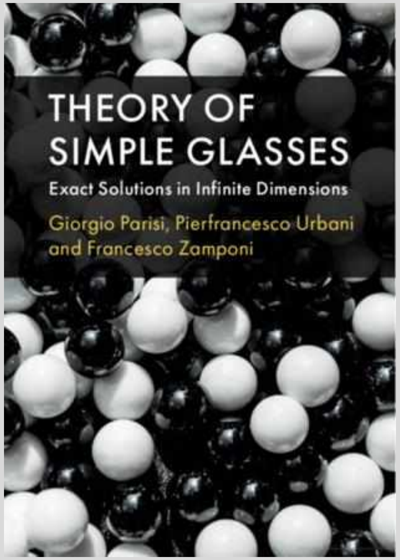
$$\mathcal{Z}_c = \sum_{l=0}^{\infty} b_l \left(\frac{z}{\lambda^d}\right)^l, \quad z = e^{\mu/k_B T} \text{ fuga}$$

$\lambda = \hbar\sqrt{2\pi/mk_B}$



(2020)

Typical scale of volume: volume of hard sphere

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$$\Rightarrow B_2 = \frac{1}{2}\mathrm{v}_d(a),\ B_{l>2} = 0$$

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$$\boxed{\frac{PV}{k_B T} = N\left(1 + \frac{1}{2}\mathrm{v}(a^*) n\right)}$$

Conclusion: only 2-particle interaction important in $d=\infty$

Correlated electrons

Electronic correlations (I):
Effects beyond factorization of the interaction (Hartree-Fock)

Wigner (1934)

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:

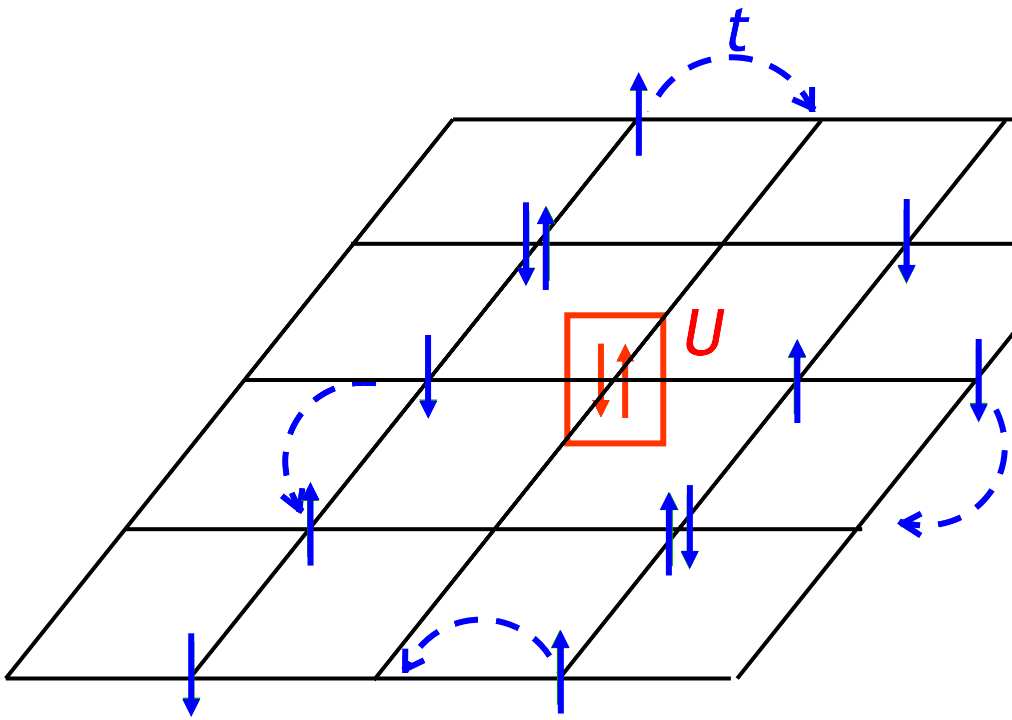
Magnetism and localized magnetic states in metals

Anderson impurity model ("single-impurity Anderson model"):
local interaction between *d*-electrons $Un_{\uparrow}^{d}n_{\downarrow}^{d}$

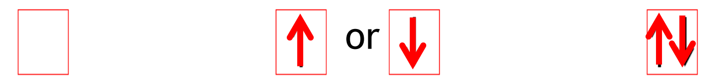
Anderson (1961)
Wolff (1961)

Single-impurity Anderson model

Anderson (1961)



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



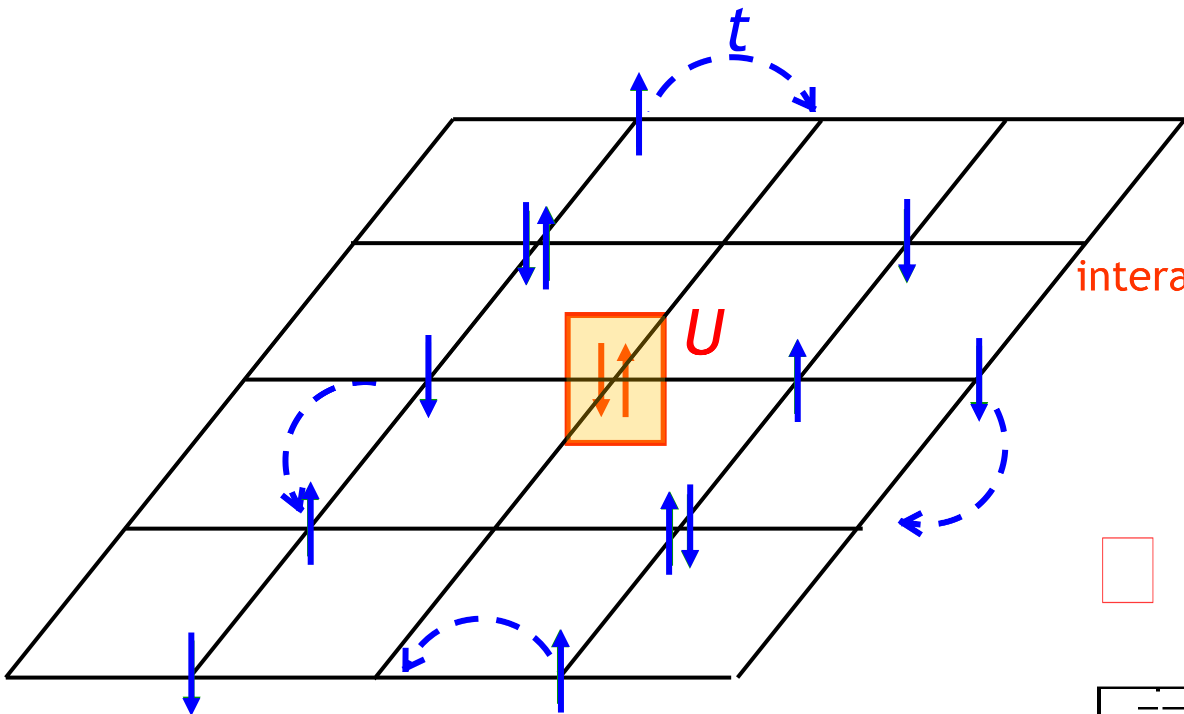
$E = \;0 \qquad \varepsilon_d \qquad 2\varepsilon_d+U$

local moment

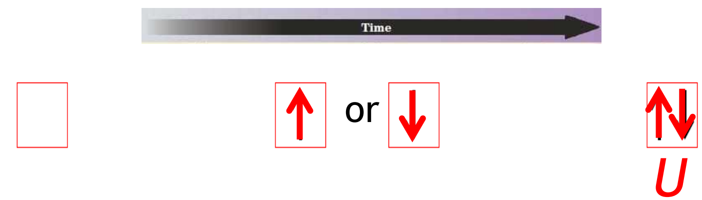
trivial eigenstates

Single-impurity Anderson model

Anderson (1961)



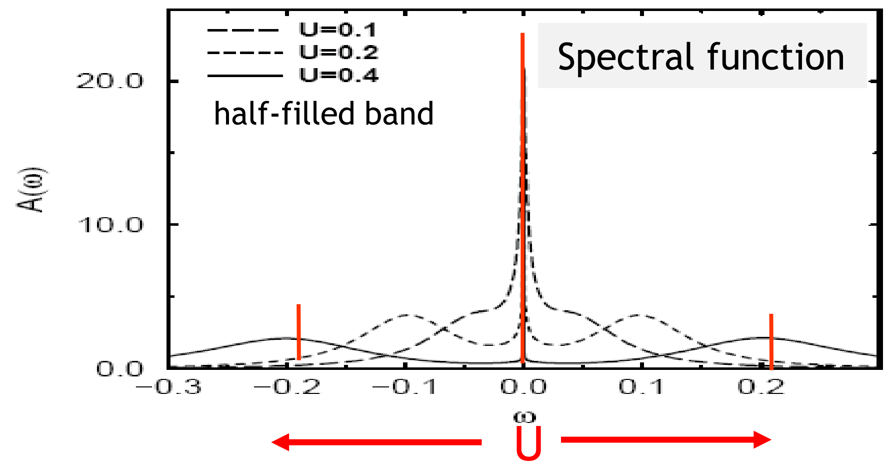
Non-interacting
conduction (*s*-) electrons
+
Immobile *d*-electrons with
interaction *U* on a single site ("impurity")
+
s,*d*-hybridization



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

→ characteristic 3-peak structure

→ Lecture Jan von Delft



Bulla, Hewson, Pruschke (1998)

1963: Minimal lattice model of correlated electrons

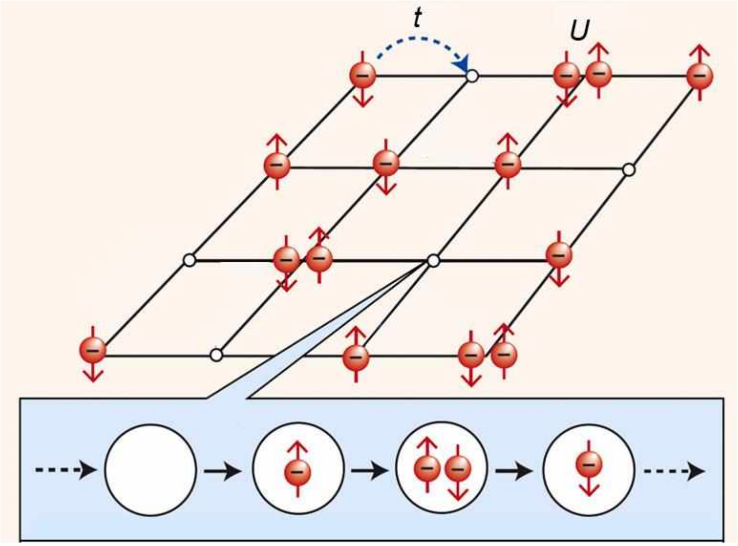
(for ferromagnetism of transition metals ?)

