COLLÈGE DE FRANCE
1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

Fermions en interaction: Introduction à la théorie de Champ Moyen Dynamique(DMFT)

Cours 3 – Différentes perspectives sur l'établissement des équations de la théorie de champ moyen dynamique et la limite de grande dimension

Lecture mostly on BOARD – see recording

Cycle 2018-2019
21 mai 2019

COLLÈGE DE FRANCE 1530

Chaire de Physique de la Matière Condensée
Antoine Georges

Interacting Fermions: Introduction to Dynamical Mean-Field Theory (DMFT)

Lecture 3 – Different perspectives on the DMFT equations, their derivation and the limit of large dimensions.

Slides will be in English

Please don't hesitate to ask questions in French or English

2018-2019 Lectures
May 21, 2019

Today’s seminar (11:30)

Jan Kuneš

Institute of Solid-State Physics, TU Wien

Institute of Physics, Czech Academy of Sciences, Praha

Excitonic Condensation of Strongly Correlated Electrons

Exceptional seminar

Wednesday May 22 at 11:00

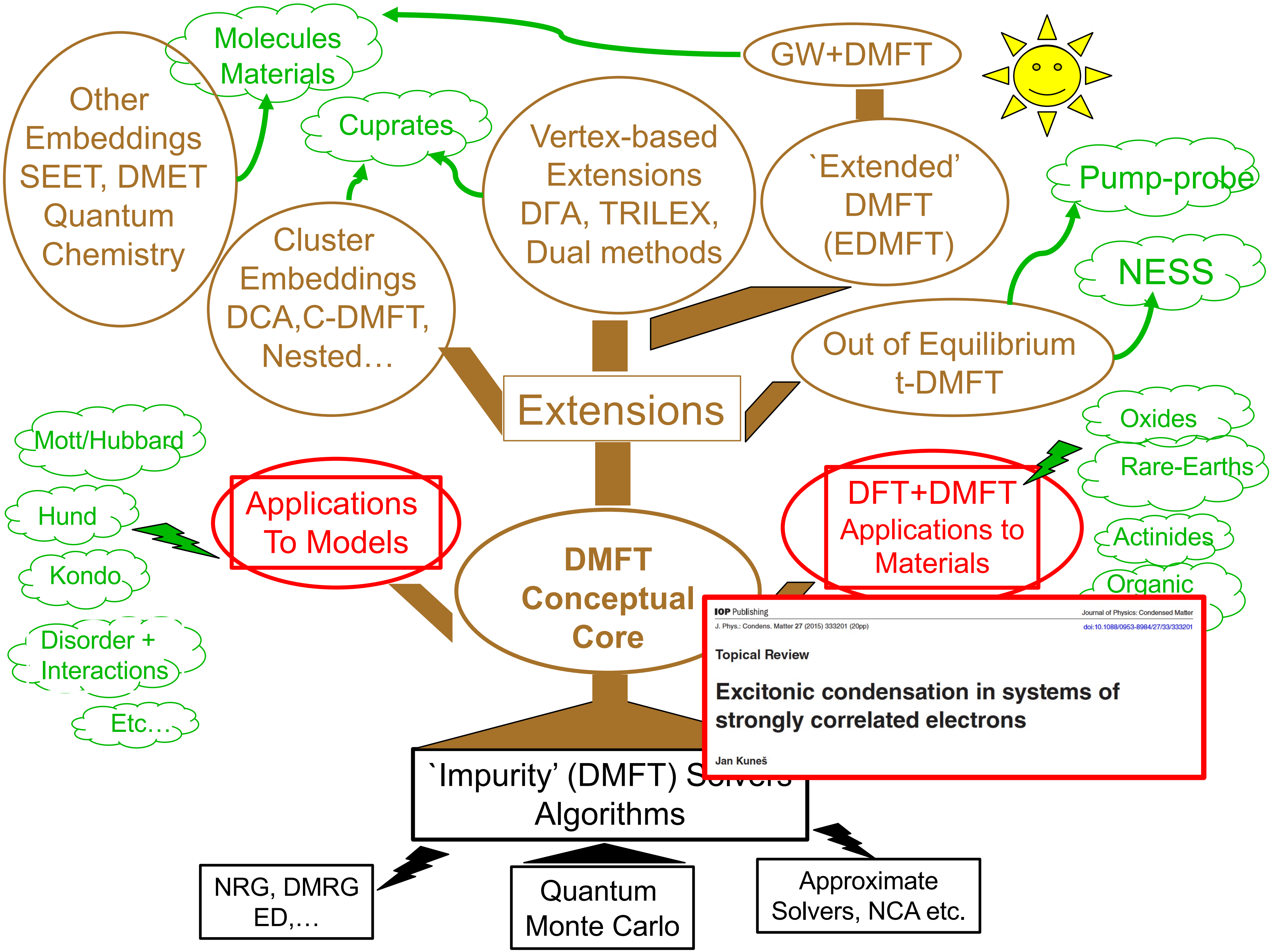
Salle 5

Andrew J. Millis

Columbia University

and CCQ-Flatiron Institute, Simons Foundation, New York

