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 2 –Equations fondamentales de la théorie du Champ Moyen Dynamique, selon différentes perspectives

Cycle 2018-2019
14 mai 2019

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1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

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

Lecture 2 – The DMFT construction: basic equations and different perspectives on their derivation

Slides will be in English

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

2018-2019 Lectures
May 14, 2019

Mailing List

(Weekly announcement of lecture and seminar, etc.)

Send email to: listes-diffusion.cdf@college-de-france.fr
Subject line: subscribe chaire-pmc.ipcdf
…ou: unsubscribe chaire-pmc.ipcdf

Website:

https://www.college-de-france.fr/site/antoine-georges/index.htm

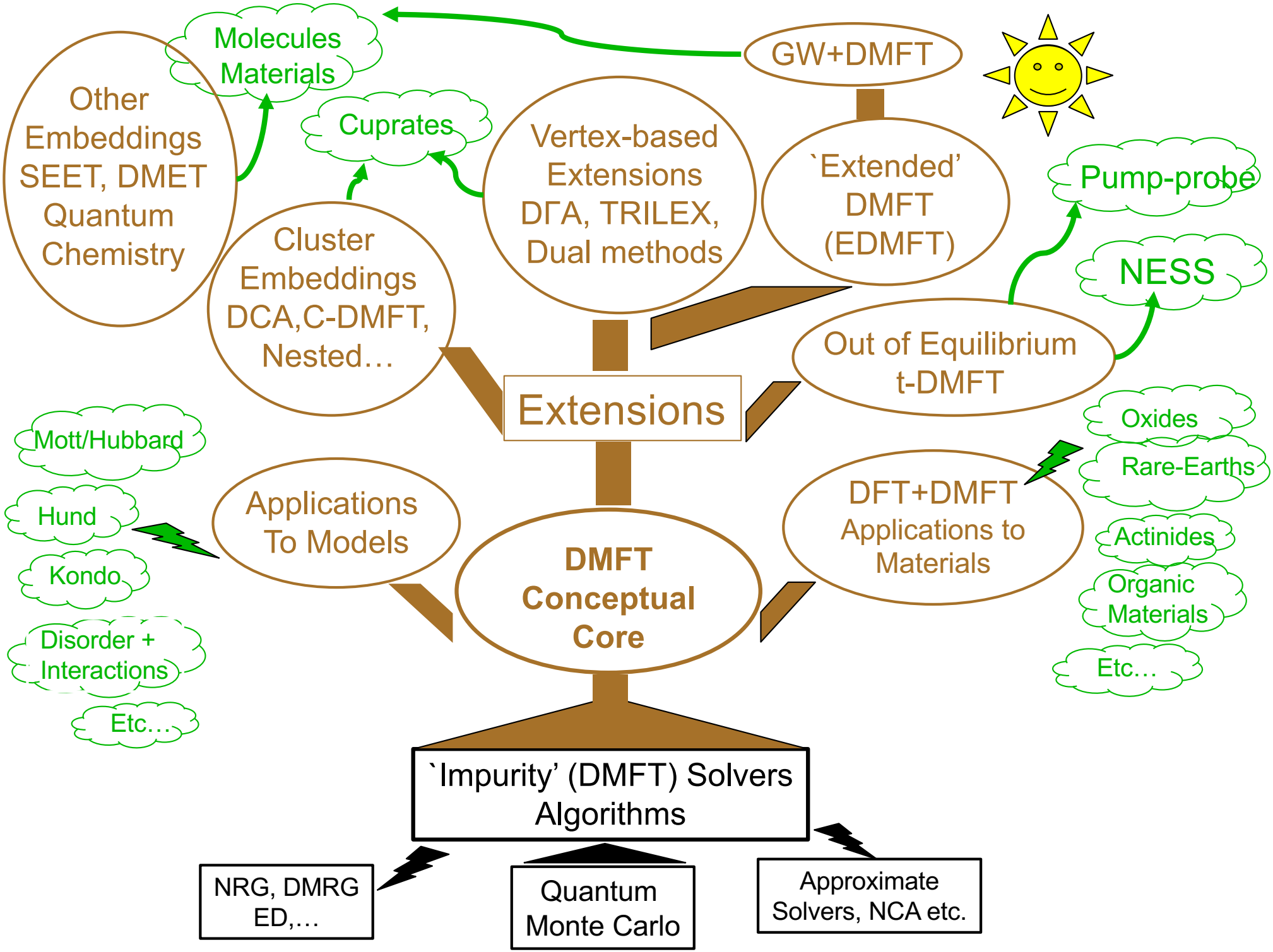
Lectures from this year (and 2016-2017) are video recorded
PDF and Audio of lectures available for all years
PDF for (almost) all seminars

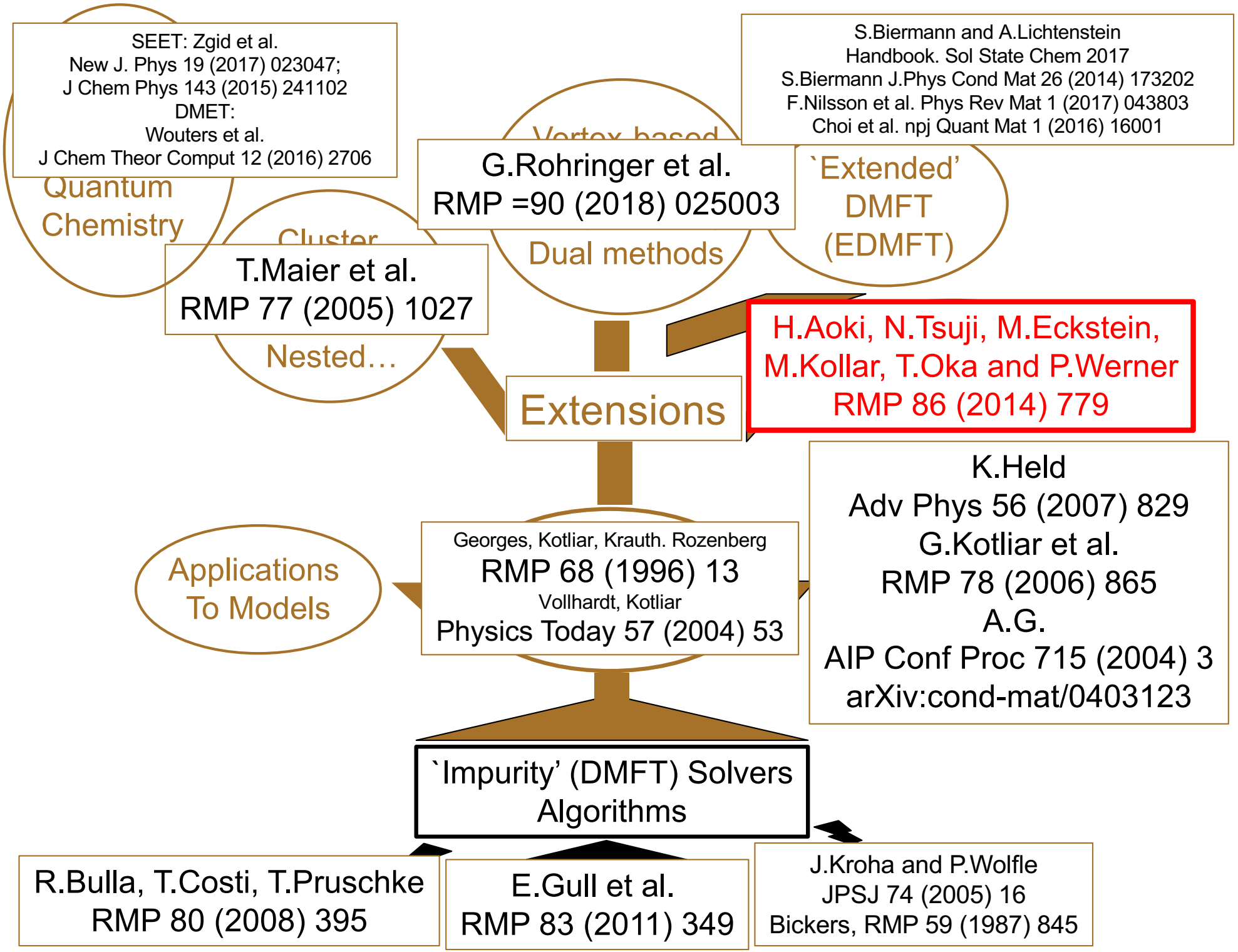
Today's seminar (11:30)

Philipp Werner

University of Fribourg, Switzerland

Non-Equilibrium Extensions of Dynamical Mean-Field Theory


Molecules
Materials
GW+DMFT
Other
Embeddings
SEET, DMET
Quantum
Chemistry
Cuprates
Vertex-based
Extensions
DΓA, TRILEX,
Dual methods
`Extended'
DMFT
(EDMFT)
Pump-probe
NESS
Cluster
Embeddings
DCA,C-DMFT,
Nested…
Out of Equilibrium
t-DMFT
Extensions
Mott/Hubbard
Hund
Kondo
Disorder +
Interactions
Etc…
Applications
To Models
DMFT
Conceptual
Core
DFT+DMFT
Applications to
Materials
Oxides
Rare-Earths
Actinides
Organic
Materials
Etc…
`Impurity' (DMFT) Solvers
Algorithms
NRG, DMRG
ED,…
Quantum
Monte Carlo
Approximate
Solvers, NCA etc.