Hubbard model

- tight binding
- extreme screening assumed:

  only local interaction

→ no classical analogue



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

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

Diagonal in momentum space (waves)

Diagonal in position space (particles)

$\langle H_{\text{int}} \rangle = 0$ in the ferromagnetic phase

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

→ Find good approximations

Gutzwiller variational approach

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \underbrace{\sum_{i} n_{i\uparrow} n_{i\downarrow}}_{D}$$

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

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

One-particle wave function

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

- Gutzwiller approximation (GA):

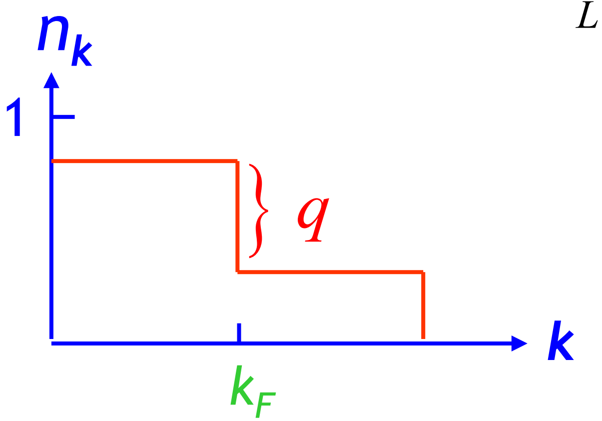
Gutzwiller (1963/65)

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

Gutzwiller variational approach

Gutzwiller (1963/65)

$$\frac{E_G(\lambda)}{L} \overset{GA}{=} q(d)\varepsilon_0 + U \underbrace{d}_{\frac{1}{L}\langle D\rangle} \;, \quad d \equiv d(\lambda) \qquad \boxed{\frac{\partial E_G}{\partial d} = 0}$$



Conditions for ferromagnetic ground state?

Brinkman, Rice (1970)

$$\boxed{d = \frac{1}{4}\left(1 - \frac{U}{U_c}\right)} \qquad \boxed{U_c = 8\varepsilon_0} \qquad \boxed{q = 1 - \left(\frac{U}{U_c}\right)^2} \qquad \boxed{E_G = -L\varepsilon_0\left(1 - \frac{U}{U_c}\right)^2}$$

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

describes
metal-insulator
("Mott") transition
→ V_2O_3

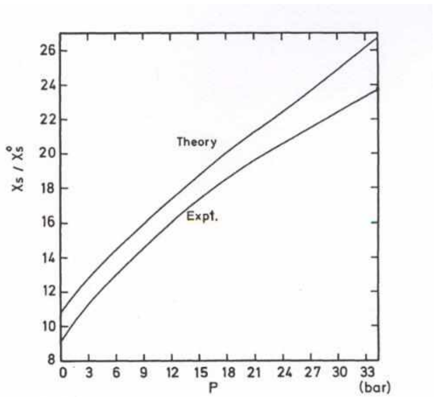
Application of Gutzwiller-Brinkman-Rice theory

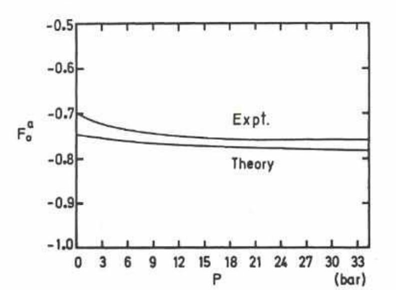
$$\frac{E_G(\lambda)}{L} \stackrel{GA}{=} q(d)\varepsilon_0 + Ud$$

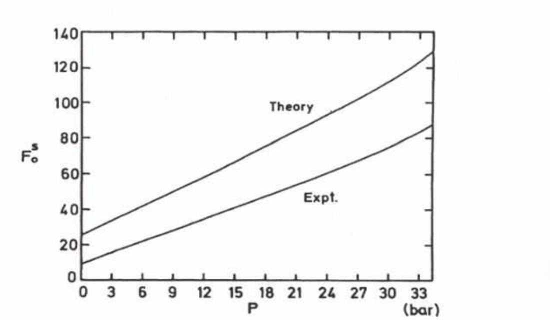
Normal liquid ^{3}He: close to Mott transition ? Anderson, Brinkman (1975)

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

→ Lecture Giovanni Vignale







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

Systematic derivation using quantum many-body methods?

- Slave boson mean-field theory Kotliar, Ruckenstein (1986)

- Infinite dimensions Metzner, DV (1987-89)

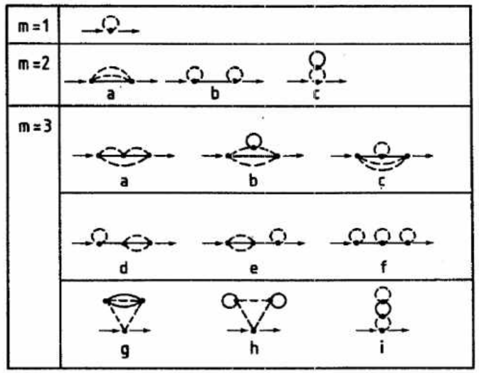
Correlated electrons in infinite dimensions

Gutzwiller wave function

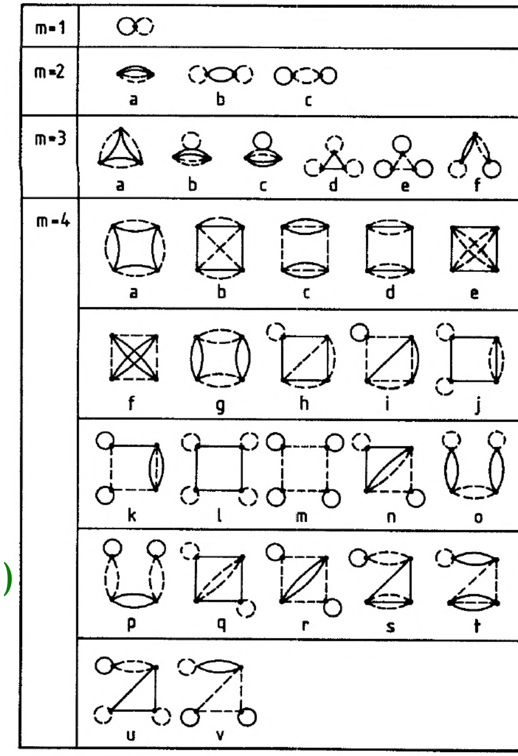
Analytic evaluation of $E_G = \frac{\langle \psi_G | H | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$ in $d=1$

Metzner, DV (1987/1988)

Walter Metzner



Diagrams (kinetic energy)



Diagrams (Hubbard interaction)

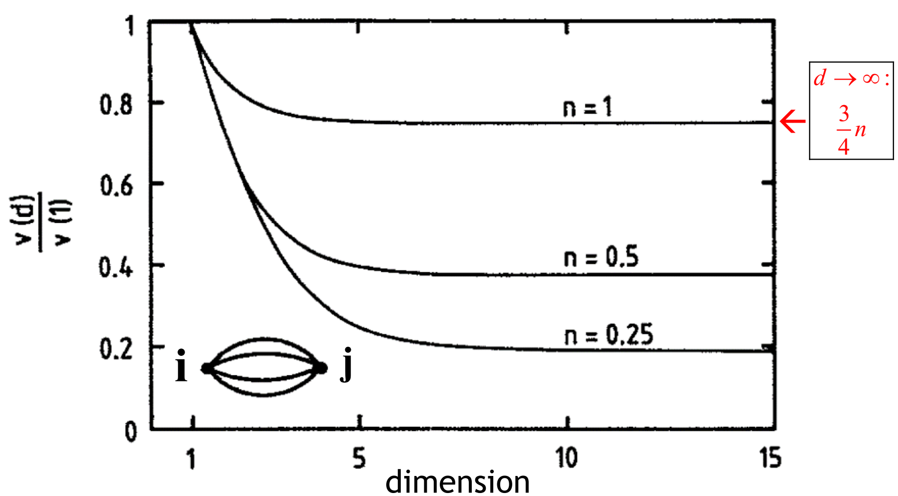
→ Exact, analytic summation of all diagrams

→ all correlation functions

Gebhard, DV (1987/1988)

d>1

Numerical calculation by Monte-Carlo integration



Great simplifications for $d \to \infty$:

- internal momenta become independent
- again all diagrams can be calculated and summed exactly
- results of GA recovered
  → fully diagrammatic derivation of the GA

VOLUME 62, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JANUARY 1989

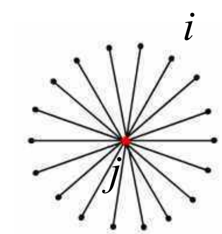
Correlated Lattice Fermions in $d=\infty$ Dimensions

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)

$$\left\langle \hat{H}_{\rm kin} \right\rangle_0 = -t \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\left\langle \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} \right\rangle_0}_{g^0_{ij,\sigma}}$$

$g^0_{ij,\sigma}$ = Probability amplitude for hopping $\mathbf{j}$ → NN $\mathbf{i}$