Correlated Electrons and the Lattice



Molecules
Materials
GW+DMFT
Other
Embeddings
SEET, DMET
Quantum
Chemistry
Cuprates
Vertex-based
Extensions
DΓA, TRILEX,
Dual methods
`Extended'
DMFT
(EDMFT)
Pump-probe
Cluster
Embeddings
DCA,C-DMFT,
Nested…
NESS
Out of Equilibrium
t-DMFT
Extensions
Oxides
Mott/Hubbard
Rare-Earths
Applications
To Models
DFT+DMFT
Applications to
Materials
Hund
Actinides
Kondo
DMFT
Conceptual
Core
Organic
IOP Publishing
Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter 27 (2015) 333201 (20pp)
doi:10.1088/0953-8984/27/33/333201
Topical Review
Excitonic condensation in systems of
strongly correlated electrons
Jan Kuneš
Disorder +
Interactions
Etc…
`Impurity' (DMFT) Solvers
Algorithms
NRG, DMRG
ED,…
Quantum
Monte Carlo
Approximate
Solvers, NCA etc.

A theoretical description of the solid-state based on ATOMS rather than on an electron-gas picture: « ***Dynamical Mean-Field Theory*** »

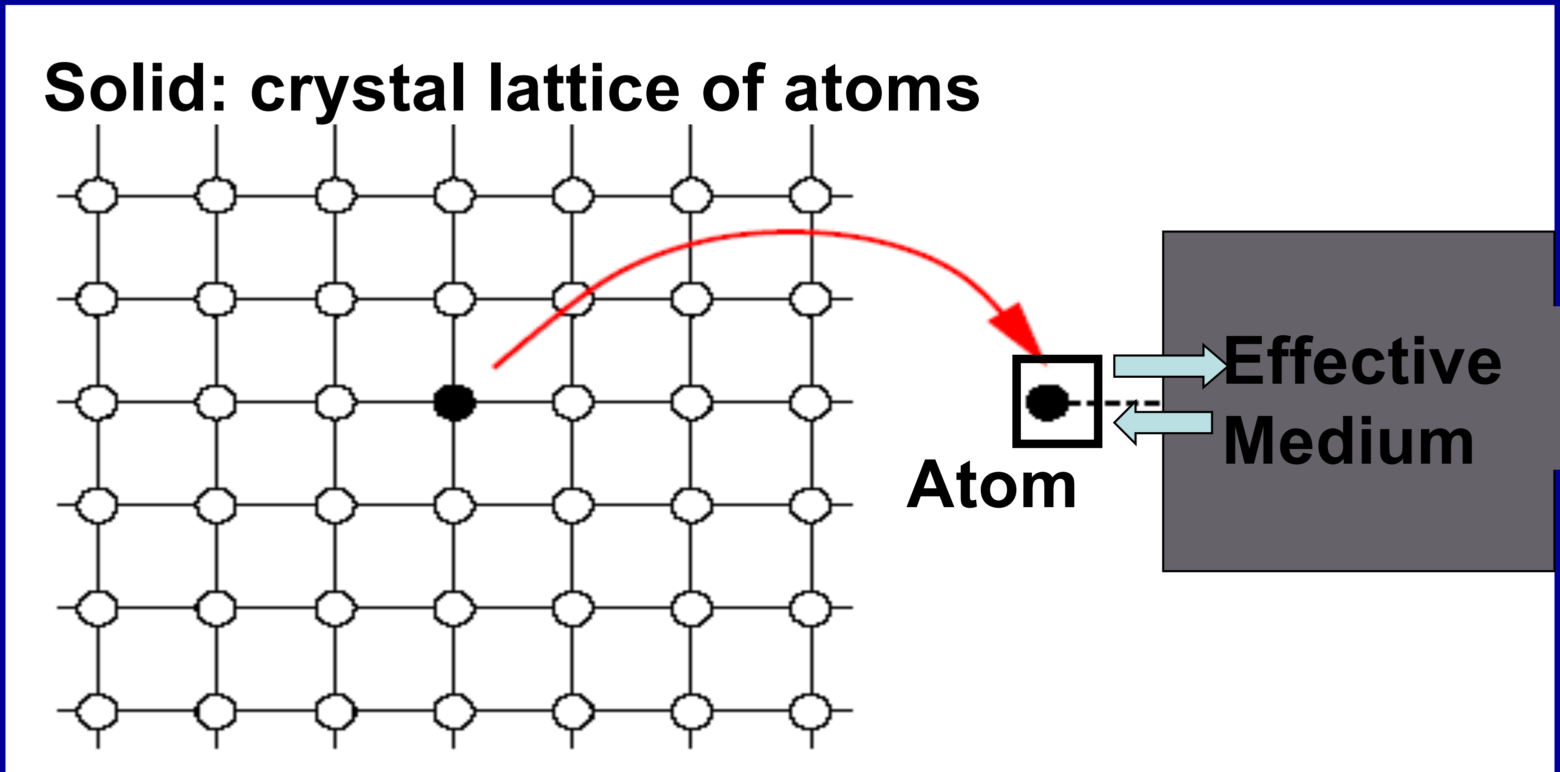
Dynamical Mean-Field Theory:
A.G. & G.Kotliar, PRB 45, 6479 (1992)
Correlated electrons in large dimensions:
W.Metzner & D.Vollhardt, PRL 62, 324 (1989)