SEET: Zgid et al.
New J. Phys 19 (2017) 023047;
J Chem Phys 143 (2015) 241102
DMET:
Wouters et al.
J Chem Theor Comput 12 (2016) 2706
Quantum Chemistry
S.Biermann and A.Lichtenstein
Handbook. Sol State Chem 2017
S.Biermann J.Phys Cond Mat 26 (2014) 173202
F.Nilsson et al. Phys Rev Mat 1 (2017) 043803
Choi et al. npj Quant Mat 1 (2016) 16001
G.Rohringer et al.
RMP =90 (2018) 025003
Dual methods
`Extended' DMFT (EDMFT)
Cluster
T.Maier et al.
RMP 77 (2005) 1027
Nested…
H.Aoki, N.Tsuji, M.Eckstein,
M.Kollar, T.Oka and P.Werner
RMP 86 (2014) 779
Extensions
K.Held
Adv Phys 56 (2007) 829
G.Kotliar et al.
RMP 78 (2006) 865
A.G.
AIP Conf Proc 715 (2004) 3
arXiv:cond-mat/0403123
Applications To Models
Georges, Kotliar, Krauth. Rozenberg
RMP 68 (1996) 13
Vollhardt, Kotliar
Physics Today 57 (2004) 53
`Impurity' (DMFT) Solvers Algorithms
R.Bulla, T.Costi, T.Pruschke
RMP 80 (2008) 395
E.Gull et al.
RMP 83 (2011) 349
J.Kroha and P.Wolfle
JPSJ 74 (2005) 16
Bickers, RMP 59 (1987) 845

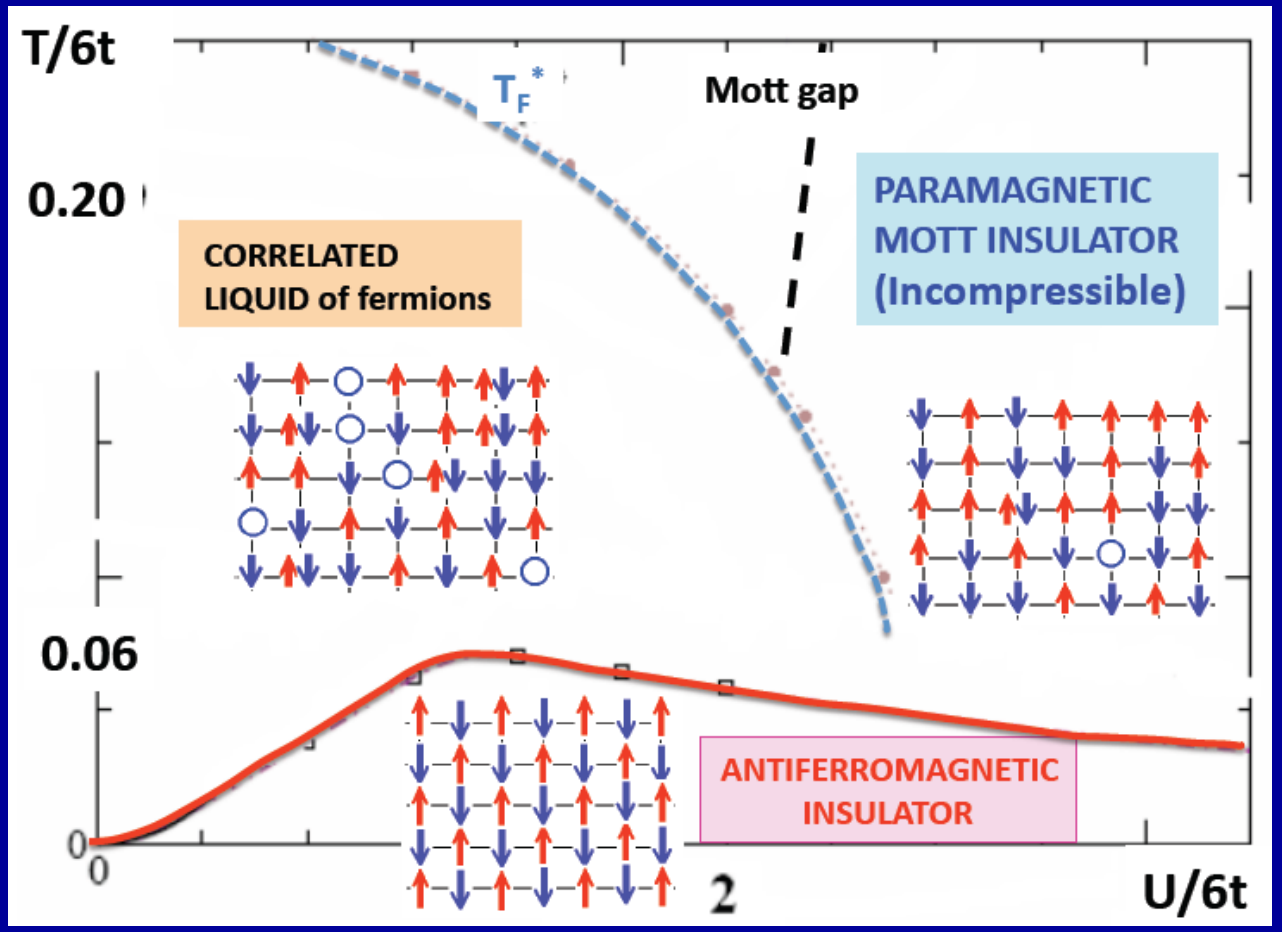
Outline of today's lecture

- Why DMFT (cont'd) ?
- Observables, basic formalism
- The DMFT construction: overview
- Limits where DMFT becomes exact
- Derivation: 1-Perturbation theory considerations (to all orders) and the Baym-Kadanoff functional
- Derivation: 2-The Cavity method (probably → lecture 3)

Why do we need to go beyond (effective) one-particle descriptions ?

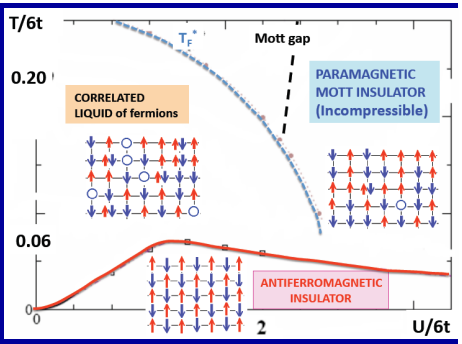
Why DMFT ?