$\left|\text{Amplitude for hopping } \mathbf{j} \to \text{NN } \mathbf{i}\right|^2$ = ***Probability*** for hopping $\mathbf{j} \to Z$ NN $\mathbf{i}$ $\propto \dfrac{1}{Z}$



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

VOLUME 62, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JANUARY 1989

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

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

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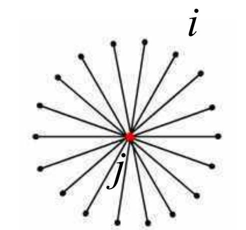

$\Rightarrow$ $\left|\text{Amplitude for hopping } \mathbf{j} \to \text{NN } \mathbf{i}\right| = g^0_{ij,\sigma} \propto \dfrac{1}{\sqrt{Z}}$ or $\dfrac{1}{\sqrt{d}}$, $Z = 2d$ (hypercubic lattice)

VOLUME 62, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JANUARY 1989

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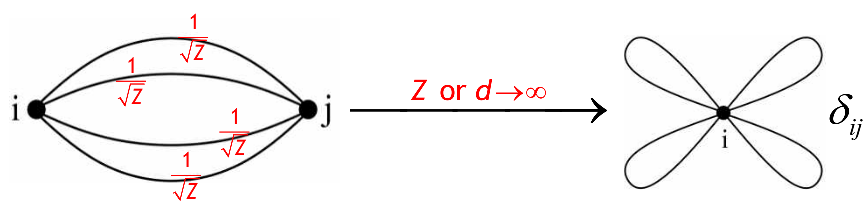
Quantum scaling $\quad t = \dfrac{t^*}{\sqrt{2d}}$

$\xrightarrow{Z \text{ or } d \to \infty}$ 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 $g^0_{ij,\sigma} = \lim_{t\to 0^-} G^0_{ij,\sigma}(t)$

VOLUME 62, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JANUARY 1989

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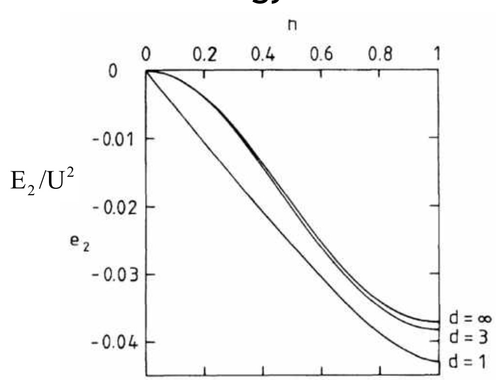
Quantum scaling $t = \dfrac{t^*}{\sqrt{2d}}$

$\xrightarrow{Z \text{ or } d \to \infty}$ 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 $d=3$

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

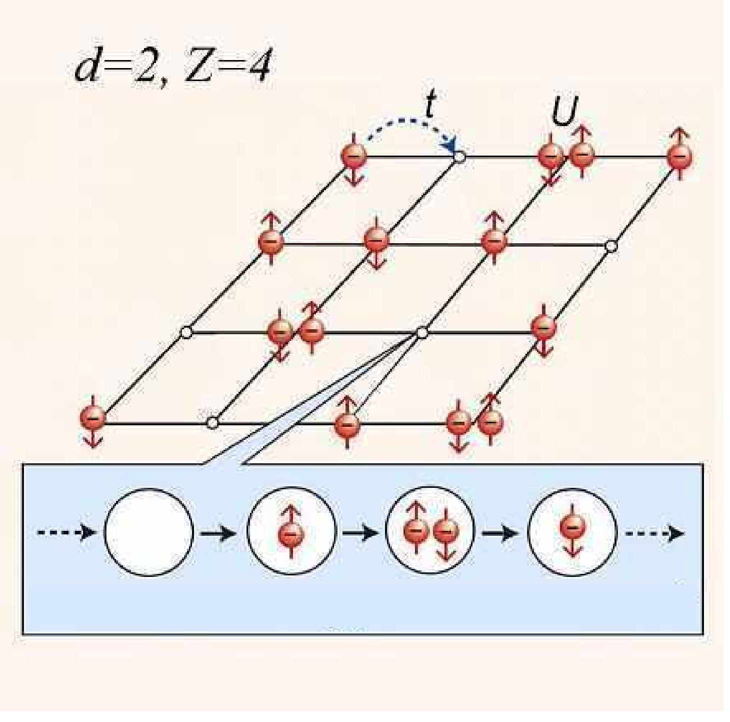
Mean-field limit of the Hubbard model in $d \to \infty$

Metzner, DV (1989)

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

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

Purely local interaction:
independent of d, Z



Thou shalt not factorize:

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

Local quantum fluctuations always present → dynamic

Quantum fluctuations neglected → static

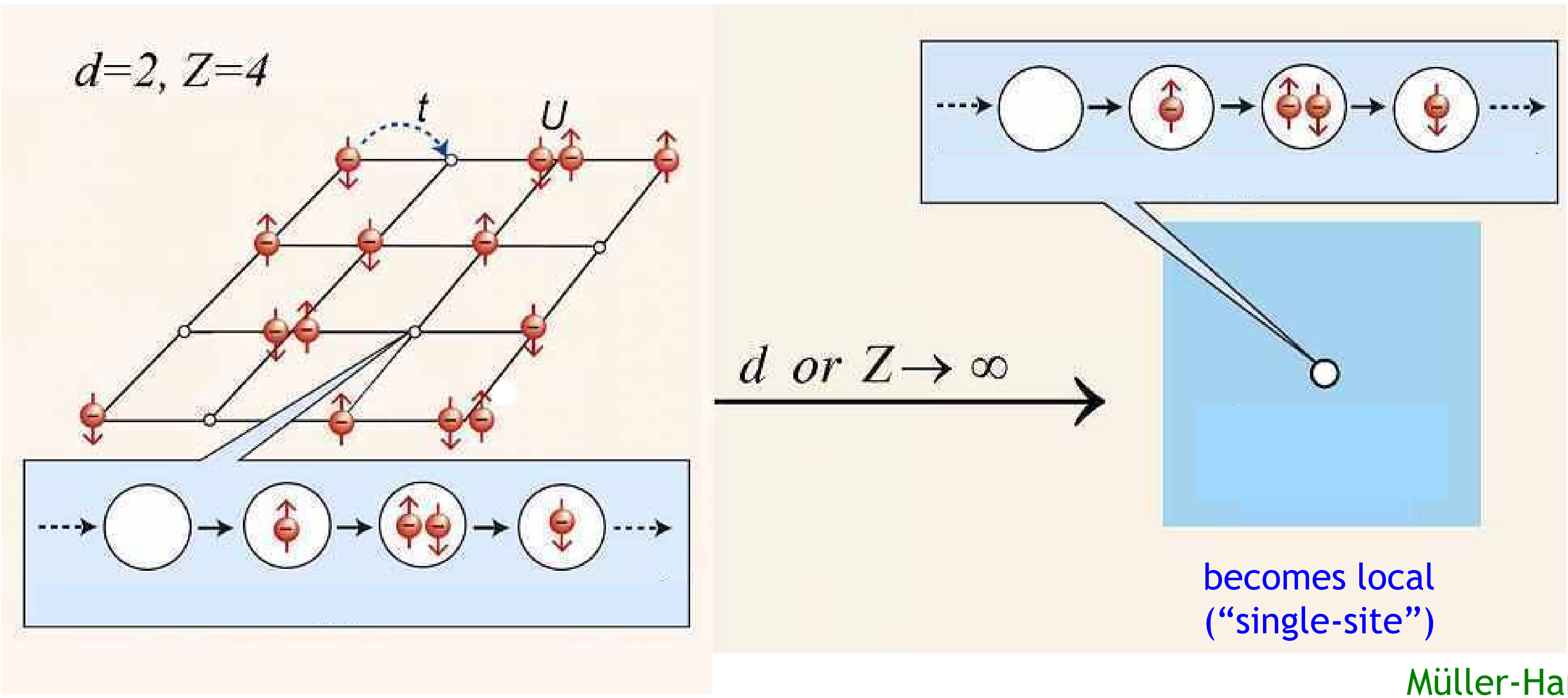
Hartree(-Fock)

Mean-field limit of the Hubbard model in $d \rightarrow \infty$

Metzner, DV (1989)

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

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



becomes local
("single-site")

