# Numerically exact Monte Carlo algorithms for quantum impurity problems


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Transregional Collaborative Research Centre SFB / TRR 49

*Condensed matter systems with variable many-body interactions*

Frankfurt / Kaiserslautern / Mainz

# Outline

Introduction: correlations in materials and ultracold gases

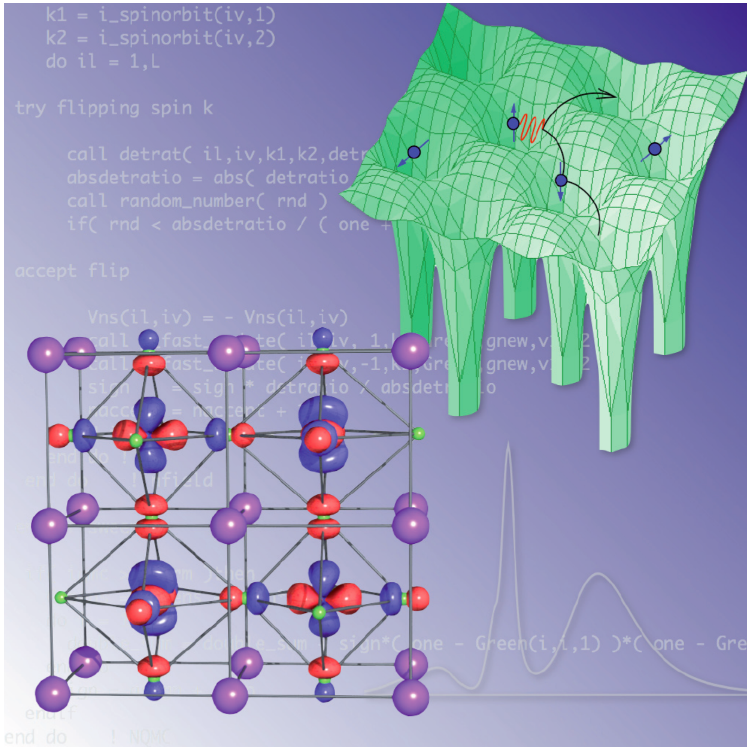
Application: signature of magnetism in fermions on optical lattices

[N. Blümer and E. V. Gorelik, CPC, in press, doi:10.1016/j.cpc.2010.07.011]

[E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, N. Blümer, PRL **105**, 065301 (2010)]

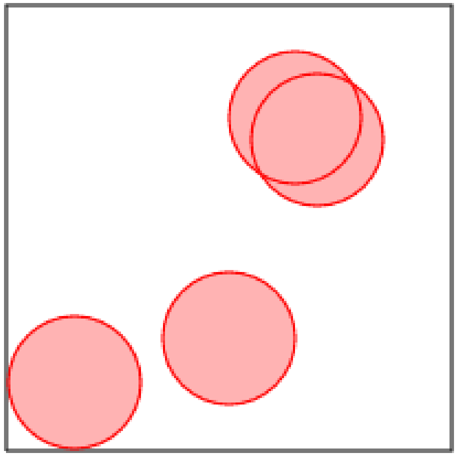
Methods: status quo and project idea

Context: SFB/TR 49, FOR 1346

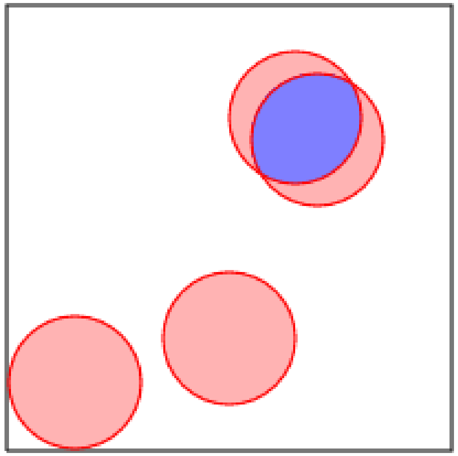


# Introduction: strong correlations and metal-insulator transition

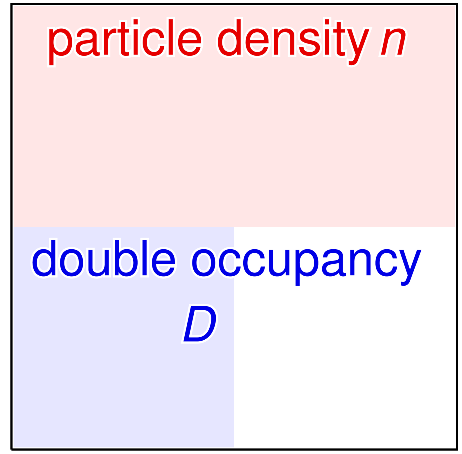
1. Classical case in continuum



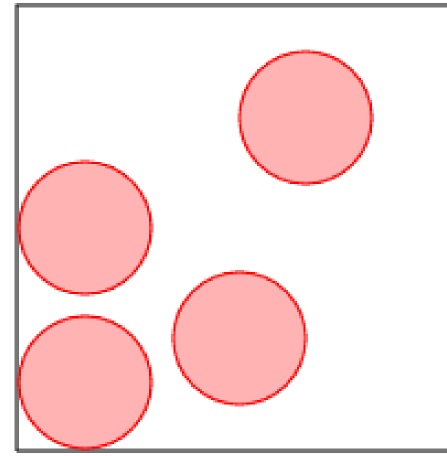
Free non-int. spherical particles in 2d box



double occupancy

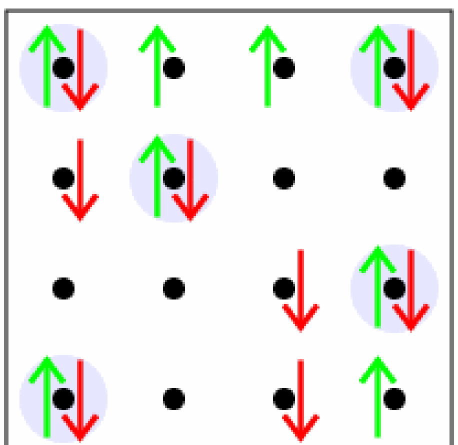



$D = n^2$ uncorrelated $\quad$ $D = 0$ max corr.