Illustrate this on a simple case:
½ filled Hubbard model on a cubic lattice



From: A.G. DMFT@25 book (Julich lectures)
T_Neel is from DQMC on the cubic lattice
Crossover lines are indicative (not quantitative)

Please note:



- Ordered phase: Crossover from Slater-like antiferromagnet to localized Heisenberg AF
- Phase without long-range order:
- Weak-coupling: Crossover corresponding to the formation of coherent quasiparticles
- Strong coupling - Two crossovers:
- - Opening of Mott gap ~ U
- - Onset of magnetic correlations ~ $J=4t^2/U$
- At strong coupling, the onset of Mott insulating regime (incompressible w/ local moments) has nothing to do with magnetism

The Mott phenomenon at strong coupling (U >> t) HAS NOTHING TO DO with magnetism It is due to blocking of density/charge

Energy scale for magnetism: superexchange $J \sim t^2/U$

Insulating gap: $\sim U > t >> J$

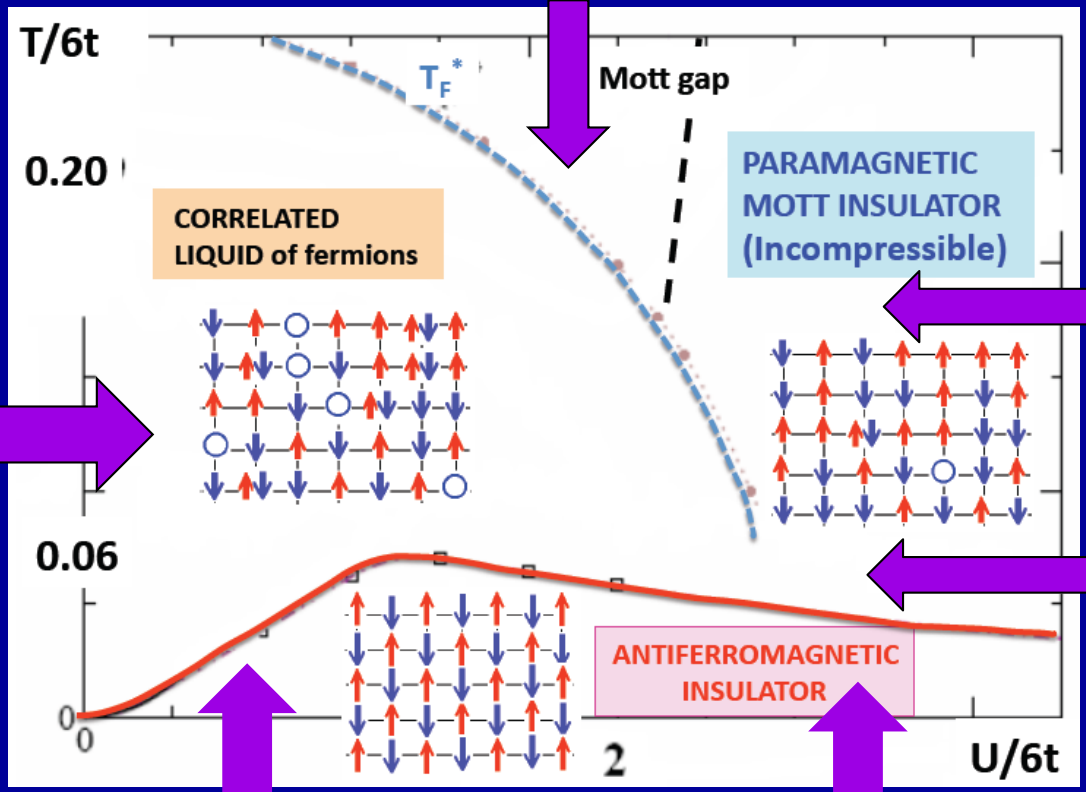
The system is basically an insulator even well above T_{Neel}

Ex: MANY oxides, e.g. NiO, $YTiO_3$, cuprates etc…

In contrast, LDA+U needs to assume ordering to describe the insulator

Hence, 6 distinct regimes:

Incoherent `soup'



Mott Insulating Paramagnet (Fluctuating Local Moments)

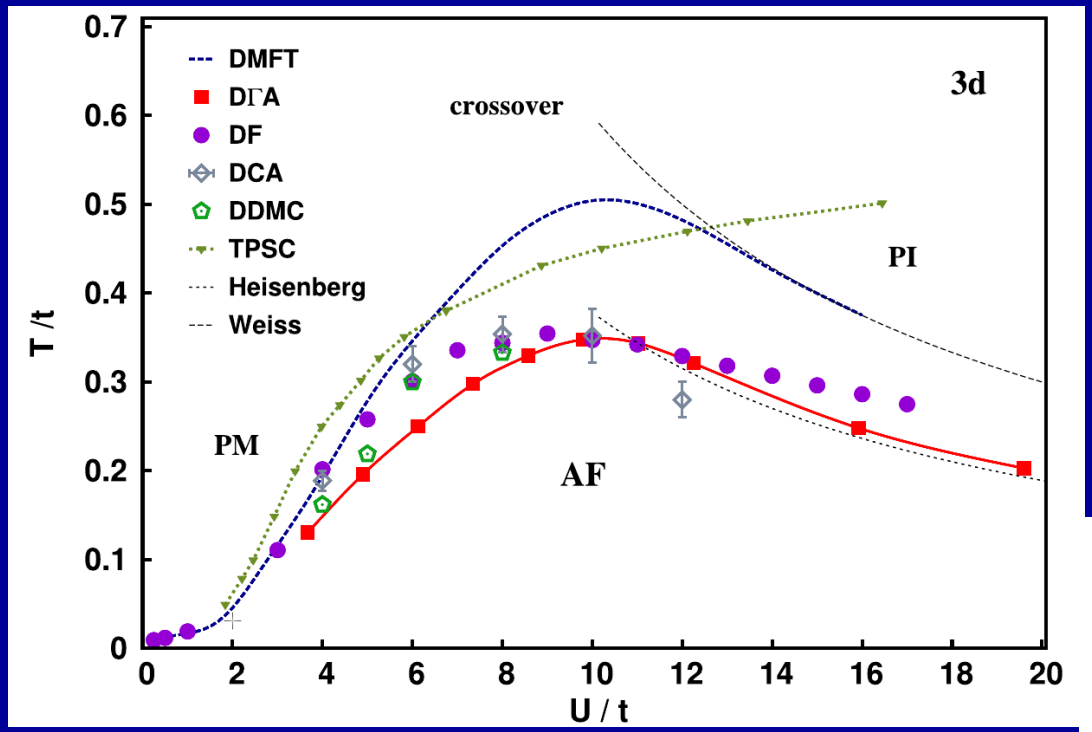
~ Fermi Liquid

Mott Insulator with short-range AF correlations

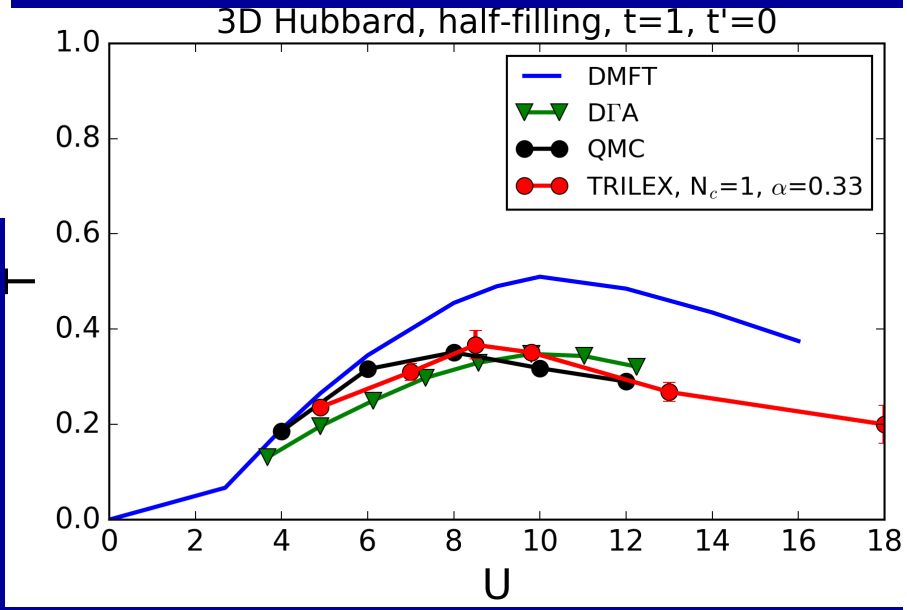
~ Slater AF

~ Heisenberg AF Ordered Mott Insulator

Fluctuations and Neel temperature



Rohringer et al. Rev Mod Phys 90, 025003 (2018)



Courtesy Thomas Schäfer, 2019

OBSERVABLES

- Since we want to also understand crossovers, we cant just rely on (static) order parameters
- Need to address nature of excited states (especially low-energy)
- Green's function
- Spectral Function
- Relation to photoemission experiments
- Two-particle response functions: charge, spin, current, etc…