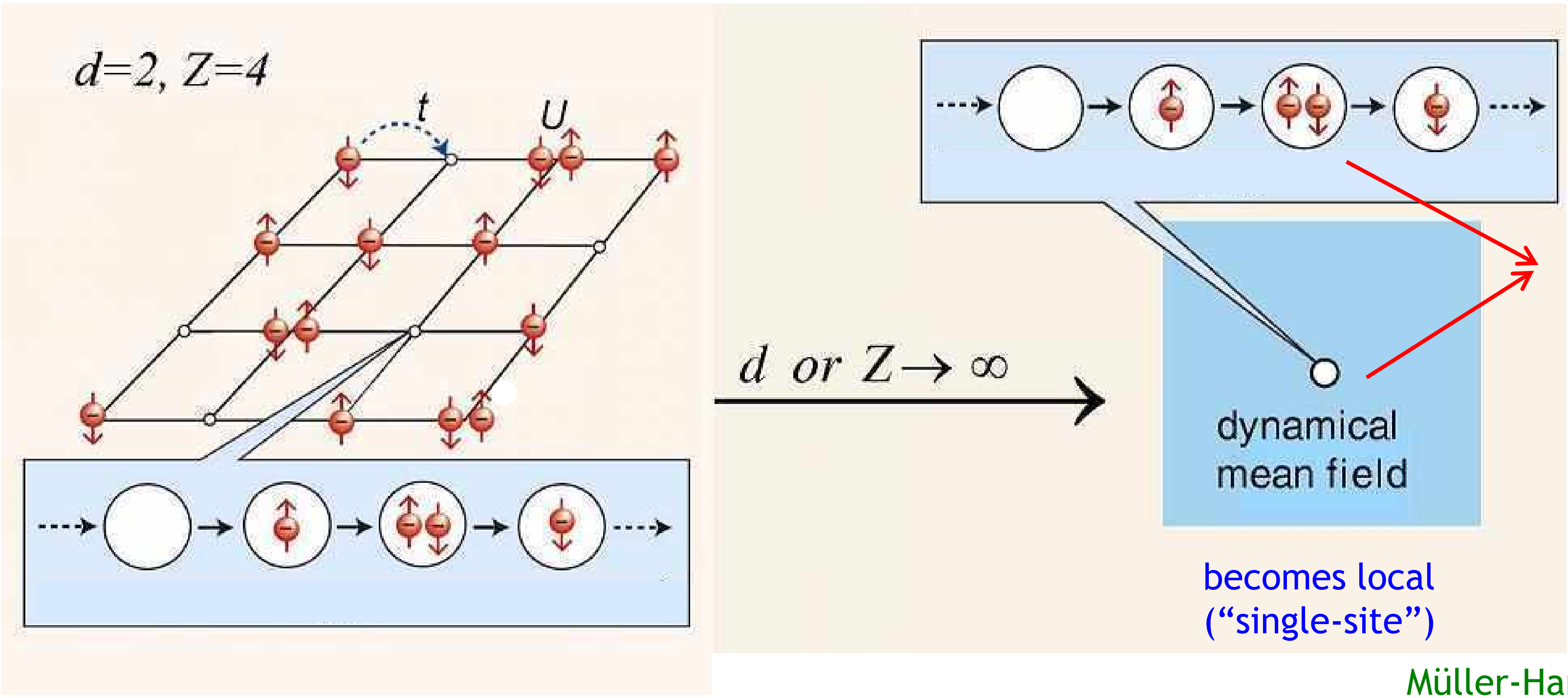
Müller-Hartmann (1989)

Mean-field limit of the Hubbard model in $d \to \infty$

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

Metzner, DV (1989)

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



mutually dependent

becomes local ("single-site")

Müller-Hartmann (1989)

CPA-type self-consistent mean-field theory

Janiš (1991)

How to solve?

Mean-field limit of the Hubbard model in $d \to \infty$

PHYSICAL REVIEW B VOLUME 45, NUMBER 12 15 MARCH 1992-II

Hubbard model in infinite dimensions

Antoine Georges*
Physics Department, Princeton University, Princeton, New Jersey 08544

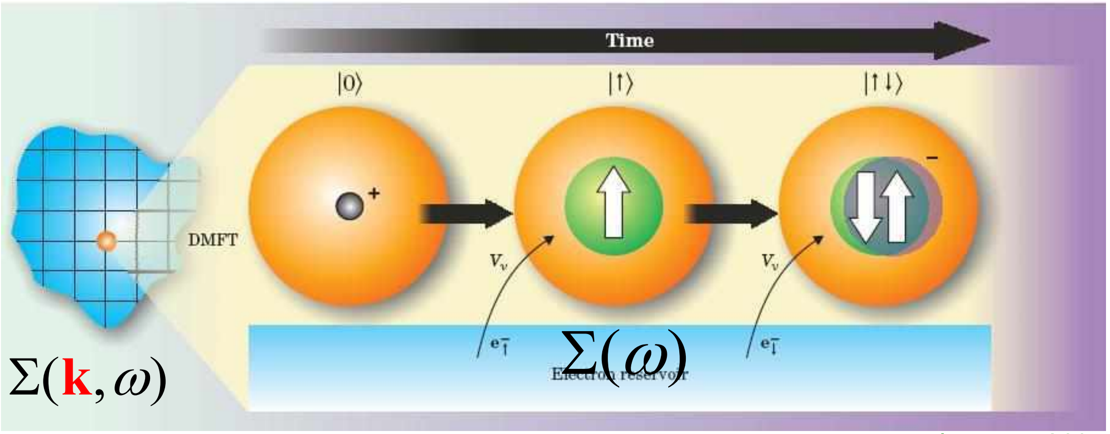
Gabriel Kotliar
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854
(Received 23 September 1991)

Hubbard model $\xrightarrow{d,Z\to\infty}$ 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 in $d \rightarrow \infty$



Kotliar, DV (2004)

Fully dynamical, but mean-field in position space

Dynamical Mean-Field Theory (DMFT)

Exact in $d, Z \rightarrow \infty$

New type of mean-field theory for quantum particles

Self-consistent equations of DMFT

(i) Impurity Green function

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

(ii) Local lattice Green function

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

→ information about lattice structure

- free electrons in a dynamic potential Σ(ω) ("mean field")
- Fermi liquid

Solve with a numerical "impurity solver":

QMC

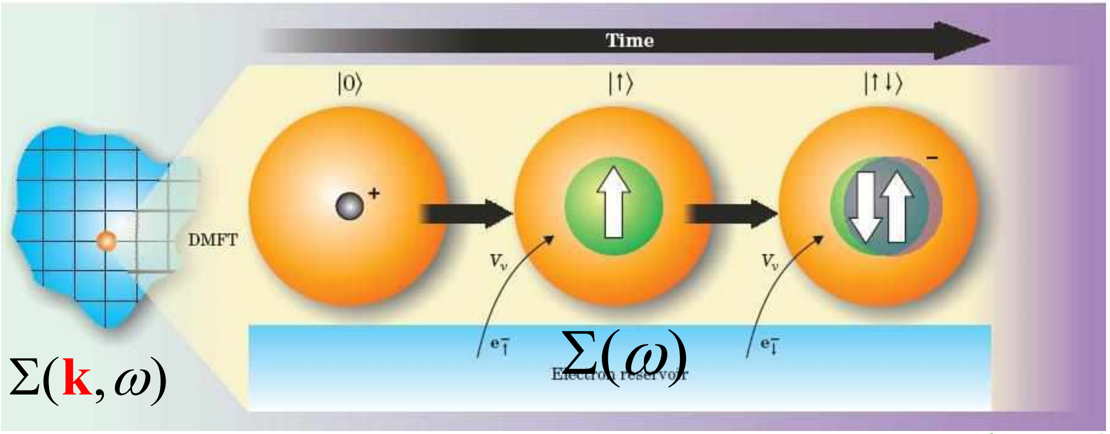
CT-QMC — Rubtsov and Lichtenstein (2004); Werner, Comanac, de'Medici, Troyer, Millis (2006)

→ Lecture Philipp Werner

Analytic continuation → Lecture Erik Koch

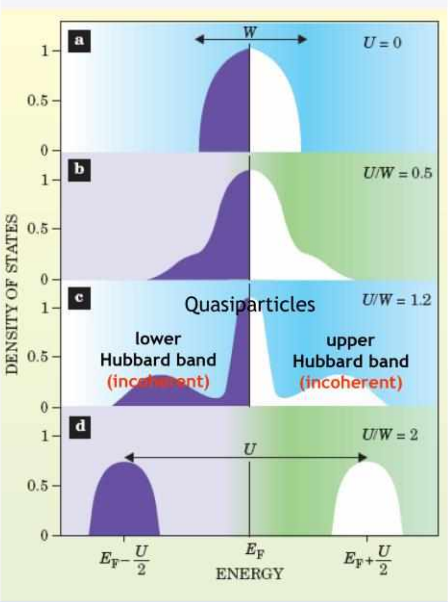
ED
Lanczos
FLEX
NRG
DMRG/tensor networks
Machine learning, … → Lecture Cedric Weber

Characteristic features of DMFT



Kotliar, DV (2004)

Spectral function (n=1)



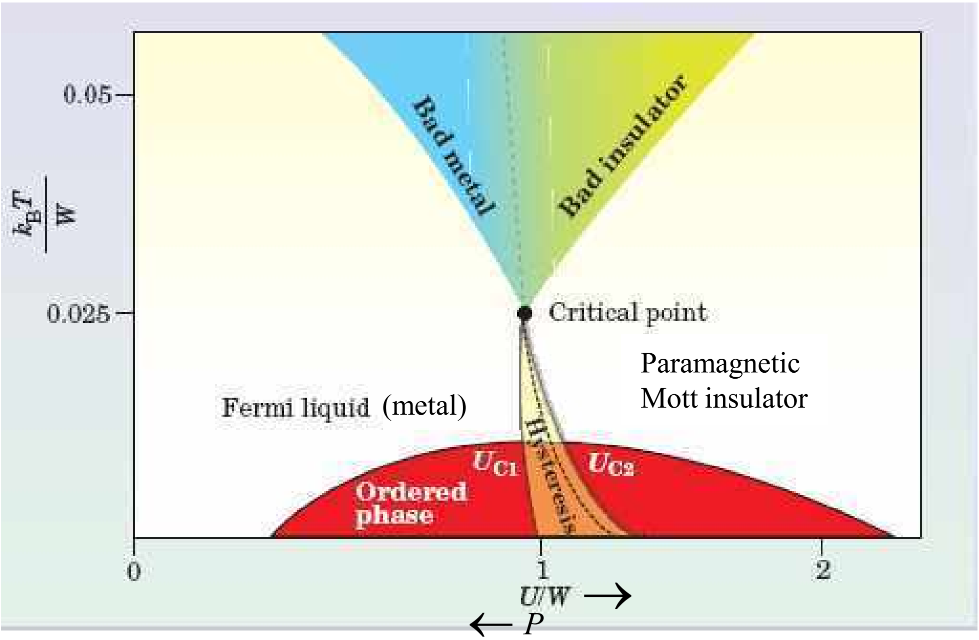
Better definition of electronic correlations:

- transfer of spectral weight
- finite lifetime of excitations

Experimentally detectable (PES, ARPES, …)