Important intermediate steps by: Müller-Hartmann, Schweitzer and Czycholl, Brandt and Mielsch, V.Janis

Early review: Georges et al. Rev Mod Phys 68, 13 (1996)

Dynamical Mean-Field Theory:

viewing a material as an (ensemble of) atoms coupled to a self-consistent medium



Correlated electrons in large dimensions: W.Metzner & D.Vollhardt, 1989

Dynamical Mean-Field Theory: A.G. & G.Kotliar, 1992

Example: DMFT for the Hubbard model (a model of coupled atoms)

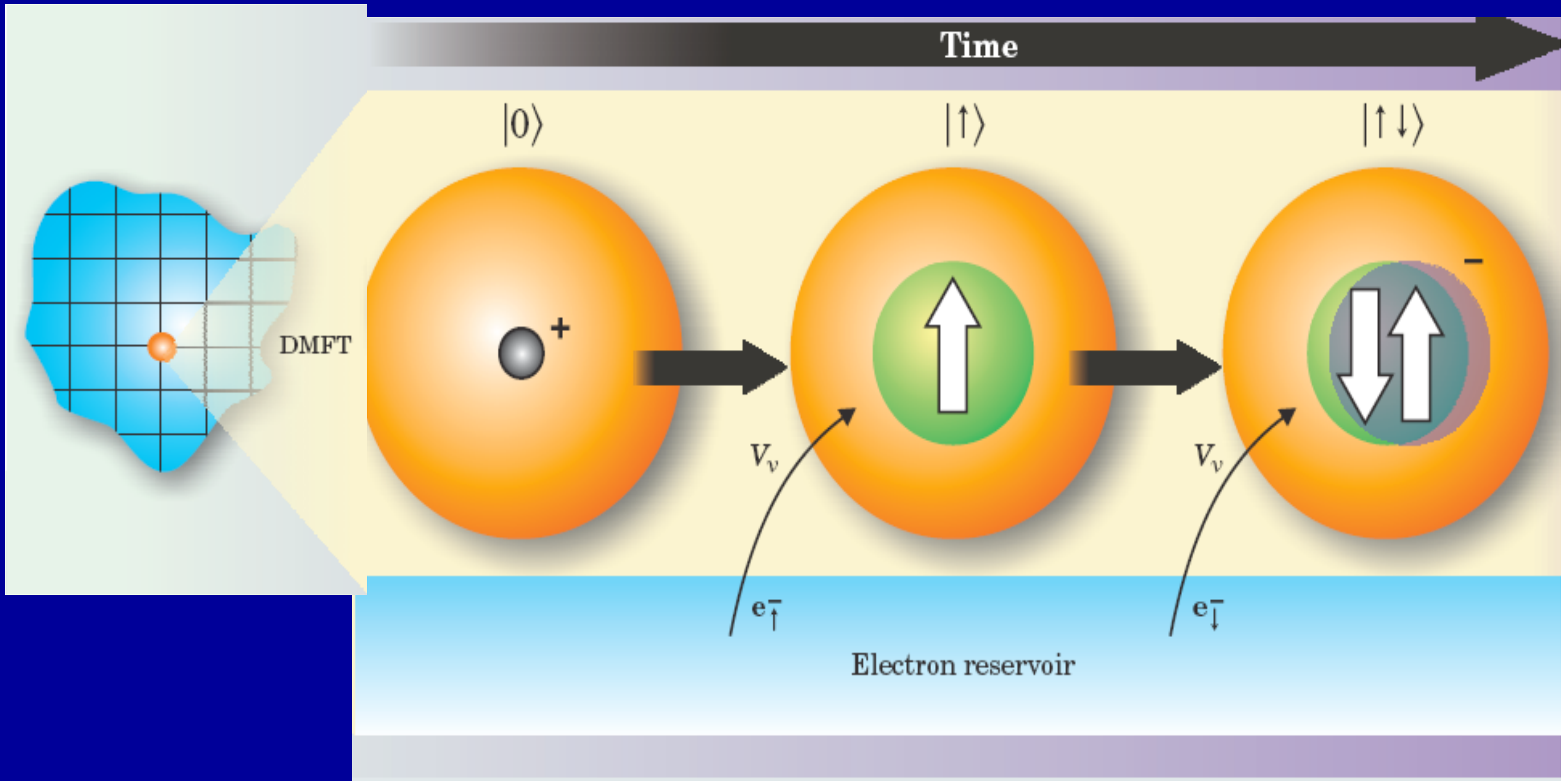
$$H = -\sum_{\mathbf{RR'}} t_{\mathbf{RR'}} d^{\dagger}_{\mathbf{R}\sigma} d_{\mathbf{R'}\sigma} + \sum_{\mathbf{R}} H^{\mathbf{R}}_{atom}$$