free particles with hard-core interaction

2. Electrons in solids: quantum lattice models, e.g. 1-band Hubbard model



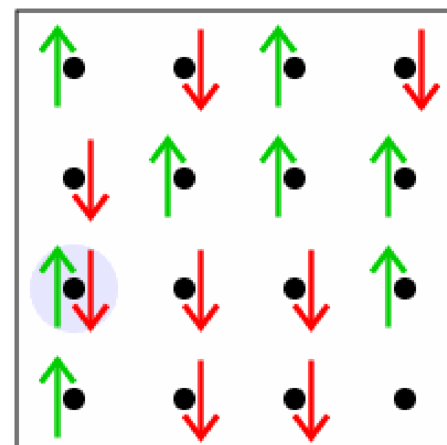
Pauli principle: max 1 $e^-$ per site/spin orientation

energy $E = E_{\text{kin}} + UD$

noninteracting case: $D = \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle$, perfect metal

at half filling: $D \overset{U\to\infty}{\longrightarrow} 0$, insulator

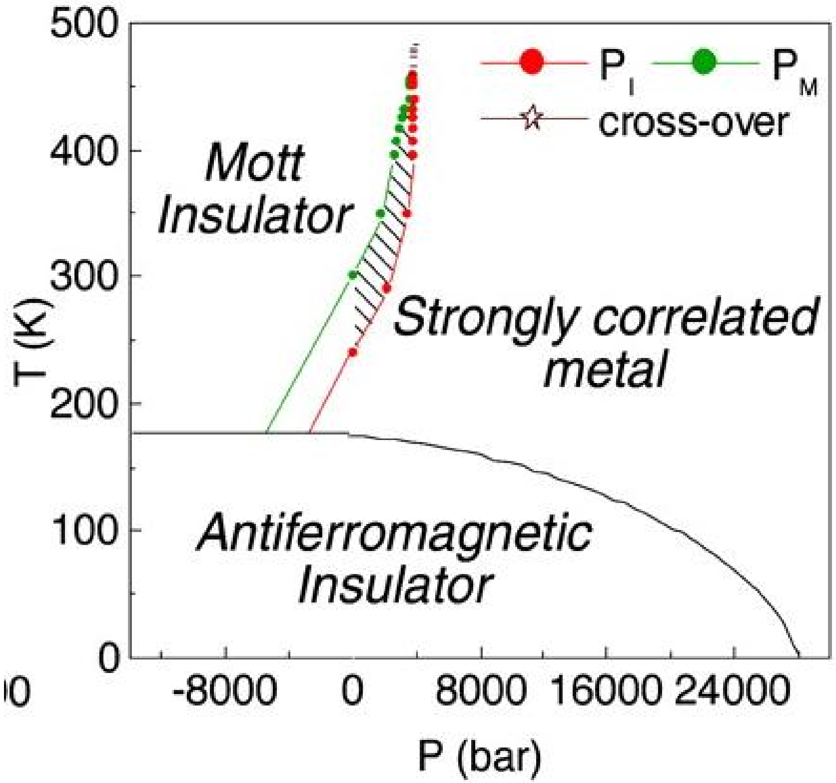
Attention: artificial dynamics ($\rightsquigarrow$ ensemble aver.)!



# Systems with strong electronic/fermionic correlations

Prototype example: $V_2O_3$ doped
with Cr/Ti and/or under pressure

## Phase diagram




[Limelette et al., Science 302, 89 (2003)]

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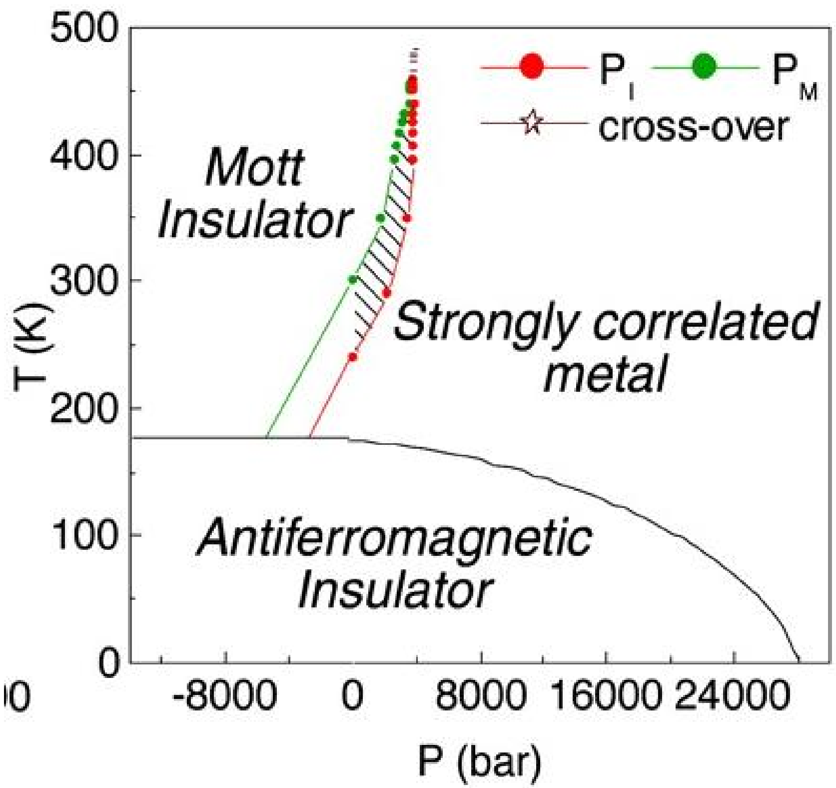
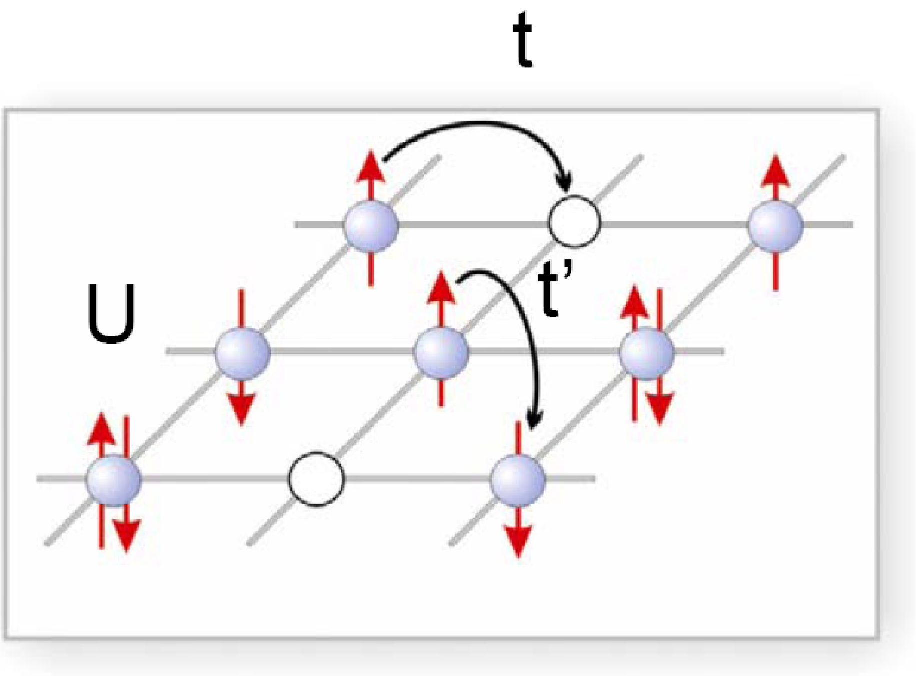