Green's function, Spectral function

$$G_{ij,\sigma}(\tau-\tau') \;=\; -\langle T\, d_{i\sigma}(\tau)\, d^{+}_{j\sigma}(\tau')\rangle$$

$$A(\mathbf{k},\omega) \;=\; \frac{1}{Z}\sum_{AB}\delta(\omega+E'_A-E'_B)|\langle A|c_{\mathbf{k}\sigma}|B\rangle|^2\;\left[e^{-\beta E'_A}+e^{-\beta E'_B}\right]$$

T=0:

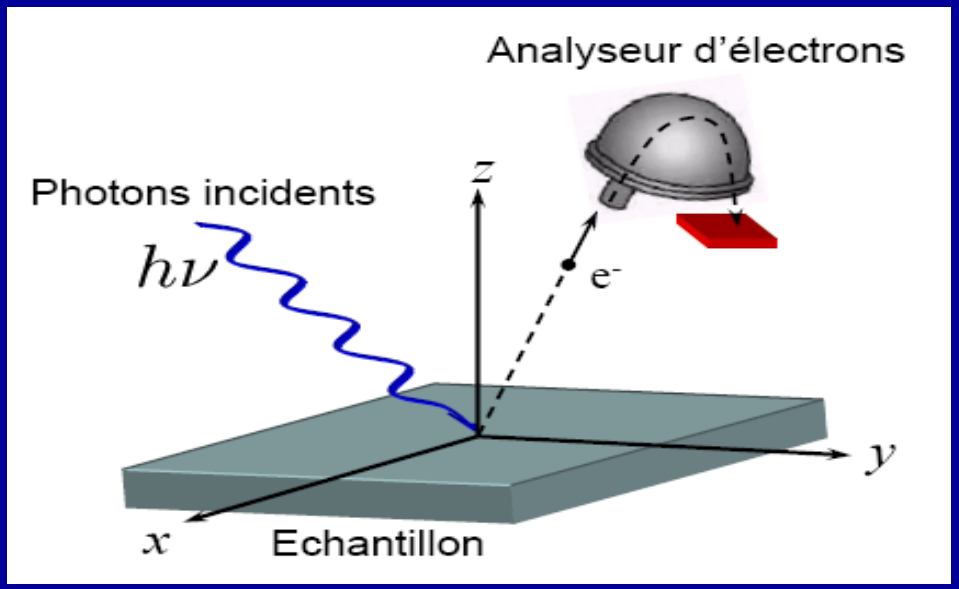
$$\omega<0:\;\; A(\mathbf{k},\omega) \;=\; \sum_{A}\delta(\omega+E_A+\mu-E_0)|\langle A|c_{\mathbf{k}\sigma}|\Psi_0\rangle|^2$$

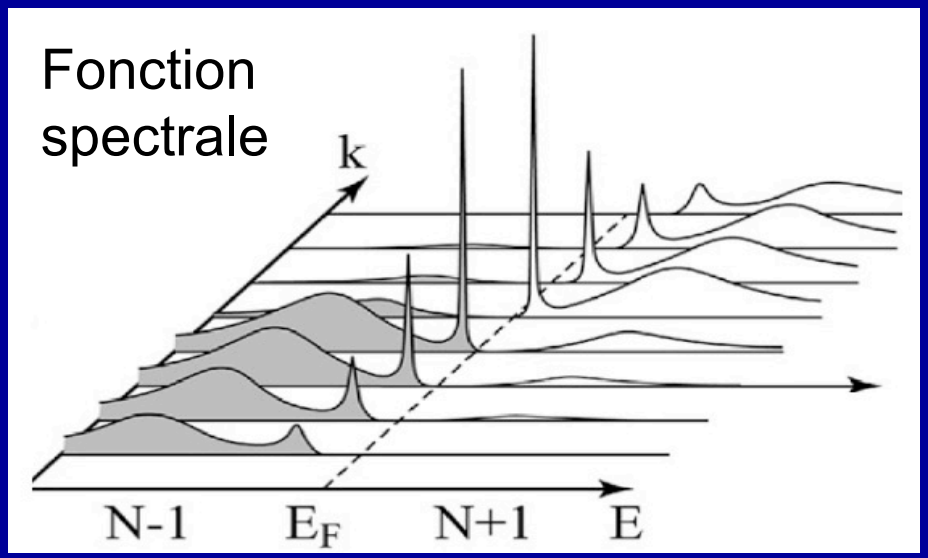
$$\omega>0:\;\; A(\mathbf{k},\omega) \;=\; \sum_{B}\delta(\omega+E_0-E_B+\mu)|\langle B|c^{+}_{\mathbf{k}\sigma}|\Psi_0\rangle|^2$$

$$G(\mathbf{k},i\omega_n) \;=\; \int d\omega\,\frac{A(\mathbf{k},\omega)}{i\omega_n-\omega}\;\;,\;\; A(\mathbf{k},\omega) \;=\; -\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega+i0^{+})$$

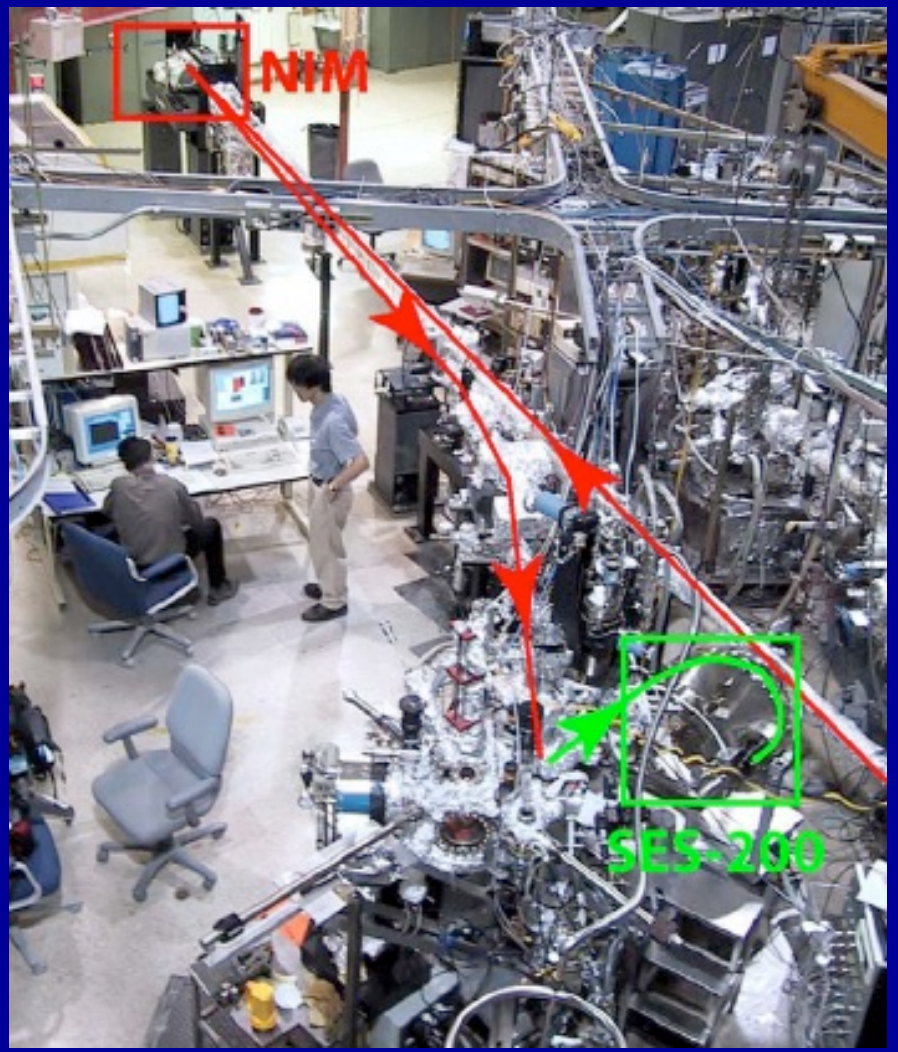
$$A^0(\mathbf{k},\omega) \;=\; \delta(\omega+\mu-\varepsilon_{\mathbf{k}})\;\;,\;\; G^0(\mathbf{k},i\omega_n)=\frac{1}{i\omega_n+\mu-\varepsilon_{\mathbf{k}}}$$