$$H_{atom} = \varepsilon_d \sum_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}$$

Focus on a given lattice site:

"Atom" can be in 4 possible configurations: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

<u>Describe ``history'' of fluctuations between those configurations</u>



Imaginary-time effective action describing these histories:

$$S \;=\; S_{at} + S_{hyb}$$

$$S_{at} = \int_0^\beta d\tau \sum_\sigma d_\sigma^+(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right) d_\sigma(\tau) + U \int_0^\beta d\tau\, n_\uparrow(\tau) n_\downarrow(\tau)$$

$$S_{hyb} = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^+(\tau)\Delta(\tau-\tau')d_\sigma(\tau')$$

The amplitude $\Delta(\tau)$ for hopping in and out of the selected site is self-consistently determined: it is the quantum-mechanical Generalization of the Weiss effective field.

$$\mathcal{G}_0^{-1}(i\omega_n) \;=\; i\omega_n + \mu - \Delta(i\omega_n)$$

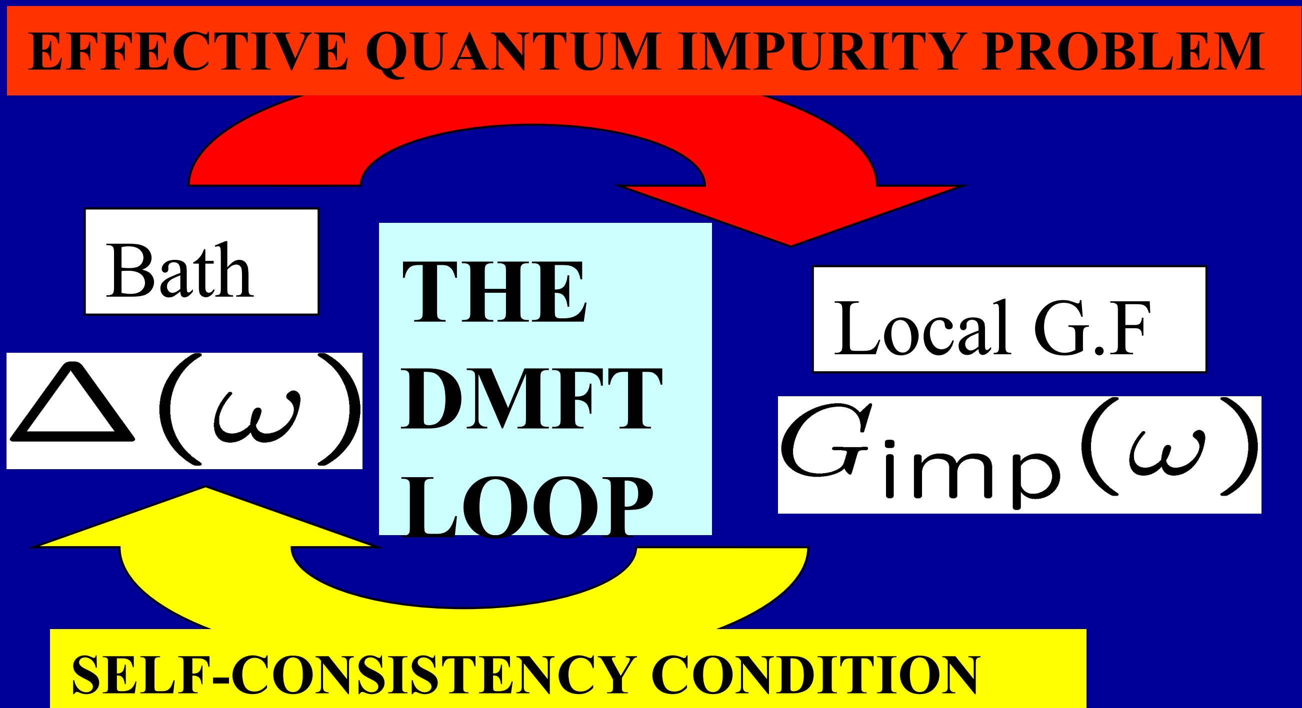
Effective `bare propagator' self-consistently determined, hence depends on U, and other parameters.