→ DMFT describes Mott metal-insulator transition

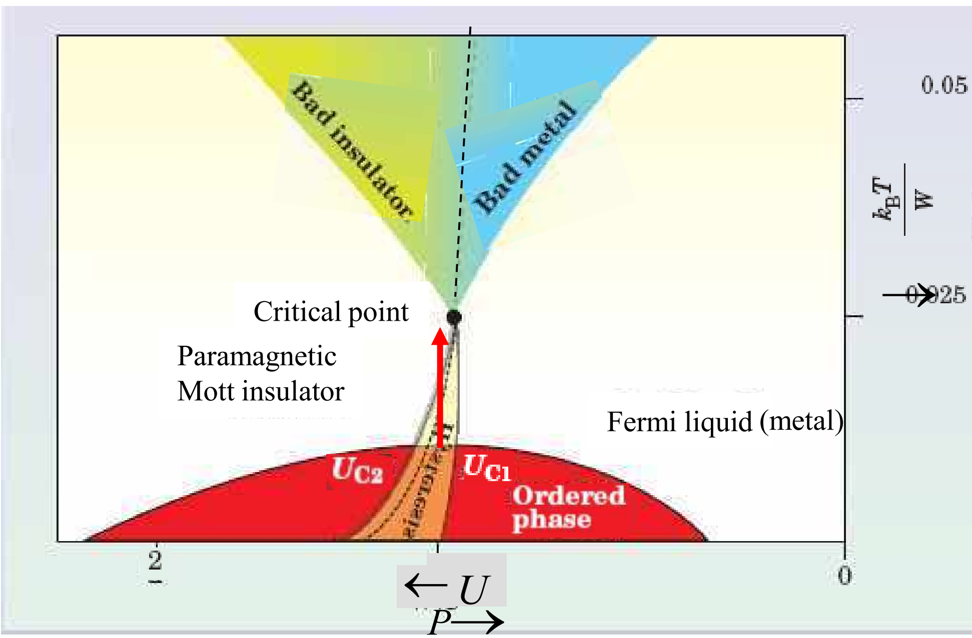
Mott metal-insulator transition: T-(U,P) phase diagram



Kotliar, DV (2004)

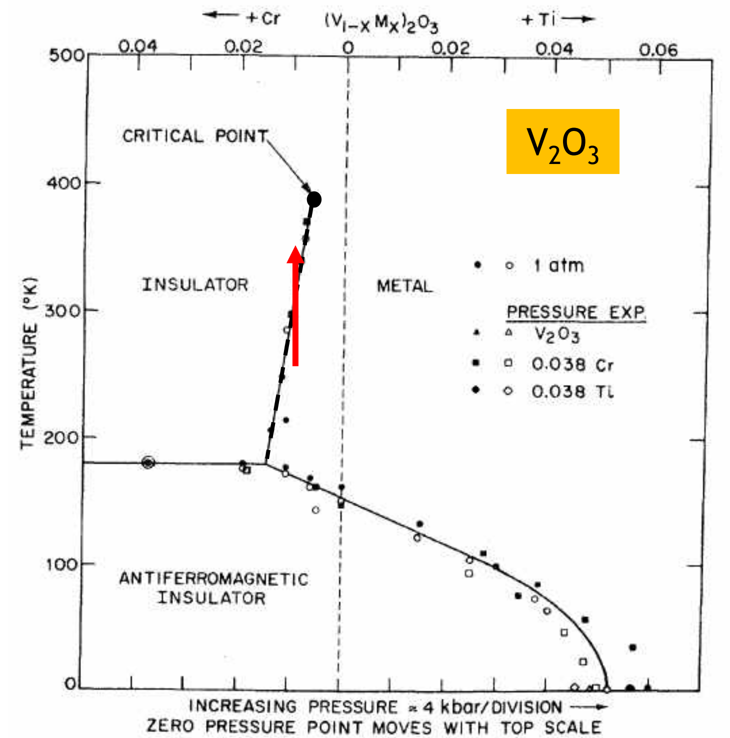
Terletska *et al*. (2011)
Radonjić *et al*. (2012)

Mott metal-insulator transition: T-(U,P) phase diagram



Terletska *et al.* (2011)
Radonjić *et al.* (2012)

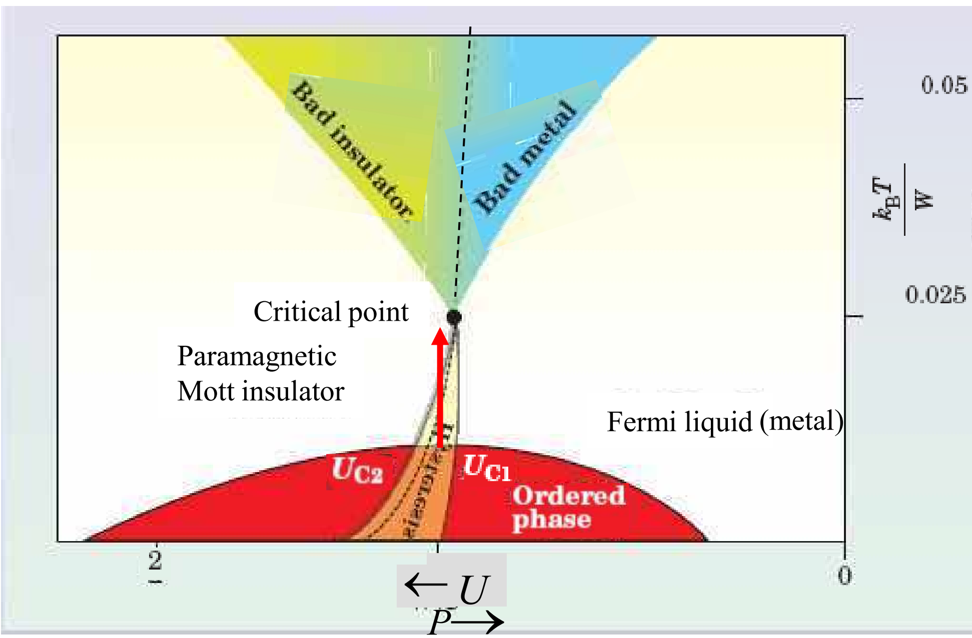
Kotliar, DV (2004)



$P \longrightarrow$

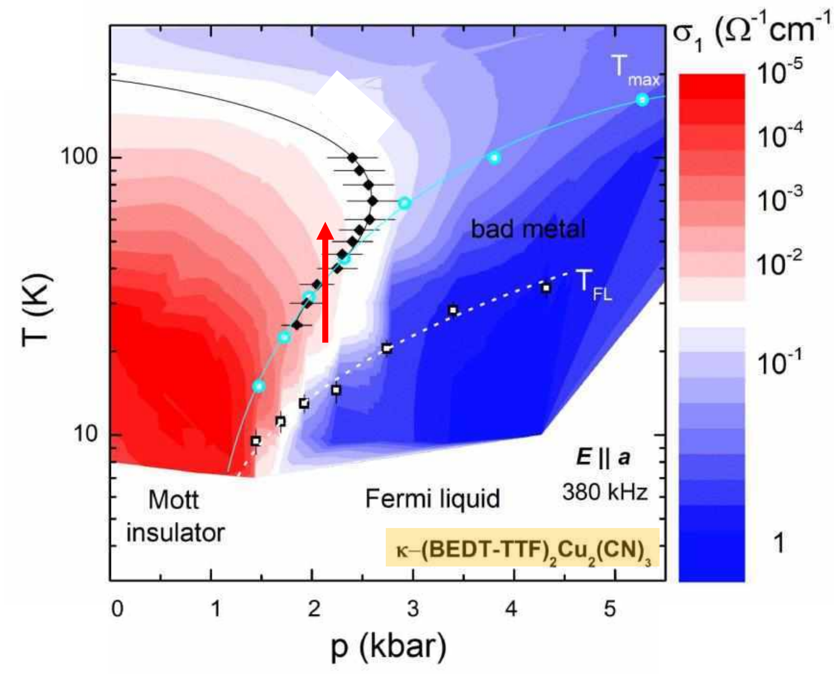
McWhan, Menth, Remeika, Brinkman, Rice (1973)

Mott metal-insulator transition: T-(U,P) phase diagram



Terletska *et al.* (2011)
Radonjić *et al.* (2012)

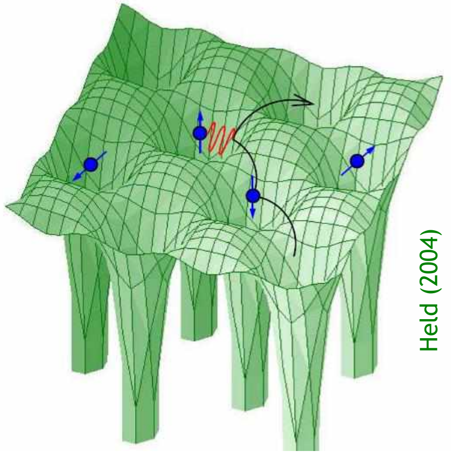
Kotliar, DV (2004)



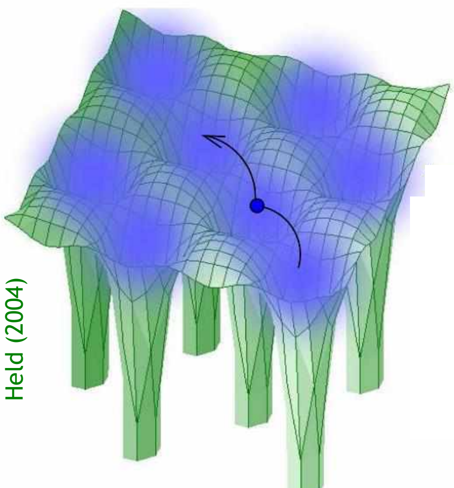
Pustogow *et al.* (2021)
Rösslhuber *et al.* (2021))

Application of DMFT to correlated electron materials

Correlated materials: Non-perturbative approaches required

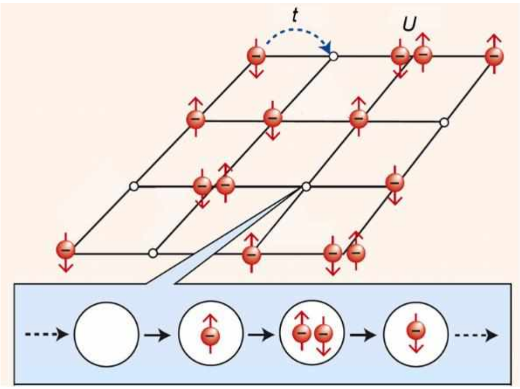


DFT/LDA, **GGA**		Model Hamiltonians	
+	material specific	−	input parameters unknown
+	fast code packages	−	computationally expensive
−	fails for strong correlations	+	systematic many-body approach



How to combine ?