Angle Resolved Photoemission Spectroscopy

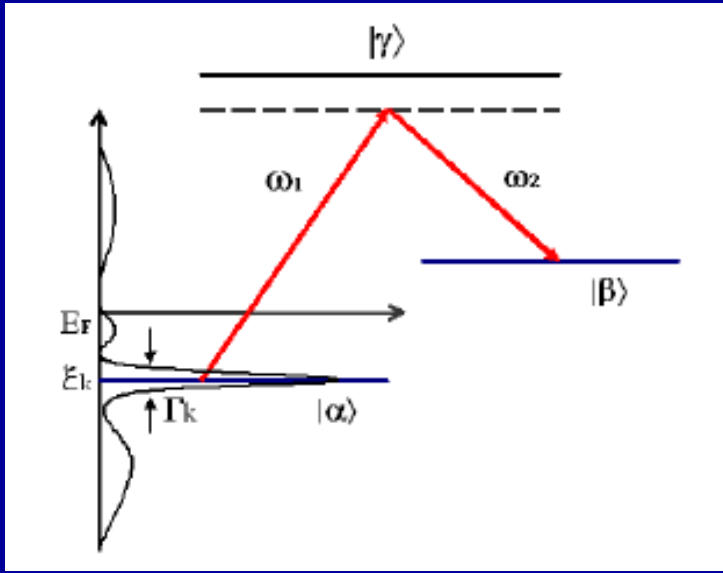




cf. APS Buckley Prize 2011
Campuzano, Johnson, Shen

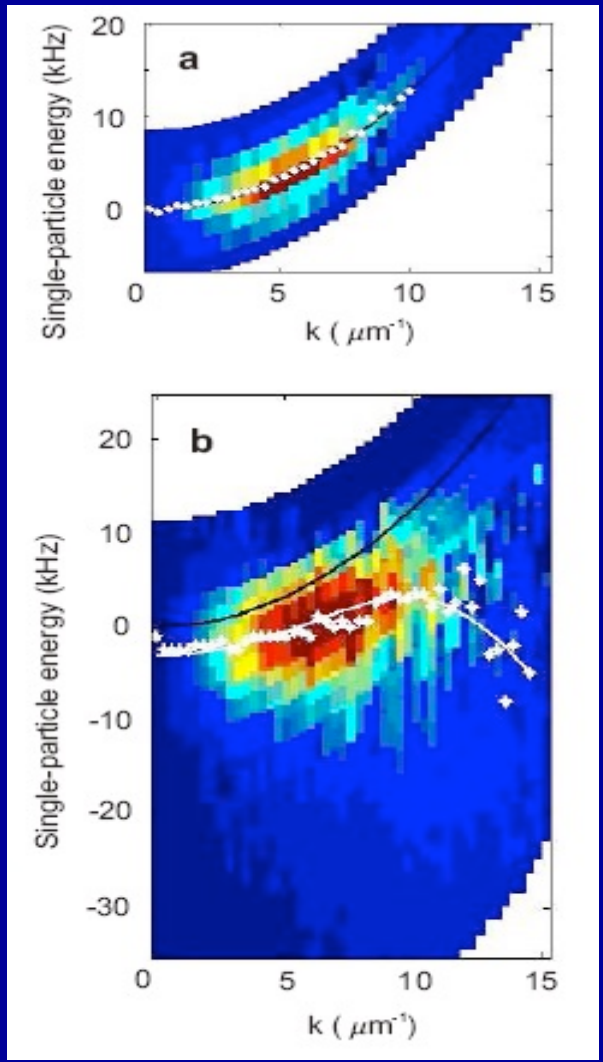


An analogue of ARPES experiments for cold atoms systems :



Raman or rf -transition
from one hyperfine state
to another weakly interacting one.

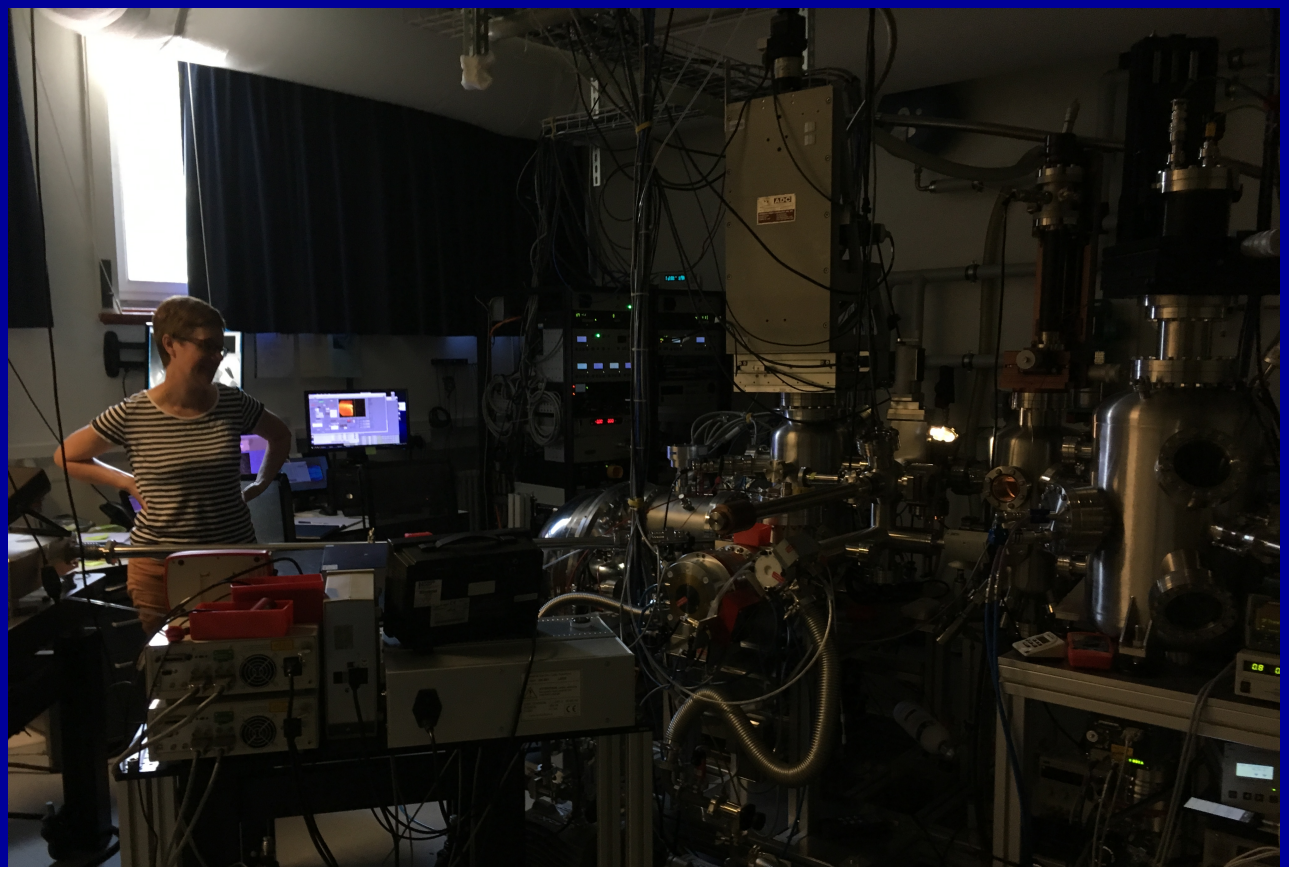
Theoretical proposal:
Dao et al. PRL 98 (2007) 240402



First experiment (in Boulder, Colorado)
Stewart, Gaebler & Jin Nature 454 (2008)

High-resolution Laser ARPES @DQMP-Geneva

(F.Baumberger, A.Tamai)