The self-consistency equation and the DMFT loop

Approximating the self-energy by that of the local problem : $\Sigma(\mathbf{k},\omega) \simeq \Sigma_{imp}(\omega)$

→ fully determines both the local G and Δ:

$$\boxed{G_{\text{imp}}[i\omega;\Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\text{imp}}[i\omega;\Delta]^{-1} + \Delta(i\omega) - \varepsilon_{\mathbf{k}}}}$$



G_{RR} is related to the exact self-energy of the lattice (solid) by:

$$G_{\mathbf{RR}}(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)} = G_{\mathrm{loc}}(\omega)$$

In which ε_k is the tight-binding band (FT of the hopping $t_{RR'}$)

High-frequency → $\varepsilon_d = -\mu + \sum_k \varepsilon_k \, (= -\mu)$

Let us now make the **APPROXIMATION** that the lattice self-energy is **k-independent** and coincides with that of the effective atom (impurity problem):

$$\Sigma(\mathbf{k}, \omega) \simeq \Sigma_{\mathrm{imp}}(\omega)$$

This leads to the following self-consistency condition:

$$\boxed{G_{\mathrm{imp}}[i\omega; \Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\mathrm{imp}}[i\omega; \Delta]^{-1} + \Delta(i\omega) - \varepsilon_{\mathbf{k}}}}$$

Δ(ω): generalizing the Weiss field to the quantum world

Pierre Weiss
1865-1940
« Théorie du Champ Moléculaire »
(1907)

Einstein, Paul Ehrenfest, Paul Langevin, Heike Kammerlingh-Onnes, and Pierre Weiss at Ehrenfest's home, Leyden, the Netherlands. From Einstein, His Life and Times, *by Philipp Frank (New York: A.A. Knopf, 1947). Photo courtesy AIP Emilio Segrè Visual Archives.*

Weiss mean-field theory
Density-functional theory
Dynamical mean-field theory

rely on similar conceptual basis

TABLE 2. Comparison of theories based on functionals of a local observable

Theory	MFT	DFT	DMFT
Quantity	Local magnetization m_i	Local density $n(x)$	Local GF $G_{ii}(\omega)$
Equivalent system	Spin in effective field	Electrons in effective potential	Quantum impurity model
Generalised Weiss field	Effective local field	Kohn-Sham potential	Effective hybridisation

- Exact energy functional of local observable

- Exact representation of local observable:
- Generalized ``Weiss field''
- Self-consistency condition, later approximated

see e.g:
A.G
arXiv cond-mat
0403123

The DMFT construction is EXACT:

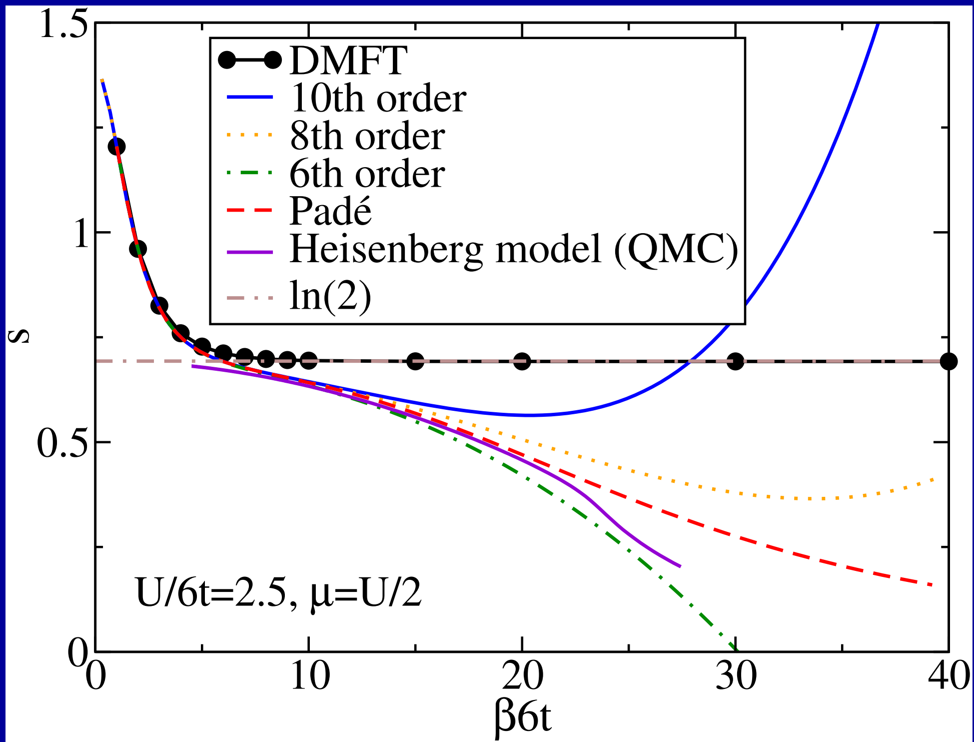
- For the non-interacting system
  (U =0 → $\Sigma = 0$!)
- For the isolated atom
  (strong-coupling limit t=0 → $\Delta = 0$)