↔



Computational scheme for correlated electron materials

LDA+DMFT

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

J. Phys.: Condens. Matter **9** (1997) 7359–7367. Printed in the UK PII: S0953-8984(97)83361-9

First-principles calculations of the electronic structure and spectra of strongly correlated systems: dynamical mean-field theory

V I Anisimov†, A I Poteryaev†, M A Korotin†, A O Anokhin† and G Kotliar‡

† Institute of Metal Physics, Ekaterinburg, GSP-170, Russia
‡ Serin Physics Laboratory, Rutgers University, Piscataway, NJ 08854, USA

Received 14 April 1997

PHYSICAL REVIEW B VOLUME 57, NUMBER 12 15 MARCH 1998-II

***Ab initio* calculations of quasiparticle band structure in correlated systems: LDA++ approach**

A. I. Lichtenstein
Forschungszentrum Jülich, D-52428 Jülich, Germany

M. I. Katsnelson
Institute of Metal Physics, Ekaterinburg 620219, Russia

(Received 11 July 1997)

Computational scheme for correlated electron materials

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**)

→ Lecture Alexander Lichtenstein

→ Lecture Eva Pavarini (+ linear response)

Computational scheme for correlated electron materials

More general:

$\boxed{\textbf{X+DMFT}}$

X= **DFT (LDA, GGA)**
GW Biermann, Aryasetiawan, Georges (2003)

→ Lecture Ferdi Aryasetiawan

=

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

+

Local electronic correlations

-

Double counting correction (LDA, GGA)

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

Contact with experiment via, e.g., the DMFT spectral function

k-integrated spectral function
→ PES

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

k-resolved spectral function
→ ARPES

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

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

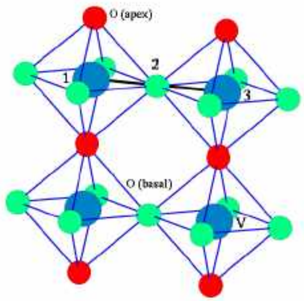
Early results of DFT+DMFT

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

Electronic structure

Crystal structure

SrVO$_3$: $\angle V - O - V = 180°$

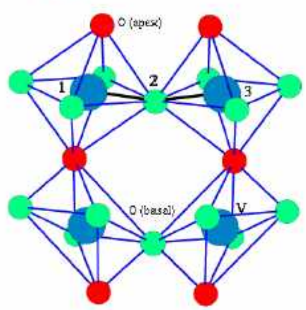


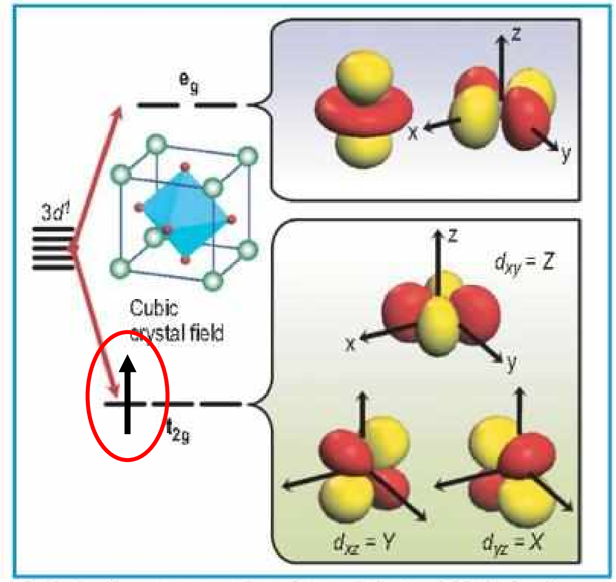
$\Downarrow$

orthorhombic distortion

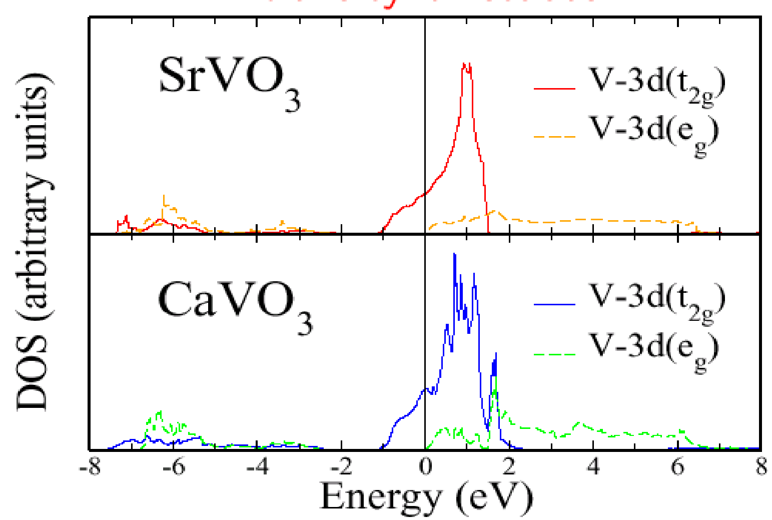
$\Downarrow$

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





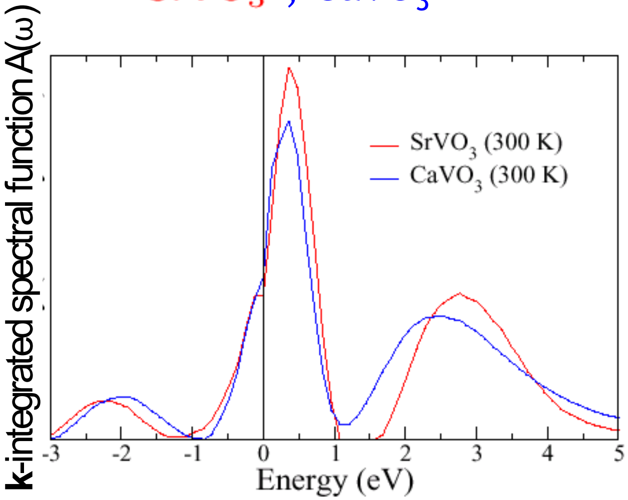
LDA density of states

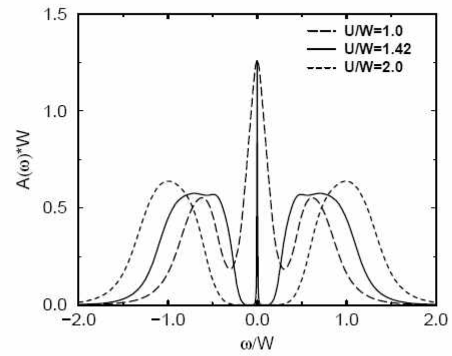


No correlation effects/spectral transfer

LDA+DMFT results

$SrVO_3$, $CaVO_3$



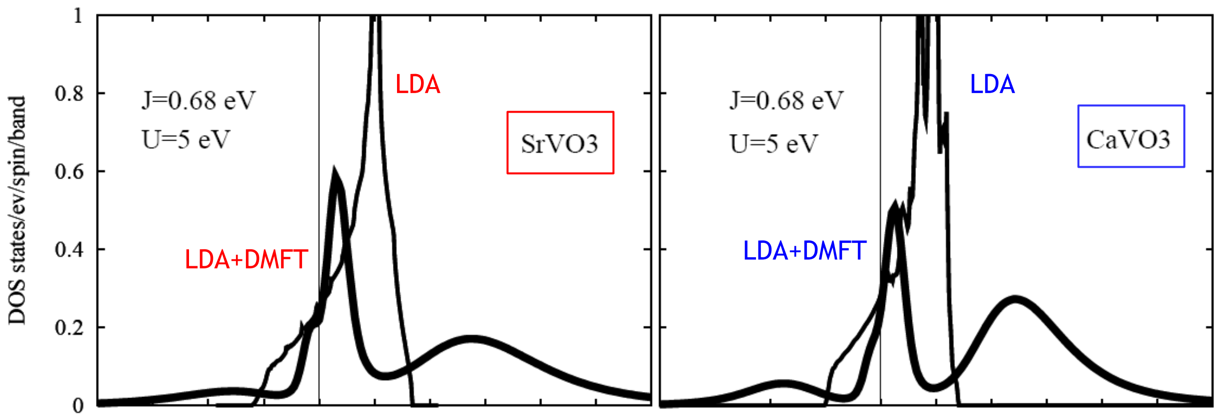


Single-band Hubbard model (DMFT)

Bulla (1999)

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

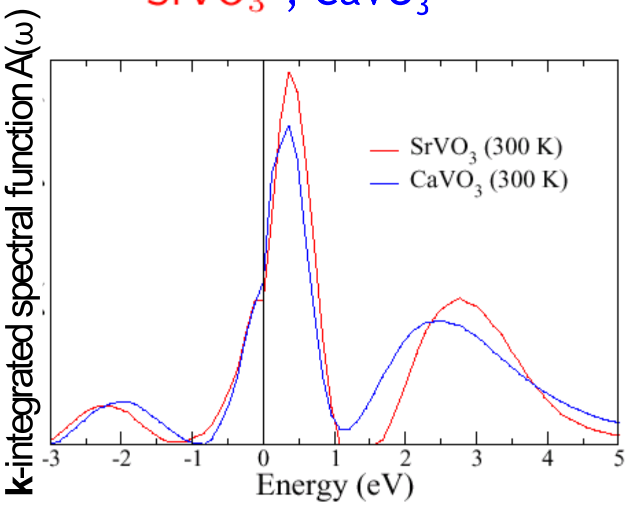
Osaka – Augsburg – Ekaterinburg collaboration: Sekiyama *et al.* (2004)