[Limelette et al., Science 302, 89 (2003)]

Mott metal-insulator transition and AF: generic physics of 1-band Hubbard model



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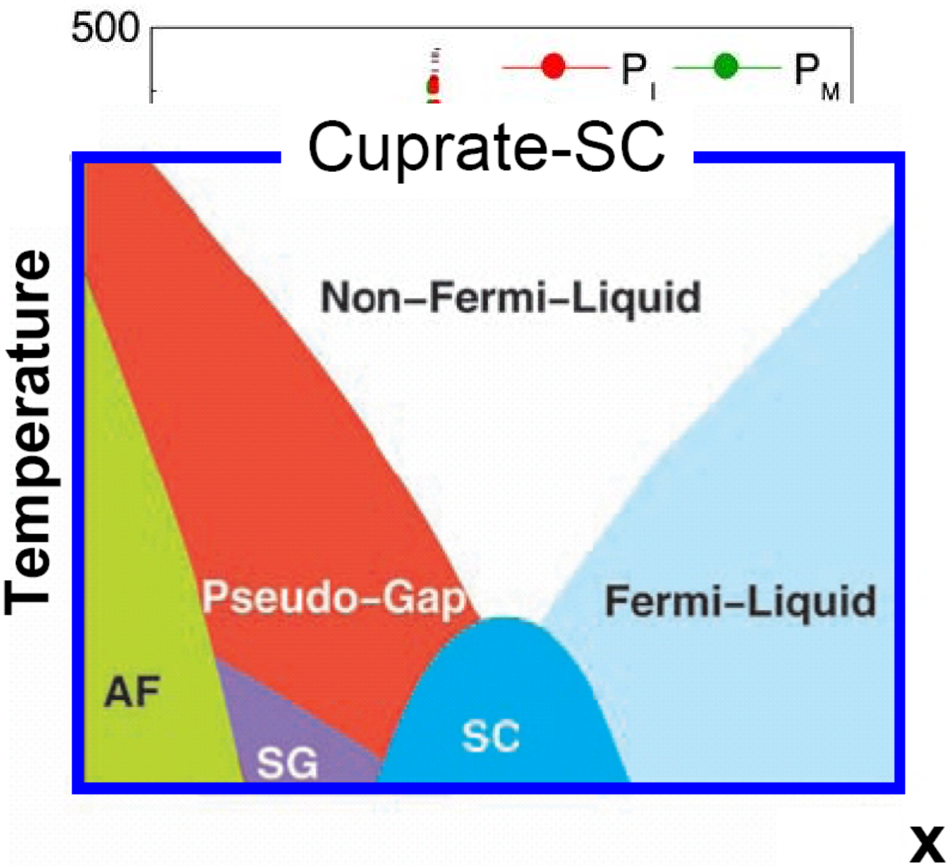


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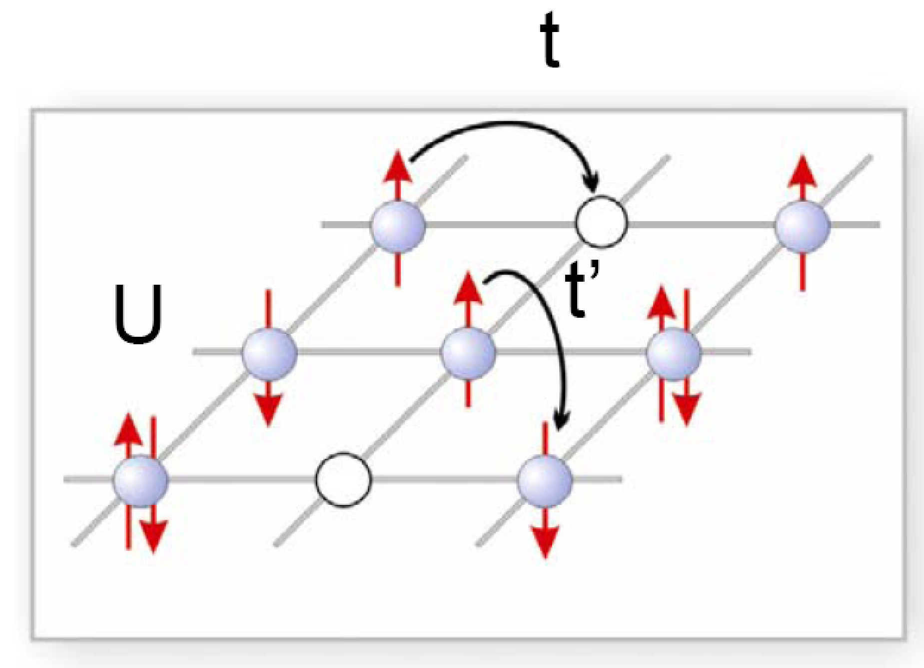


Are AF and Mott phases essential for superconductivity?