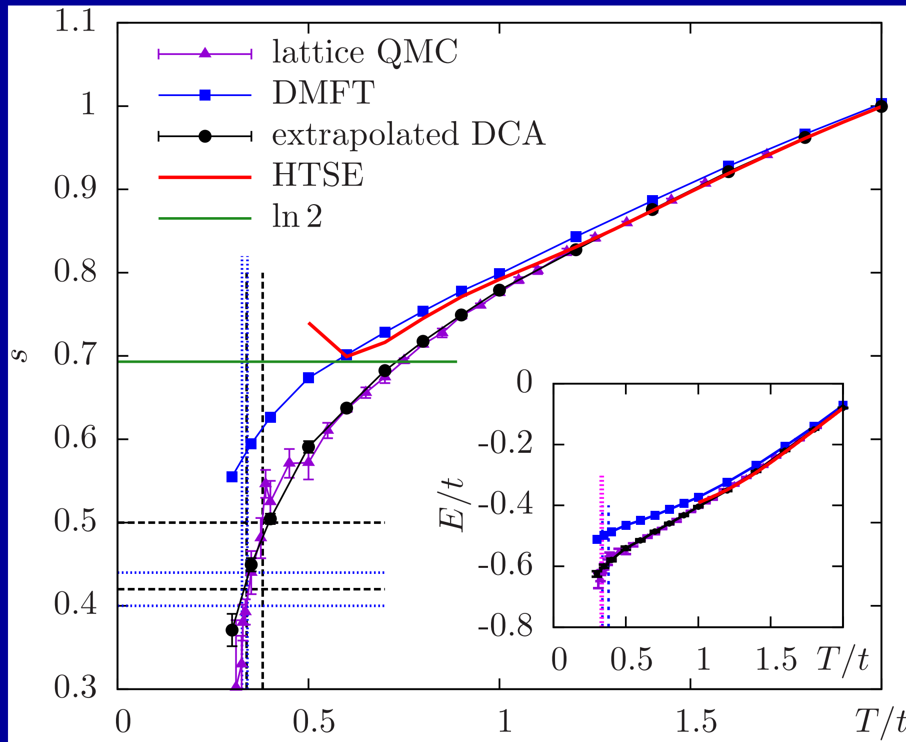
→ Hence provides an interpolation from weak to strong coupling

- <u>In the formal limit of infinite dimensionality (infinite lattice coordination)</u> [introduced by Metzner and Vollhardt, PRL 62 (1989) 324]

Proofs: LW functional, Cavity construction (more on board)