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

LDA+DMFT results

$SrVO_3$, $CaVO_3$

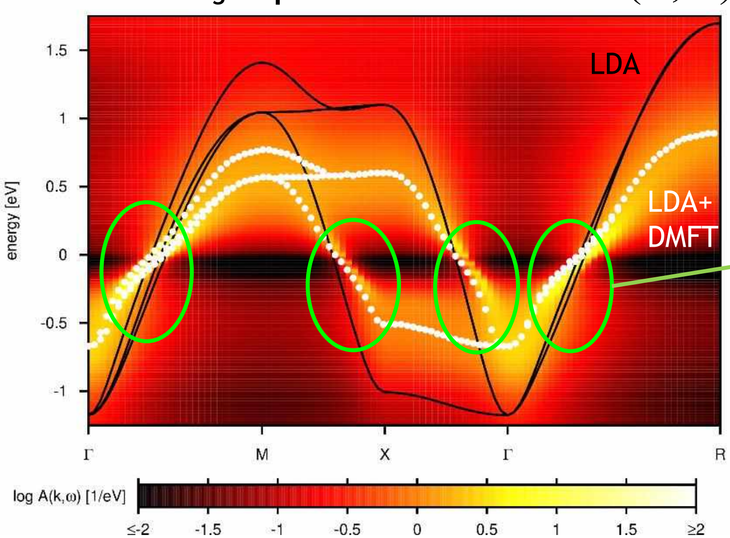


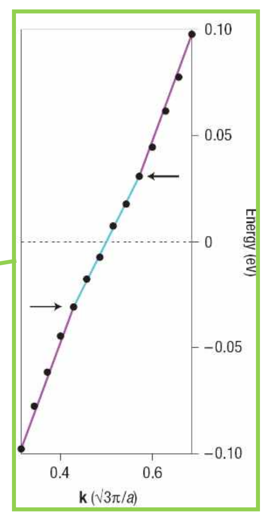
Constrained LDA: U=5.55 eV, J=1.0 eV

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

$SrVO_3$: Spectral function $A(\mathbf{k},\omega)$

Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV (2007)





Electronic correlations →

- quasiparticle damping
- band narrowing

- "kinks"

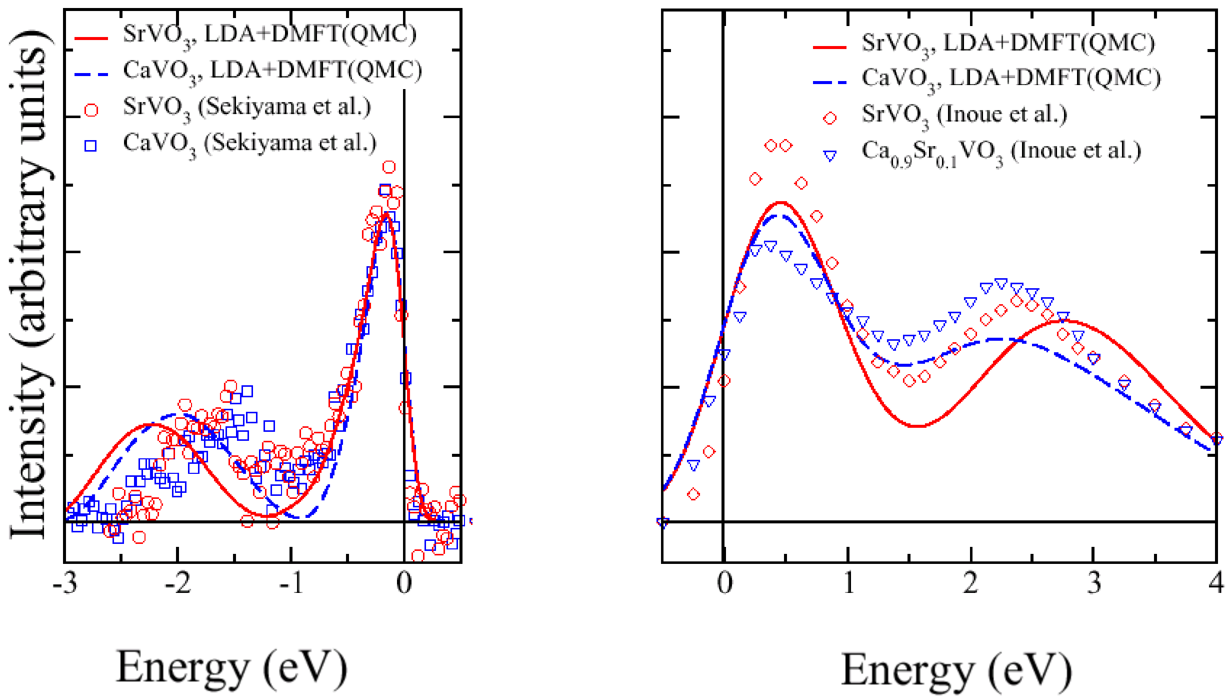
- at energy $\omega_* = Z_{FL} \times$(bare energy scale)
- sharpen with increasing interaction $\propto (Z_{FL})^{-2}$
- Fermi liquid regime terminates at ω_*

LDA+DMFT for (Sr,Ca)VO_3: 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



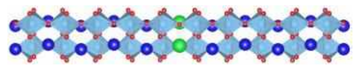
Correlation-induced 3-peak structure confirmed

Applications of DMFT during 1997-2022: Current status

DMFT used to investigate/explain electronic correlations in:

- Many bulk materials

- Heterostructures, interlayers, surfaces

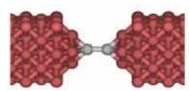


Lechermann, Obermeyer (2015)

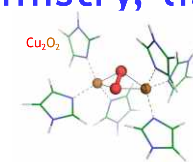
Okamoto, Millis (2004)
Peters, Tada, Kawakami (2016)
Janson, Held (2018)
Chen, Hampel, Karp, Lechermann, Millis (2022)

→ Lecture Frank Lechermann

- Molecular electronics, quantum chemistry, ligand binding



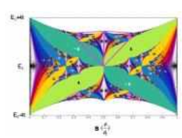
Jacob, Haule, Kotliar (2010)



al-Badri, Linscott, Georges, Cole, Weber (2020)

Weber *et al*. (2013)
Chioncel *et al*. (2015)
Pudleiner, Kauch, Held, Li (2019)

- Topological materials

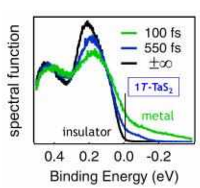


Markov, Rohringer, Rubtsov (2019)

Tada *et al*. (2012)
Irsigler, Grass, Zheng, Barbier, Hofstetter (2021)
Krüger, Potthoff (2021)

→ Lecture Michael Potthoff

- Nonequilibrium



Perfetti *et al*. (2006)

Turkowski, Freericks (2005)
Eckstein, Kollar (2008)
Freericks, Krishnamuthy, Pruschke (2009)
Aoki, Tsuji, Eckstein, Kollar, Oka, Werner (2014)
Ligges *et al*. (2018)

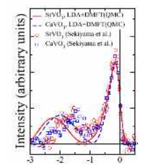
→ Lecture Martin Eckstein

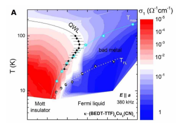
DMFT: Preliminary summary

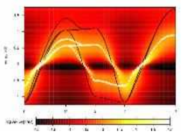
Dynamical, local self-energy $\Sigma_{ij}(\omega) = \delta_{ij}\Sigma(\omega)$

can describe

- Spectral transfer, Mott-MIT
- Quasiparticle renormalization + damping
- Orbital, charge, magnetic LRO, …



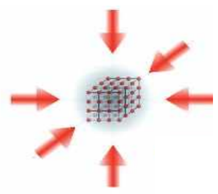




and is often accurate in $d=3$, as demonstrated for

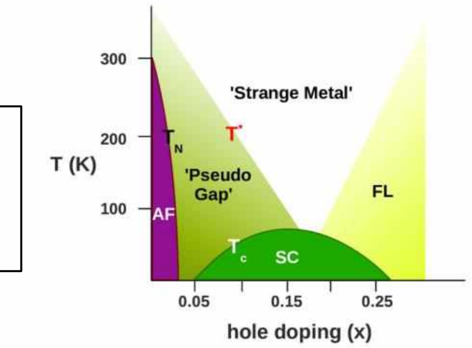
- Fermionic atoms in 3D optical lattices

Schneider *et al.* (2008)



cannot describe

- Non-local/long-range interactions
- Critical behavior near thermal or quantum phase transitions
- Low-T physics of 2-dim. systems, *e.g.*, high T_C superconductivity



Beyond mean-field theory

$1/d$ corrections

$d = \infty$ mean-field result $O(1/d^0)$

$d < \infty$ beyond mean-field via expansion in $1/d$?