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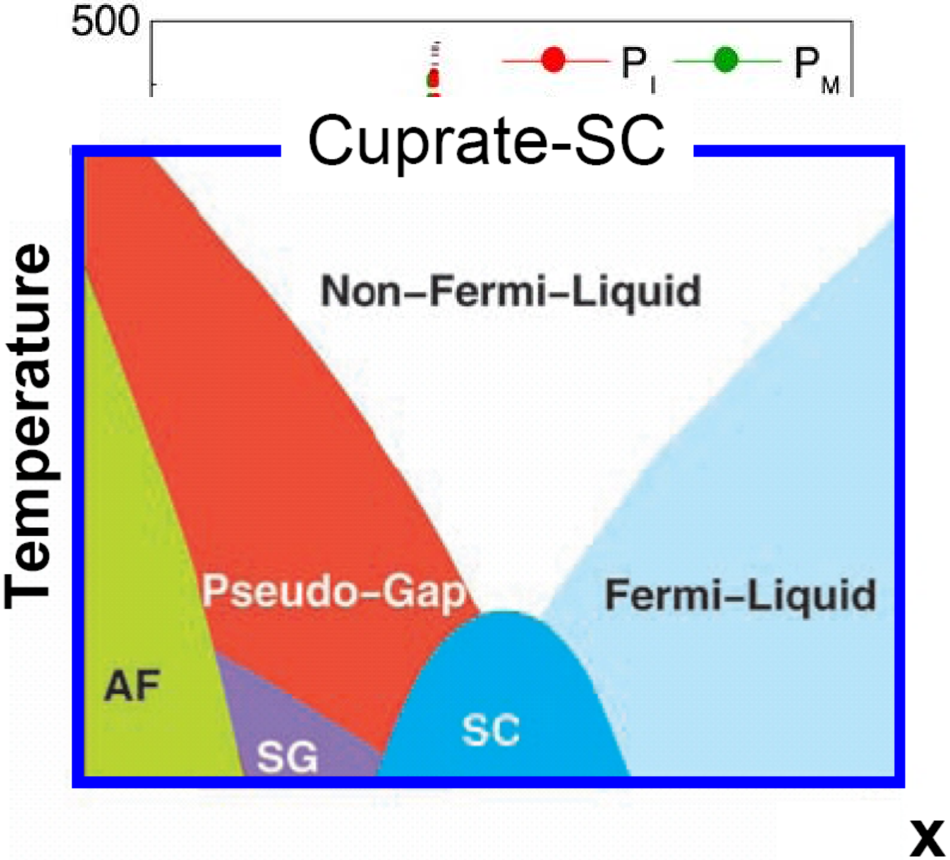


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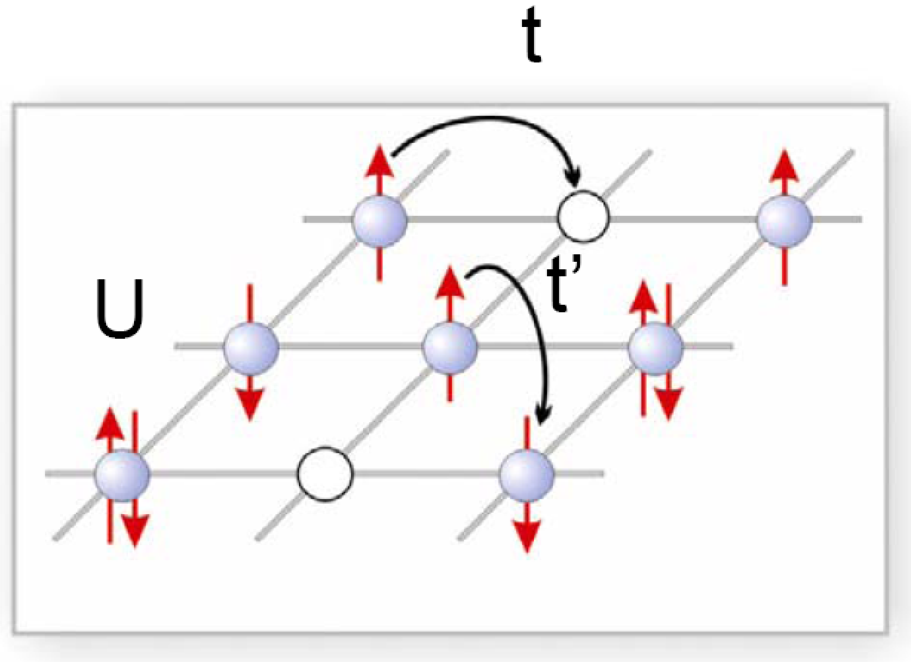
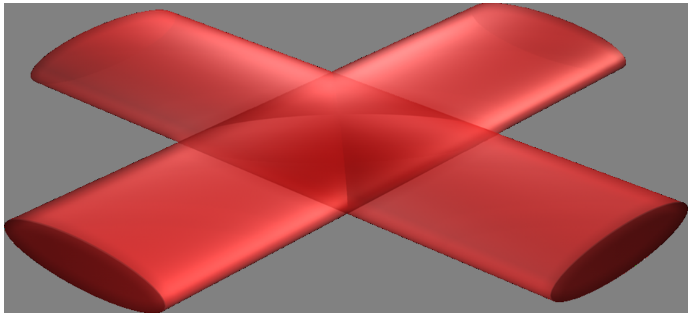



Are AF and Mott phases essential for superconductivity?

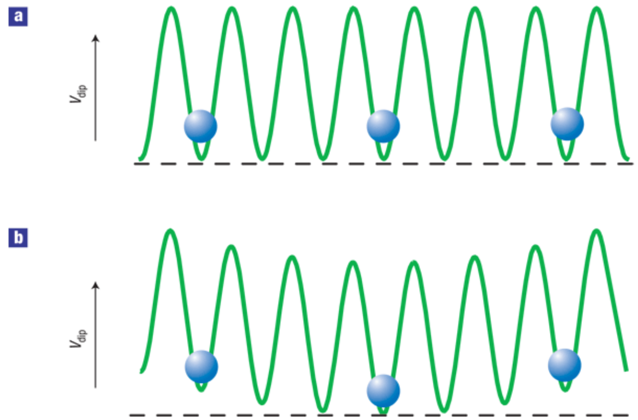
Claim: cold atoms $\rightsquigarrow$ quantum simulators

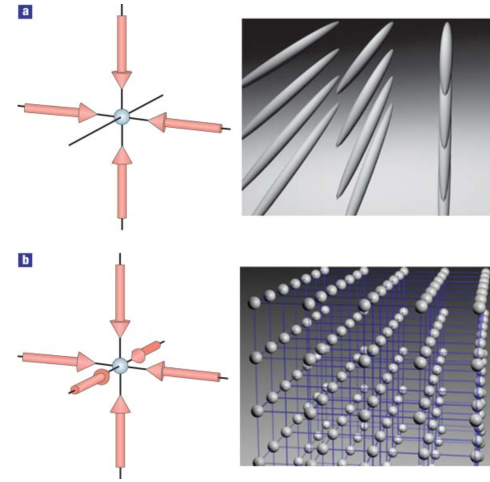
# Correlated ultracold quantum gases: traps and optical lattices