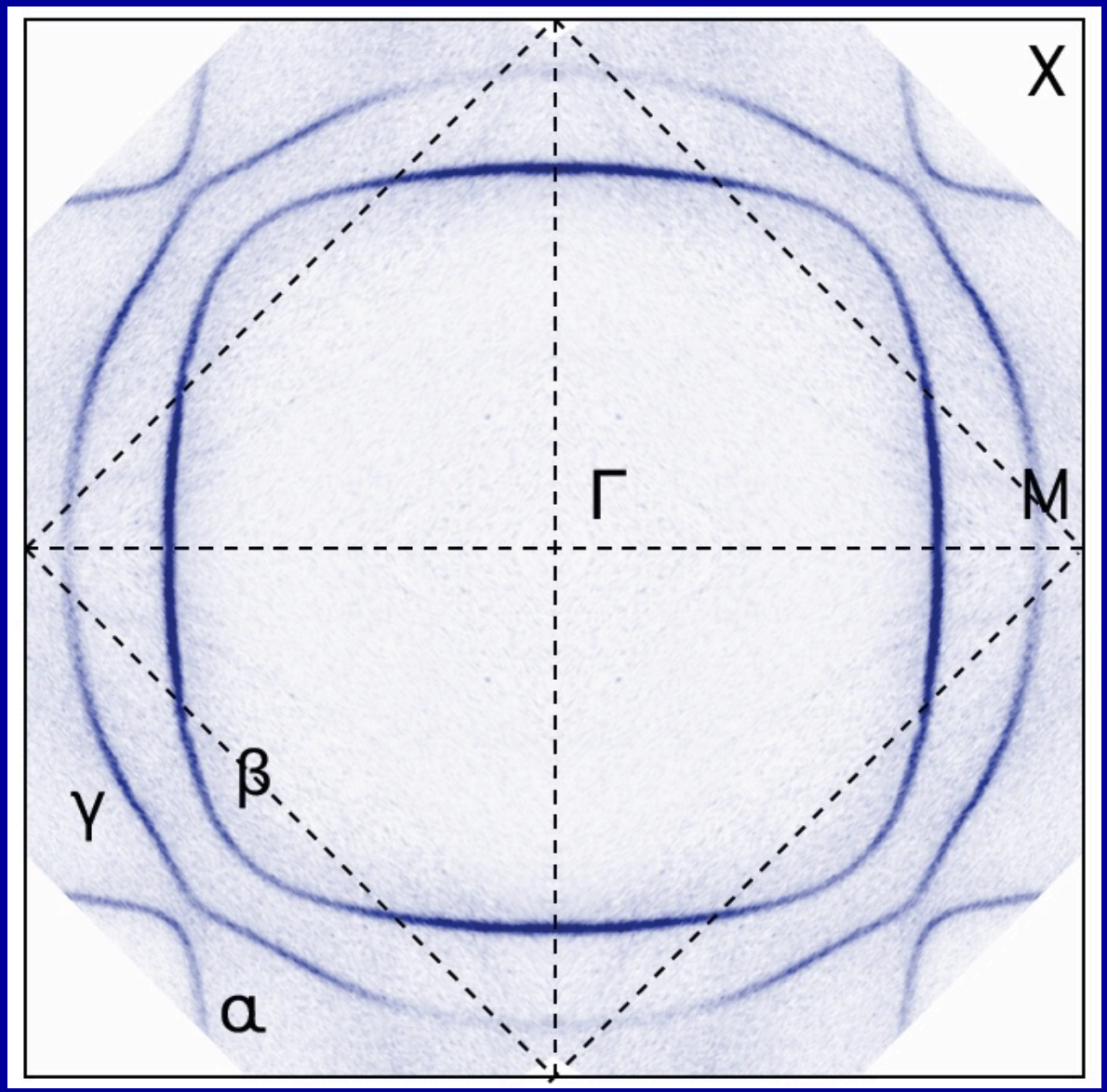
11eV Laser !
Resolution:
ΔE ~ 3meV
Δθ ~ 0.2 deg.

arXiv:1812.06531
(→ PRX 2019)

High-resolution photoemission on Sr_2RuO_4 reveals correlation-enhanced effective spin-orbit coupling and dominantly local self-energies

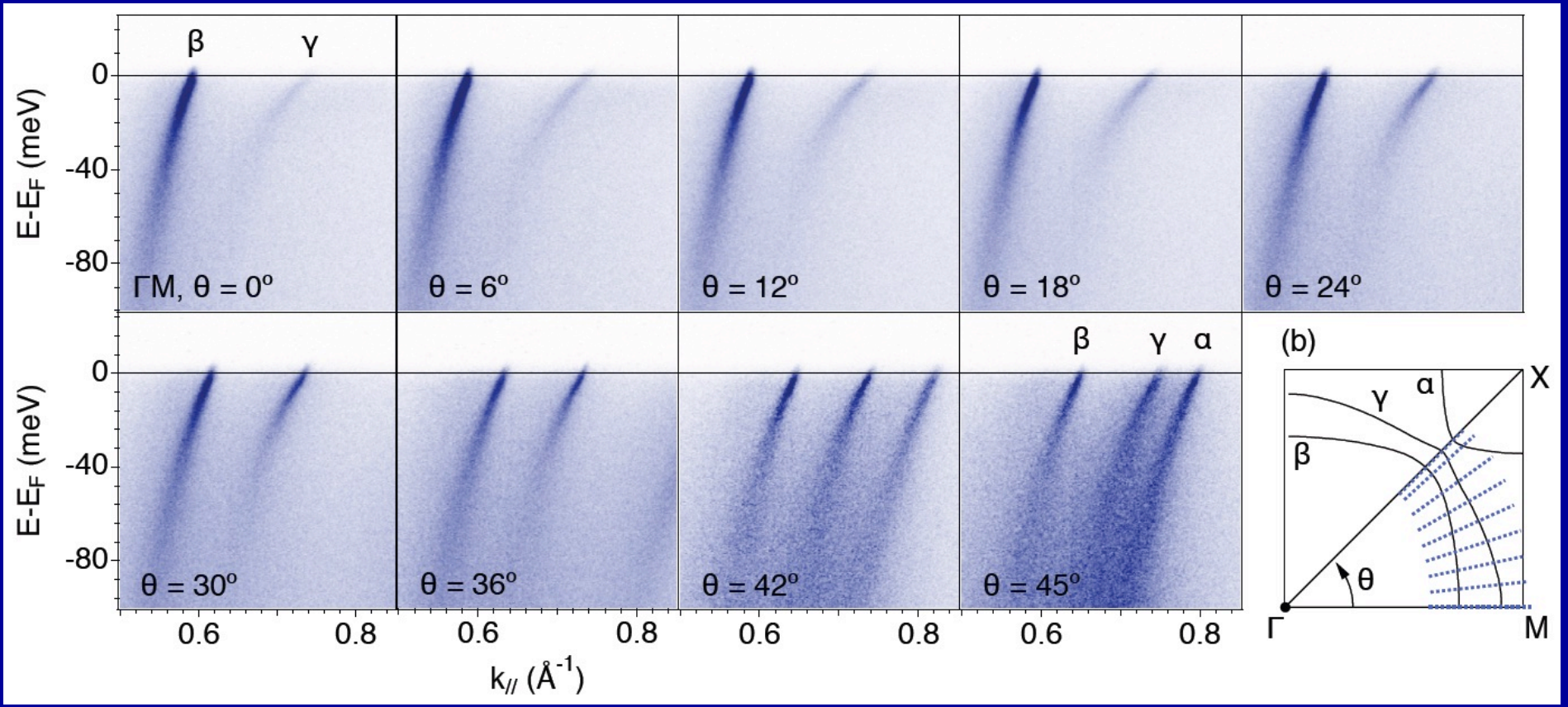
A. Tamai,[1] M. Zingl,[2] E. Rozbicki,[3] E. Cappelli,[1] S. Riccò,[1] A. de la Torre,[1] S. McKeown Walker,[1] F. Y. Bruno,[1] P.D.C. King,[3] W. Meevasana,[4] M. Shi,[5] M. Radović,[5] N.C. Plumb,[5] A.S. Gibbs,[3,*] A.P. Mackenzie,[6,3] C. Berthod,[1] H. Strand,[2] M. Kim,[7,8] A. Georges,[9,2,8,1] and F. Baumberger[1,5]