Ising model

$$H = -\frac{1}{2} J \sum_{\langle i,j \rangle} S_i S_j \qquad J \to \frac{J^*}{2d},\ J^* \equiv 1$$

- interaction along bonds
- no dynamics, but thermodynamics

High-order expansion of free energy, susceptibilities … in $1/d$ possible

(i) high-T (paramagnetic) phase — Fisher, Gaunt (1964)

(i) low-T (ferromagnetic) phase, high T $\Leftrightarrow 1/d$ expansion (valid even in low-T phase)
Georges, Yedidia (1991)

$1/d$ corrections

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Ising model

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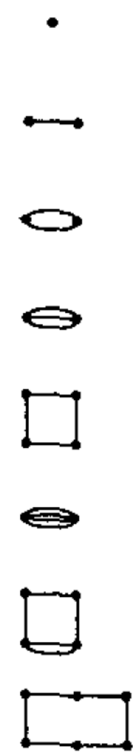
- interaction along bonds
- no dynamics, but thermodynamics

$A(T,m)$: Magnetization-dependent free energy
N: # spins

$$\begin{aligned}
-\frac{\beta A}{N} = & -\left[\frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2}\right] \\
& + \frac{\beta}{2d}\, d\, m^2 \\
& + \frac{1}{2}\left(\frac{\beta}{2d}\right)^2 d\,(1-m^2)^2 \\
& + \frac{2}{3}\left(\frac{\beta}{2d}\right)^3 d\, m^2 (1-m^2)^2 \\
& + \left(\frac{\beta}{2d}\right)^4 \frac{d(d-1)}{2}\,(1-m^2)^4 \\
& - \frac{1}{12}\left(\frac{\beta}{2d}\right)^4 d\,(1-m^2)^2 (1+6m^2-15m^4) \\
& + 2\left(\frac{\beta}{2d}\right)^5 2d(d-1)\, m^2 (1-m^2)^4 \\
& + \left(\frac{\beta}{2d}\right)^6 \left[d(d-1) + \frac{8}{3} d(d-1)(d-2)\right](1-m^2)^6
\end{aligned}$$



Georges, Yedidia (1991)

(i) high-T (paran

Fisher, Gaunt (1964)

(i) low-T (ferrom

(valid even in low-T phase)

$$\boxed{T_c = 1 - \frac{1}{2d} - \frac{1}{3d^2} - \frac{13}{24d^3} - \ldots}$$

asymptotic expansion (at best)

Fisher, Singh (1990)
Halvorsen, Bartkowiak (2000)

$1/d$ corrections

$d = \infty$ mean-field result $O(1/d^0)$

$d < \infty$ beyond mean-field via expansion in $1/d$?

Hubbard model: Gutzwiller wave function

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \qquad t \to \frac{t^*}{\sqrt{2d}},\ t^* \equiv 1$$

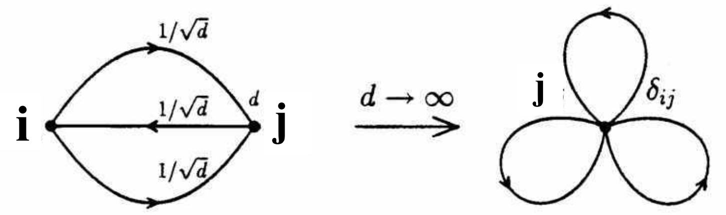
- local interaction
- no dynamics, T=0

$$g^0_{ij,\sigma} \sim O(1/d^{\|\mathbf{i}-\mathbf{j}\|/2}),\ \ \|\mathbf{i}\| = \sum_{n=1}^{d} |\mathbf{i}| :$$

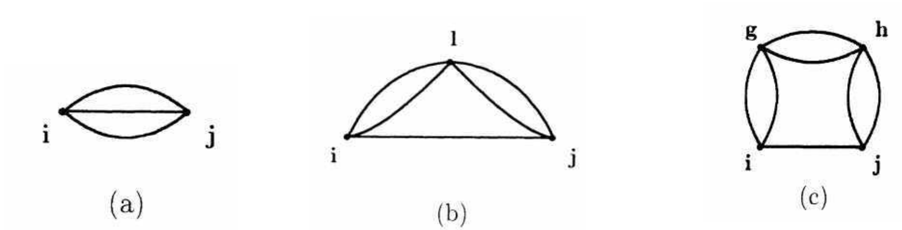
Length of $\mathbf{i}$ ("Manhattan metric")

$d = \infty$ Diagrammatic collapse → only local ("single-site") diagrams

Self-energy $\Sigma^{(2)}_{ij} =$



$d < \infty$ 2,3,... -site diagrams ("pull local diagrams apart")



Gebhard (1990)

$1/d$ corrections

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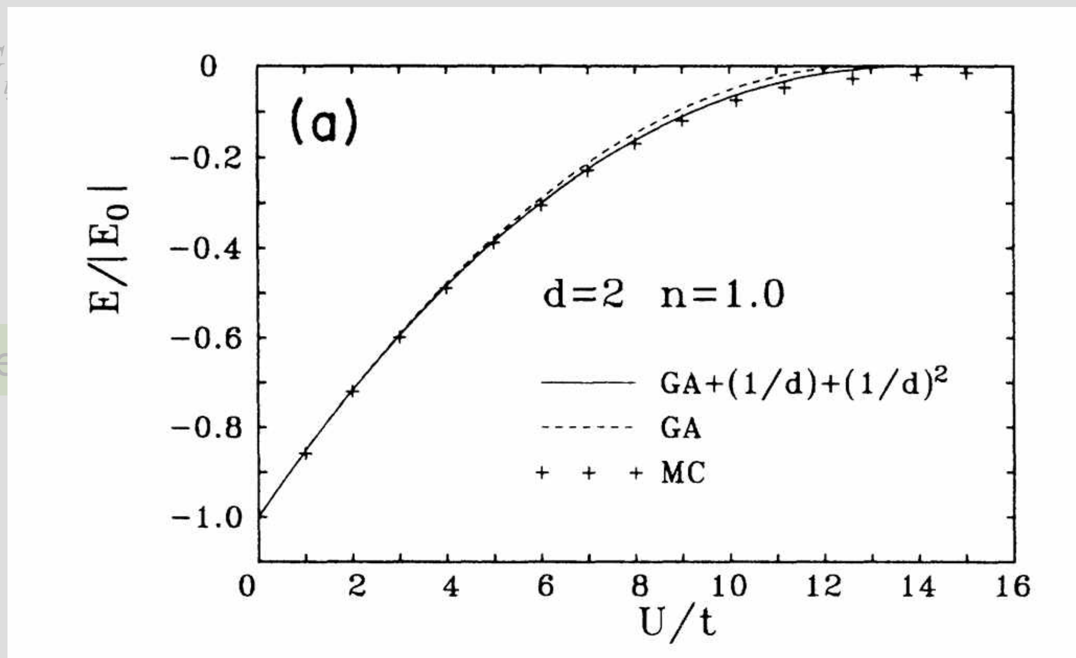

Gebhard (1990)

Gutzwiller-Brinkman-Rice transition MIT not removed in finite order $1/d$

van Dongen, Gebhard, DV (1990)

$1/d$ corrections

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$d < \infty$ beyond mean-field via expansion in $1/d$?

Hubbard model: DMFT

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \qquad t \to \frac{t^*}{\sqrt{2d}},\ t^* \equiv 1$$

- local interaction
- quantum dynamics

$1/d$ expansion using Luttinger-Ward functional $\Phi[G_{ij\sigma}]$

Sum of all vacuum-to-vacuum skeleton diagrams

Cluster approximation in $O(1/d)$

Schiller, Ingersent (1995)

Expand Φ:

$$\Phi[G] = (1 - \underbrace{2d}_{\text{Prevents overcounting}}) \sum_{i,\sigma} \underbrace{\Phi_{1-\text{imp}}}_{\Uparrow\ S_{1-\text{imp}}}[G_{ii\sigma}] + \sum_{\langle ij \rangle, \sigma} \underbrace{\Phi_{2-\text{imp}}}_{\Uparrow\ S_{2-\text{imp}}}[G_{ii\sigma}, G_{jj\sigma}, G_{ij\sigma}]$$

Self-consistent formulation possible

Problems: - DOS $N(\omega) \Longrightarrow G^0_{ij\sigma}$ non-analytic in $1/d$ → take actual d-dimensional $G^0_{ij\sigma}$

- Required exact diagrammatic cancellations violated in approx. treatments → acausal behavior

- Assure exact cancellation at each iteration step
- tested with FLEX, but success not guaranteed

Zarand, Cox, Schiller (2000)

$1/d$ corrections

$d = \infty$ mean-field result $O(1/d^0)$

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Hubbard model: DMFT

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Prevents overcounting

Self-consistent formulation possible

Problems: - DOS $N(\omega) \Rightarrow G^0_{ij\sigma}$ non-analytic in $1/d$ → take ...

- Required exact di... ...d in approx. treatments → acausal behavior

- Ass... ...ulation at each iteration step

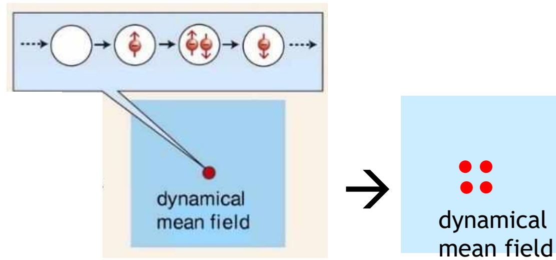
- tested with FLEX, but success not guaranteed

Zarand, Cox, Schiller (2000) ...chiller (2000)

$1/d$ expansion around DMFT possible, but not fully understood

Non-local effects: Beyond *1/d* expansions

- "Extended" DMFT   includes intersite quantum fluctuations → RKKY interaction
  Si, Smith (1996)
- Cluster extensions



Systematic, but limited numerically in cluster size

- <u>Momentum space</u>: Dynamical cluster approx. (DCA)   Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy (1998)

- <u>Real space</u>: Cellular DMFT (CDMFT)   Lichtenstein, Katsnelson (2000)
  Kotliar, Savrasov, Pálsson, Biroli (2001)

- Diagrammatic extensions, e.g.:

Dynamical vertex approximation (DΓA)   Toschi, Katanin, Held (2007)

→ Lecture Karsten Held

Local two-particle vertex → local + non-local self-energy diagrams

Dual fermion approach (DF)   Rubtsov, Katsnelson, Lichtenstein (2008)

Lattice problem: Local reference system + coupling to nonlocal degrees of freedom

- DMFT+fRG:

Start fRG flow from DMFT solution   Taranto *et al.* (2014); Vilardi, Taranto, Metzner (2019)

Conclusion on DMFT

- Hubbard model in infinite dimensions

  $\equiv$

  Dynamical mean-field theory (DMFT)

- DMFT is the natural mean-field theory of correlated lattice fermions

- DMFT can be extended beyond mean-field level

- DMFT now used to explain and predict the properties of correlated electron materials

Conclusion on infinite dimensions

Q: Why calculate in infinite dimensions?

A: Only accessible solution of many-body systems in $d > 1,2$

- thermodynamic limit
- closed form (self-consistent mean-field theory)
- thermodynamically consistent, controlled approximation