Physical Limits in which DMFT is accurate: small correlation lengths





Hubbard d=3 ½ filled
U/t=15
De Leo et al.
PRA 83 (2011) 023606

Hubbard d=3 ½ filled
U/t=8
Fuchs et al.
PRL 106 (2011) 030401

Doped: smaller correlation length

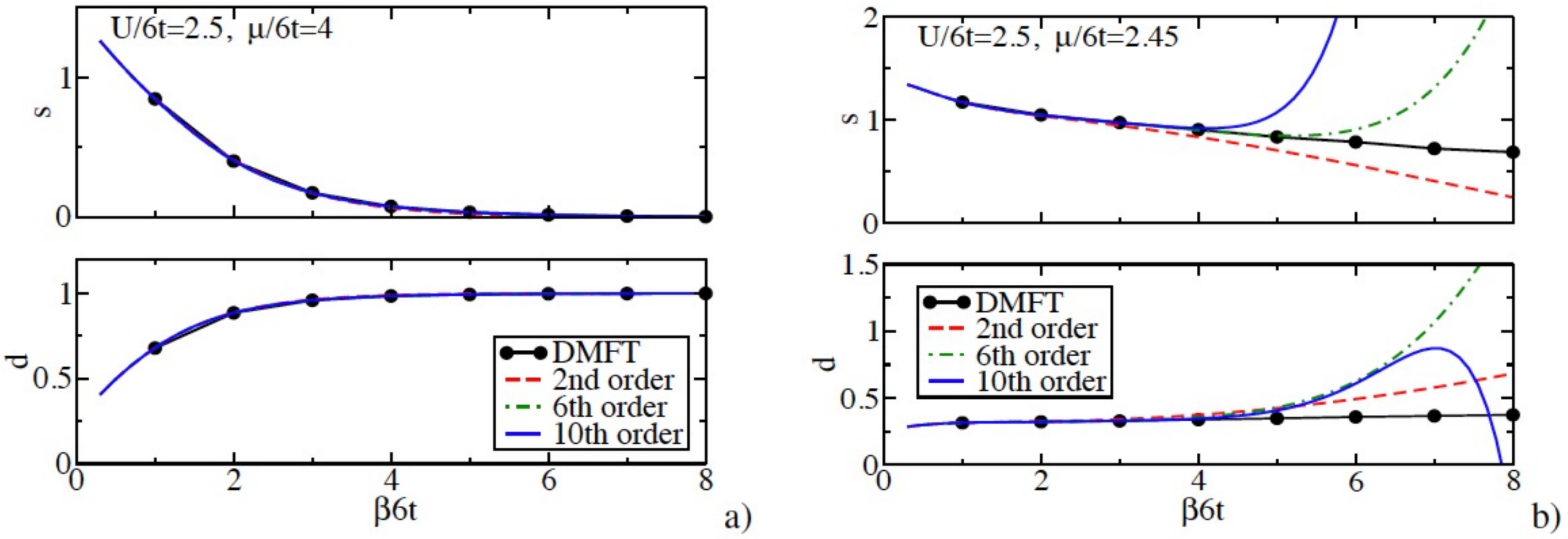
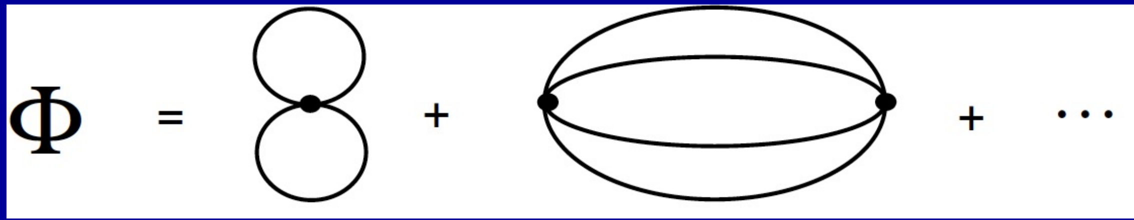


Fig. 1 Comparison between DMFT and high-temperature series for the double occupancy $d = \langle n_\uparrow n_\downarrow \rangle$ and entropy per site as a function of inverse temperature $\beta 6t = 6t/kT$, for $U/6t = 2.5$. **a):** At $\mu/6t = 4$ (corresponding to the high-density regime). **b):** At $\mu/6t = 2.45$ (corresponding to an intermediate density $n \simeq 1.25$). Reproduced and adapted from Ref. [10]

cf. A.G. Ann. Phys (Berlin) 523 (2011) 672

The Luttinger-Ward Functional



Does it really exist ? ☺

PRL **114,** 156402 (2015) PHYSICAL REVIEW LETTERS week ending 17 APRIL 2015

Nonexistence of the Luttinger-Ward Functional and Misleading Convergence of Skeleton Diagrammatic Series for Hubbard-Like Models

Evgeny Kozik,[1,2,*] Michel Ferrero,[2] and Antoine Georges[3,2,4]

IOP Publishing Journal of Physics A: Mathematical and Theoretical

J. Phys. A: Math. Theor. **48** (2015) 485202 (6pp) doi:10.1088/1751-8113/48/48/485202

Skeleton series and multivaluedness of the self-energy functional in zero space-time dimensions

Riccardo Rossi[1] and Félix Werner[2]

Classical StatMech Model in which an infinite series of terms must be summed in d=infty: fully frustrated Ising

J. Phys. A: Math. Gen. **23** (1990) 2165–2171. Printed in the UK

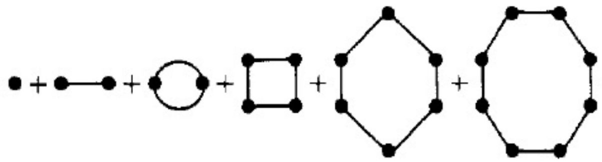
The fully frustrated Ising model in infinite dimensions

Jonathan S Yedidia† and Antoine Georges‡

† Department of Physics, Jadwin Hall, Princeton University, Princeton, NJ 08544, USA
‡ Laboratoire de Physique Théorique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

Received 28 September 1989

Abstract. We solve, subject to the validity of some reasonable assumptions, the 'fully frustrated' Ising model in the limit of infinite dimensions using an extension of the TAP theory for spin glasses. In contrast to the TAP theory of the infinite-range spin glass, an infinite summation of diagrams is required to recover the Gibbs free energy for this model. The model undergoes a first-order transition. The method used to solve the model should have many applications to other physical problems.