Optical dipole trap (2 beams)



Interference $\rightsquigarrow$ modulation



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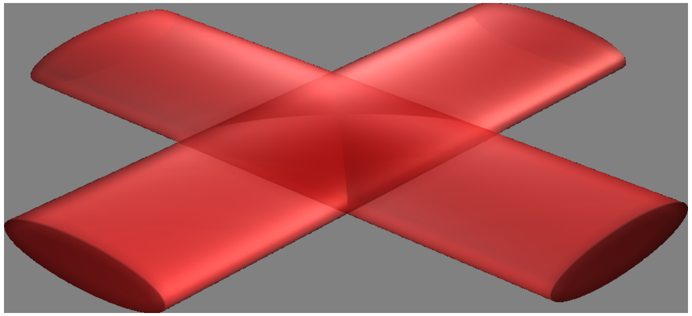

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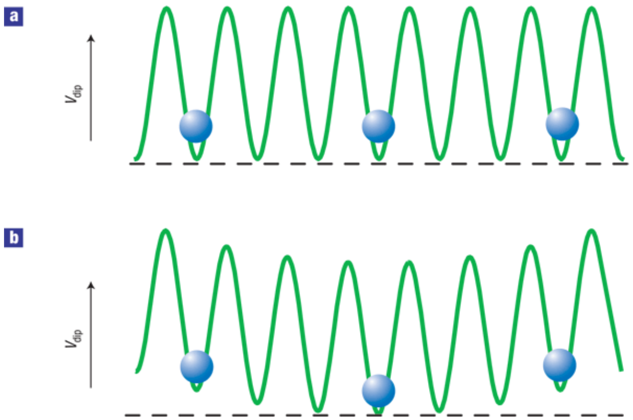
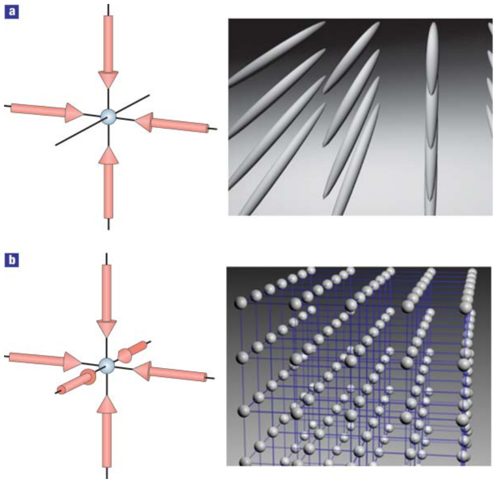
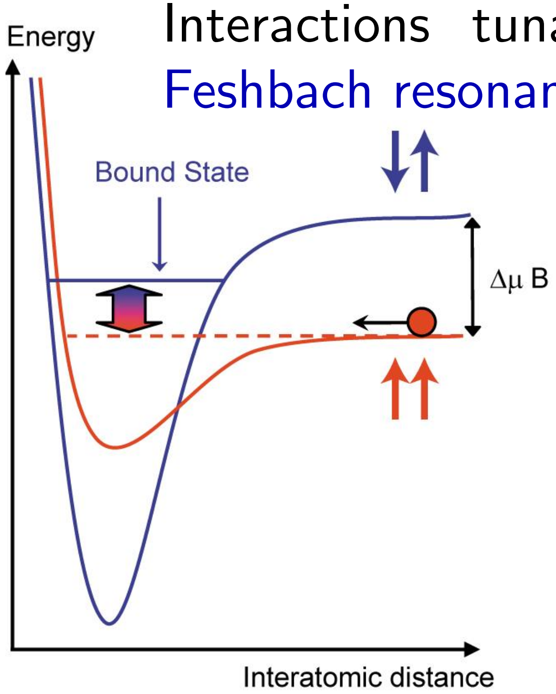




Interactions tunable via Feshbach resonances



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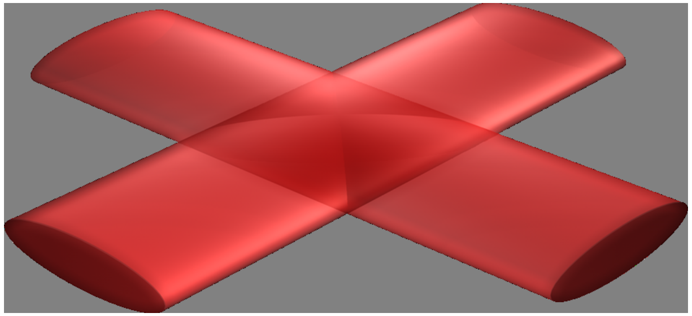

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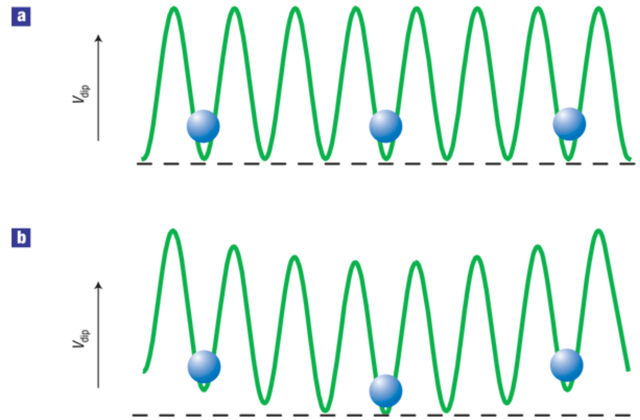