Fermi surface of Sr_2RuO_4 from high-resolution ARPES



Tamai et al. 2019

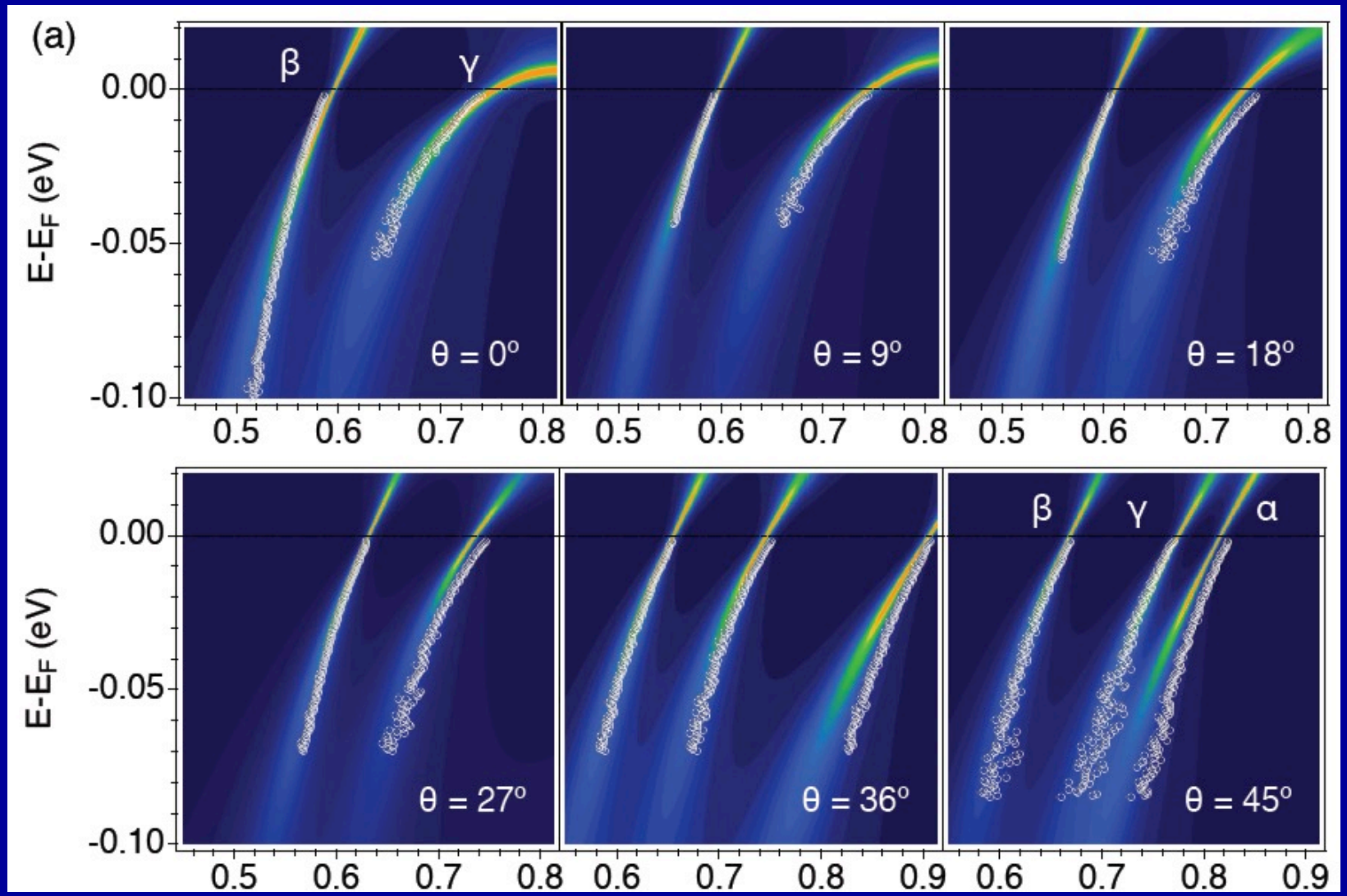
Quasiparticle Dispersions along several angular cuts



Tamai et al. 2019

Comparing DMFT to ARPES

(Dots: ARPES MDCs. Colors: DMFT spectral intensity)



Tamai et al. 2019 (calculations: M.Zingl)

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

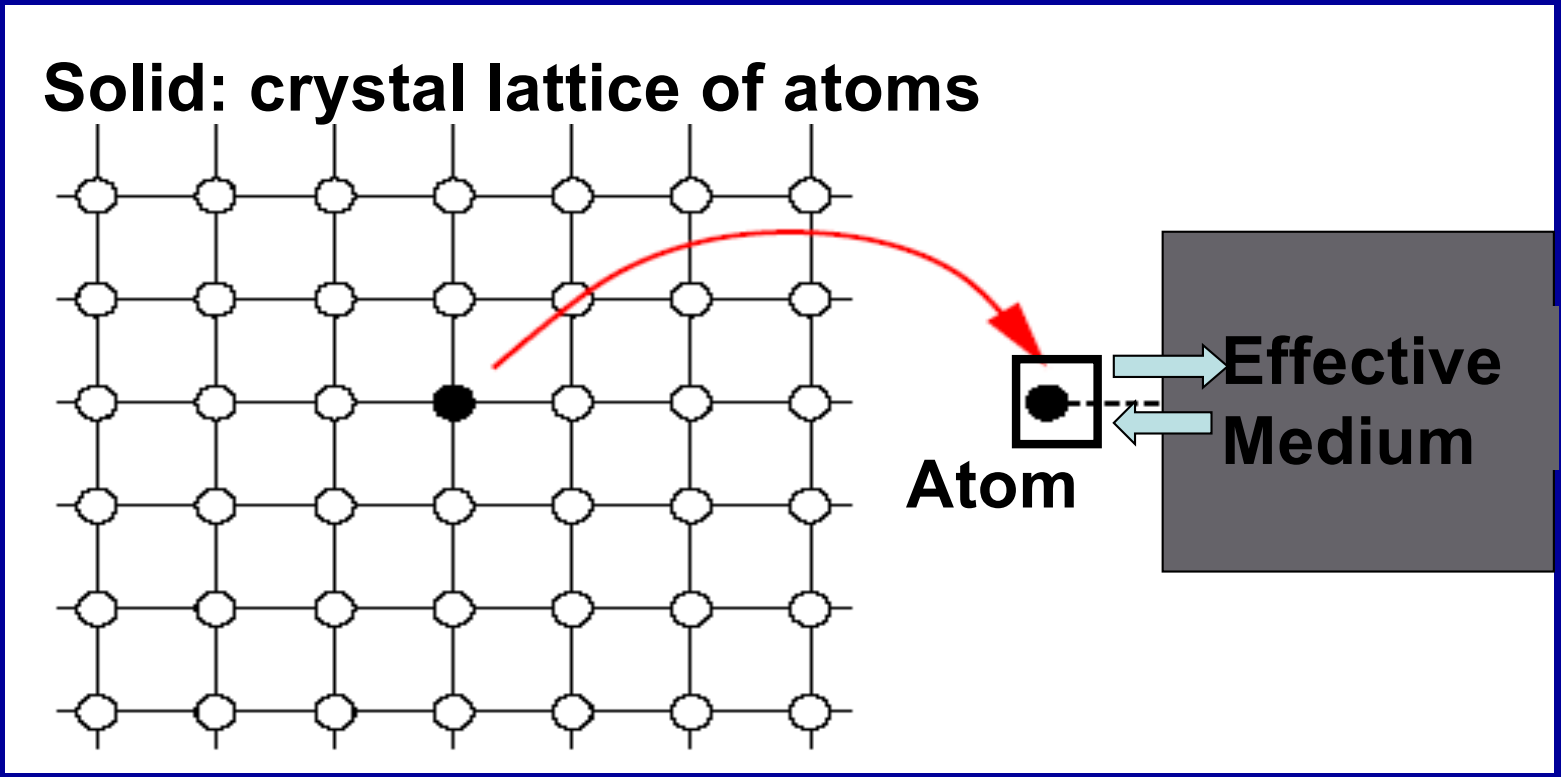
Dynamical Mean-Field Theory:
A.G. & G.Kotliar, PRB 45, 6479 (1992)
Correlated electrons in large dimensions:
W.Metzner & D.Vollhardt, PRL 62, 324 (1989)