$-\beta G =$  $+ \dots$

$$= -\sum_i \left(\frac{1+m_i}{2}\right)\ln\left(\frac{1+m_i}{2}\right) + \left(\frac{1-m_i}{2}\right)\ln\left(\frac{1-m_i}{2}\right)$$

$$+\beta \sum_{(ij)} J_{ij} m_i m_j + \frac{\beta^2}{2}\sum_{(ij)} J_{ij}^2 (1-m_i^2)(1-m_j^2)$$

$$+\beta^4 \sum_{(ijkl)} J_{ij} J_{jk} J_{kl} J_{li} (1-m_i^2)(1-m_j^2)(l-m_k^2)(1-m_l^2) + \dots .$$

Figure 1. The Gibbs free energy of the 'fully frustrated' Ising model on a hypercubic lattice in the limit of infinite dimensions.

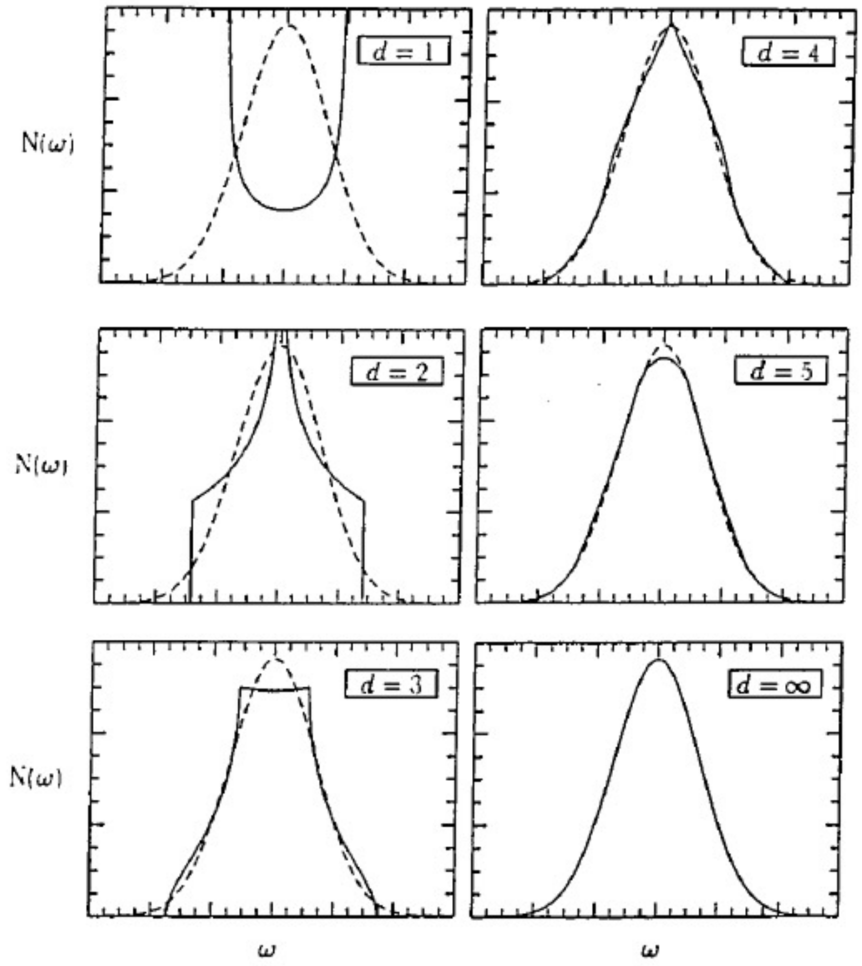


FIG. 84. Density of state $D(\epsilon)$ for tight-binding electrons with nearest neighbor hopping on a hypercubic lattice of various dimensionalities. From Vollhardt (1994).

Density of states of a tight-binding band
on a d-dimensional cubic lattice, as d increases.

MERCI POUR VOTRE ATTENTION !

PROCHAINE SEANCE:
MARDI 28 Mai 9:30

Two Lectures:

- *Atom in a bath: introduction to the Anderson impurity model with a DMFT perspective*
- *The Mott transition*

No seminar