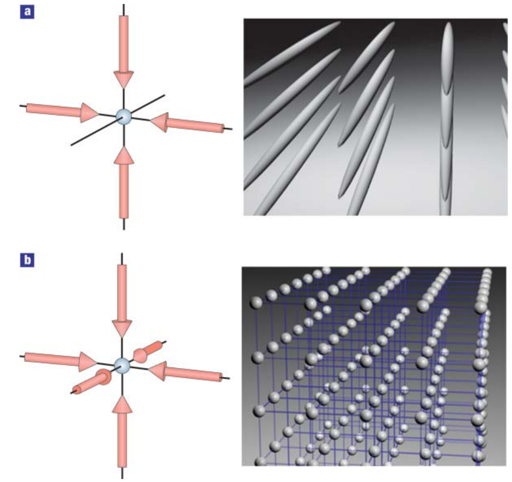


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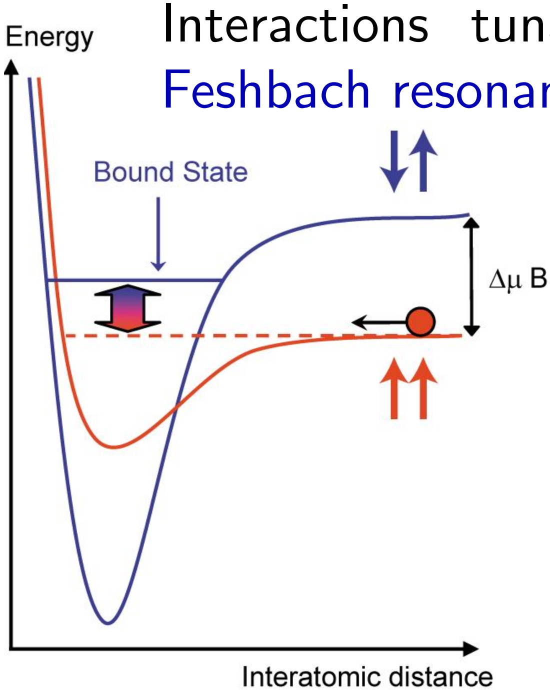
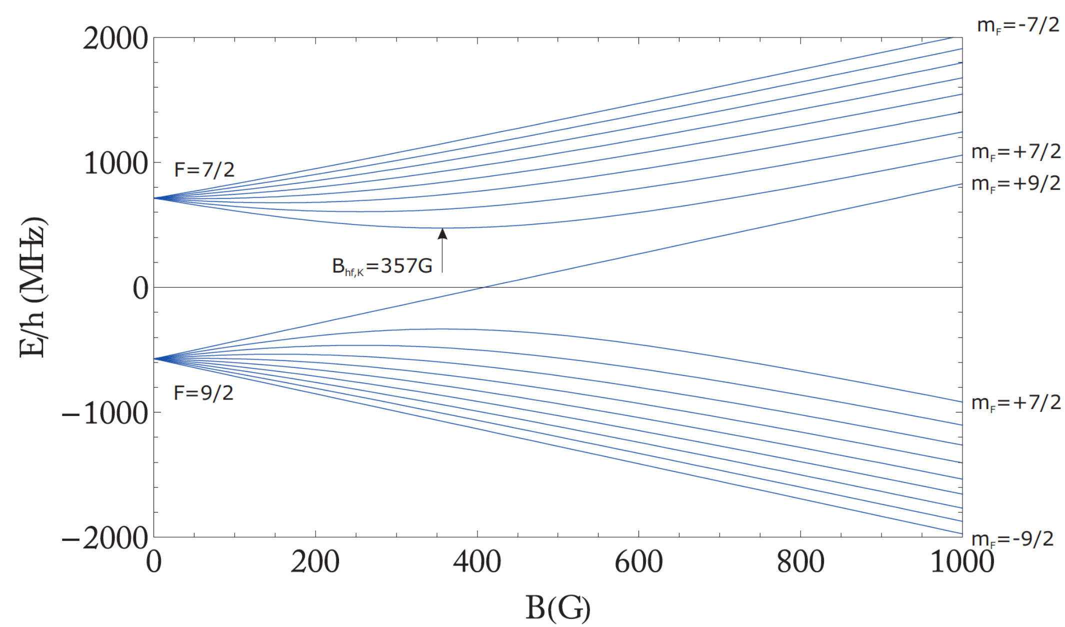



Large multiplets accessible (here $^{40}K$)



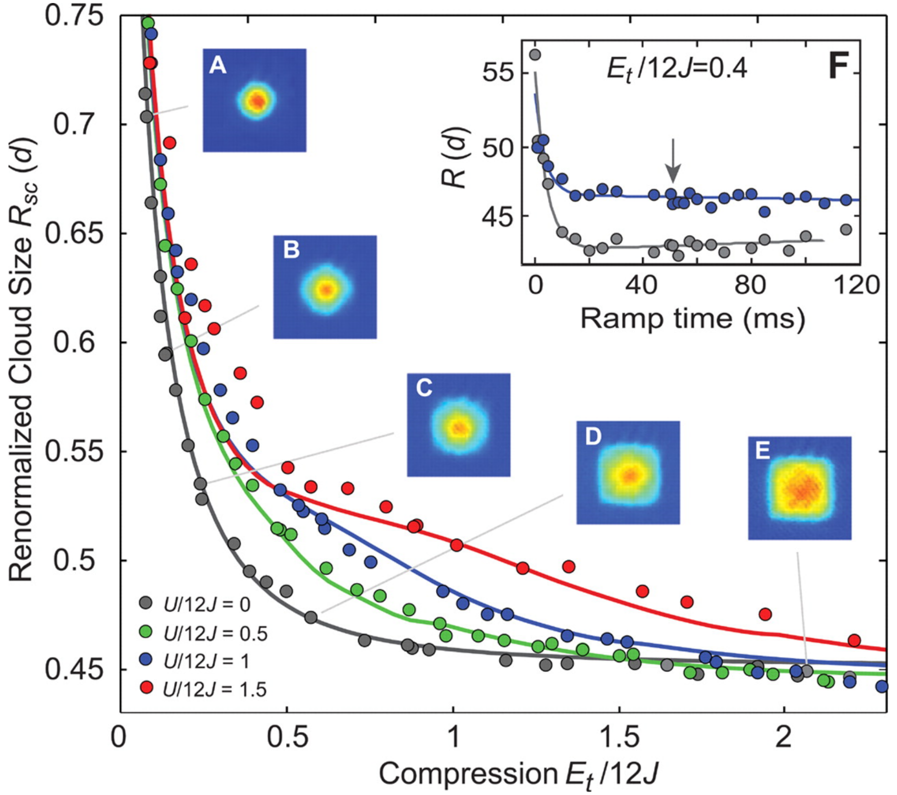
# Correlations in ultracold fermions on optical lattices

Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

Detection: cloud diameter vs. trap strength $\rightsquigarrow$ incompress. Mott phase

Simulations (here DMFT+NRG) essential for interpretation of data!