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

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

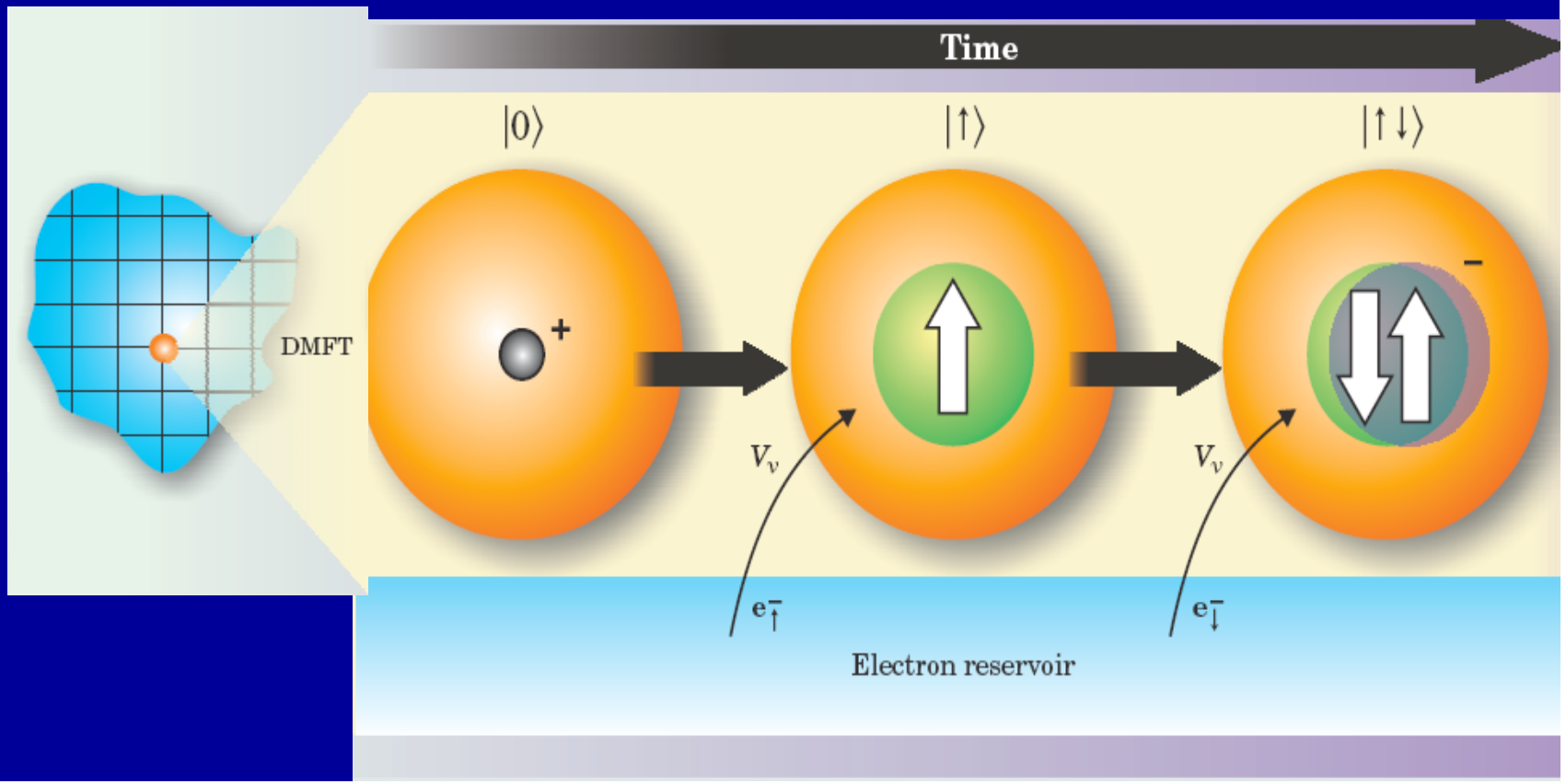
$$H = -\sum_{\mathbf{R}\mathbf{R}'} t_{\mathbf{R}\mathbf{R}'} d^{\dagger}_{\mathbf{R}\sigma} d_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} H^{\mathbf{R}}_{atom}$$

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

Focus on a given lattice site:

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

Describe ``history'' of fluctuations between those configurations



Imaginary-time effective action describing these histories:

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

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

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

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

$$\mathcal{G}_0^{-1} \equiv \omega + \mu - \Delta(i\omega)$$ Effective `bare propagator'

Focus on energy-dependent local observable :

$$G_{RR}(\omega) \equiv G_{\rm loc}$$

On-site Green's function (or spectral function) of the `solid'

Use atom-in-a-bath as a reference system to represent this observable:

→ IMPOSE that ε_d and Δ should be chosen such that:

$$G_{\rm imp}[\omega; \varepsilon_d, \Delta(\omega)] = G_{\rm loc}(\omega)$$

At this point, given G_{loc} of the lattice Hubbard model, we have just introduced an exact local representation of it

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:

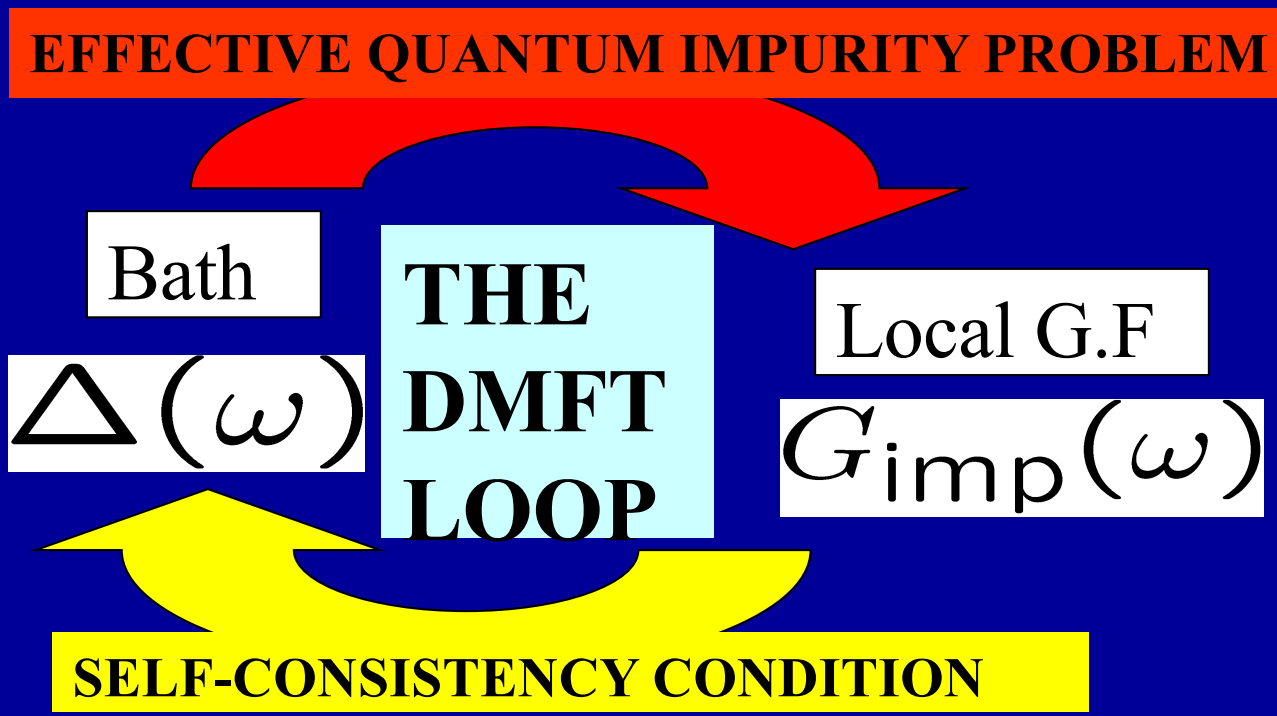
$$G_{\mathrm{imp}}[i\omega; \Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\mathrm{imp}}[i\omega; \Delta]^{-1} + \Delta(i\omega) - \varepsilon_{\mathbf{k}}}$$

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:

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



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

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.*

The DMFT construction is EXACT:

- For the non-interacting system
  (U =0 → Σ = 0 !)
- For the isolated atom
  (strong-coupling limit t=0 → Δ = 0)

→ Hence provides an interpolation from weak to strong coupling

- In the formal limit of infinite dimensionality (infinite lattice coordination) [introduced by Metzner and Vollhardt, 1989]

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

MERCI POUR VOTRE ATTENTION !

PROCHAIN COURS:

MARDI 21 Mai 9:30

Séminaire: Jan Kunes