[Schneider et al, Science **322**, 1520 (2008)]



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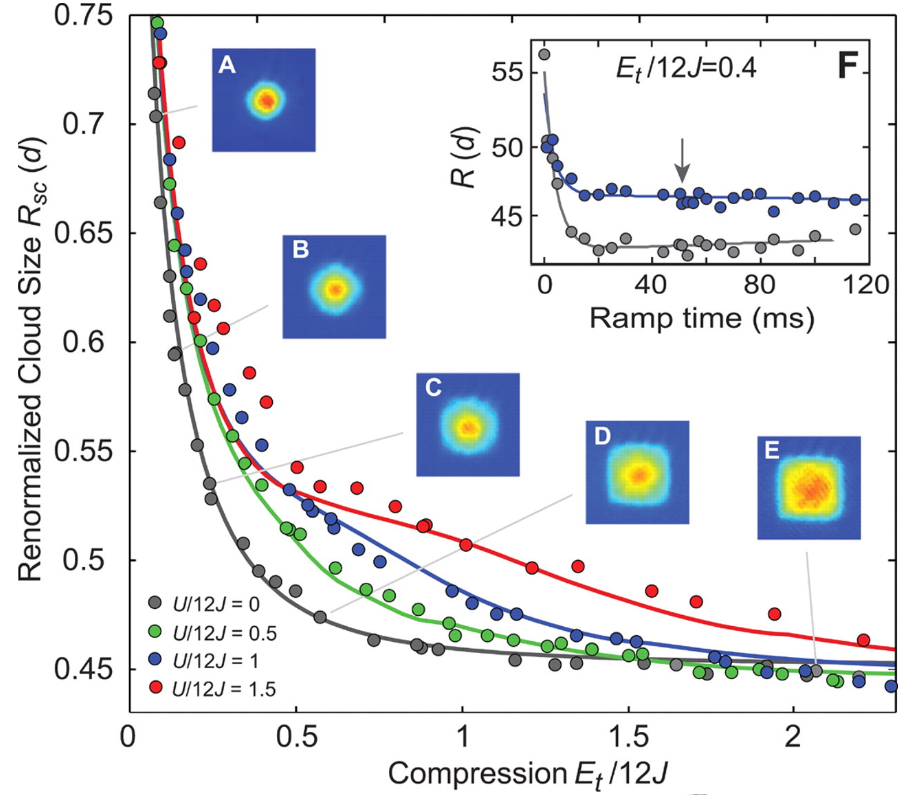


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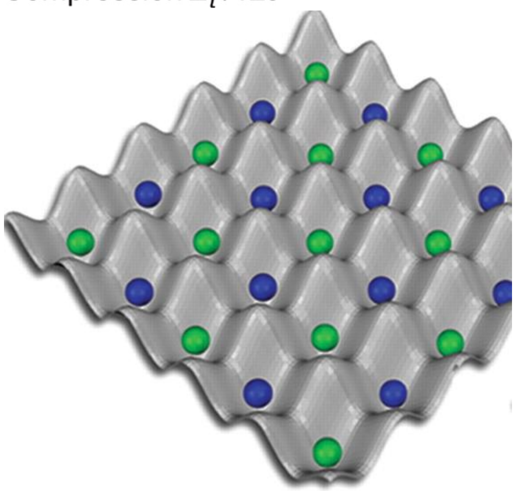
## Next grand challenge: AF

Antiferromagnetism = staggered order in 2-flavor mixtures of ultracold fermions

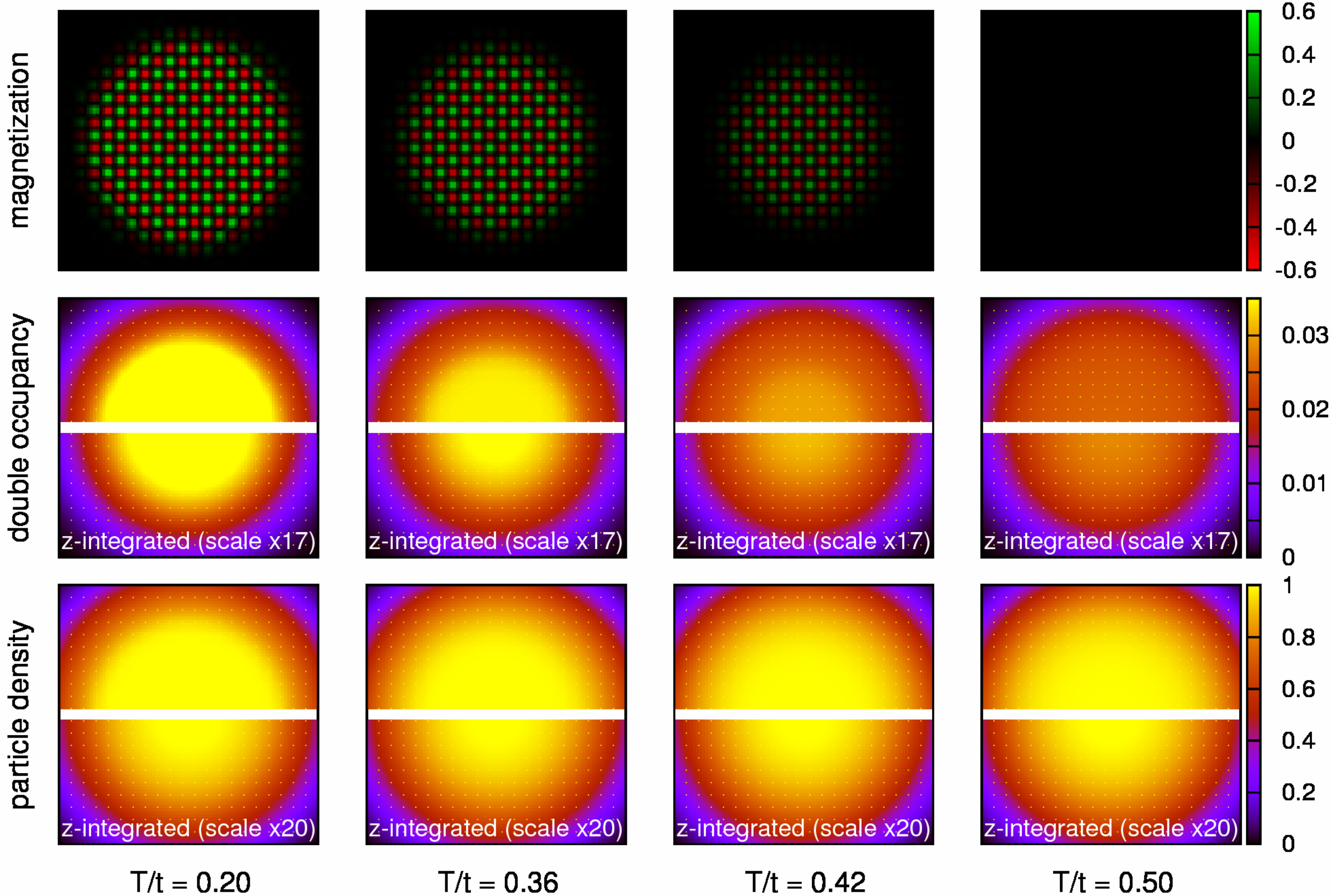


Problems:

(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of order parameter is not straightforward

# Results: RDMFT-QMC (cubic lattice, $V = 0.05t$, $U = W = 12t$)



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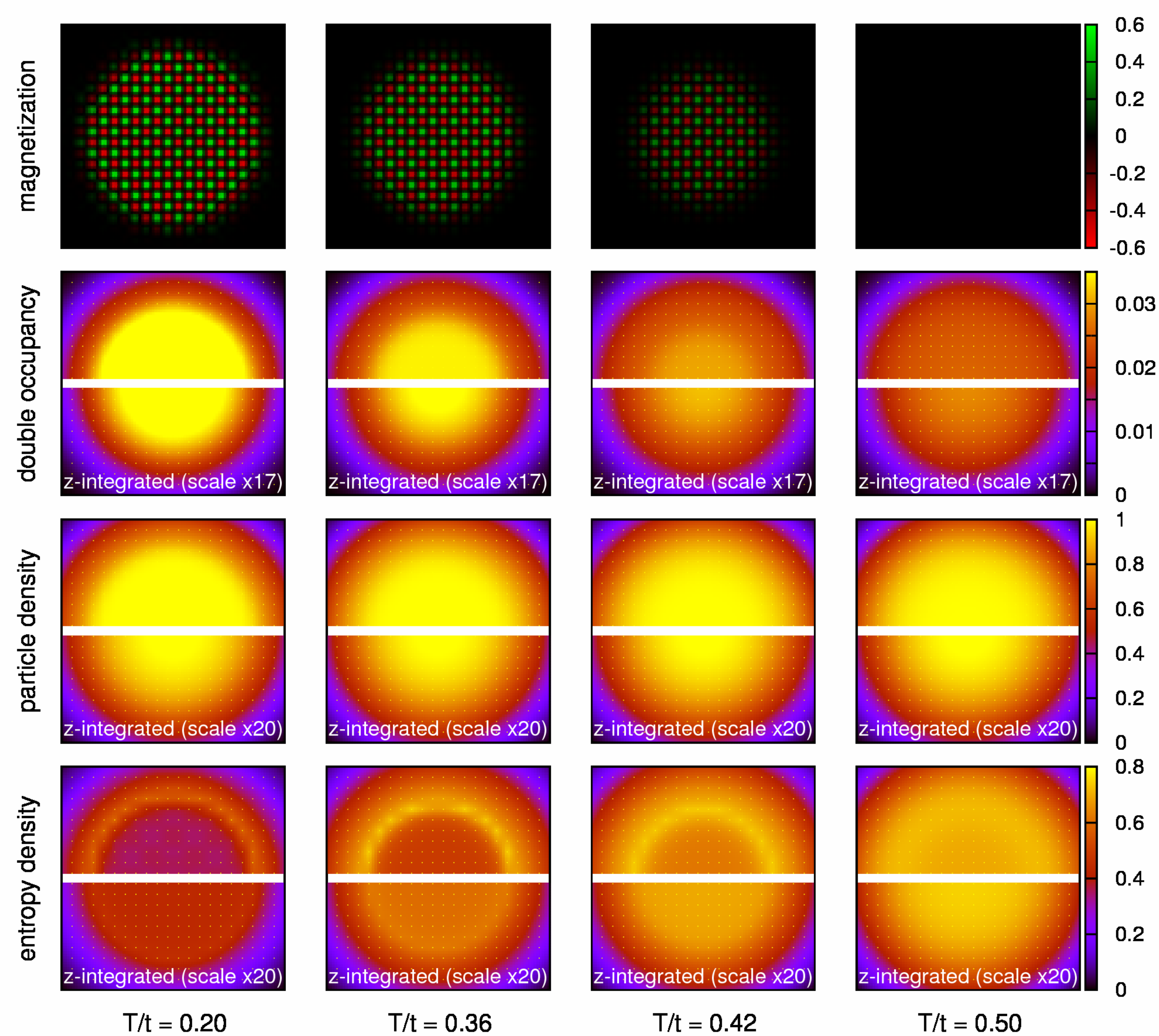



AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced $D$!

$\sim$ 6000 atoms (naively $\sim 30^3 = 27000$ sites needed)

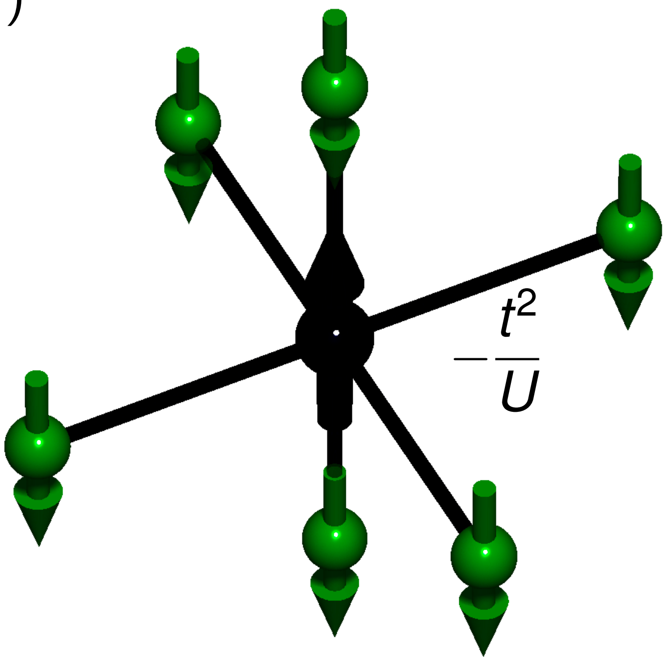
Entropy

$$S = \int_{-\infty}^{0} d\mu' \frac{dN}{dT}$$

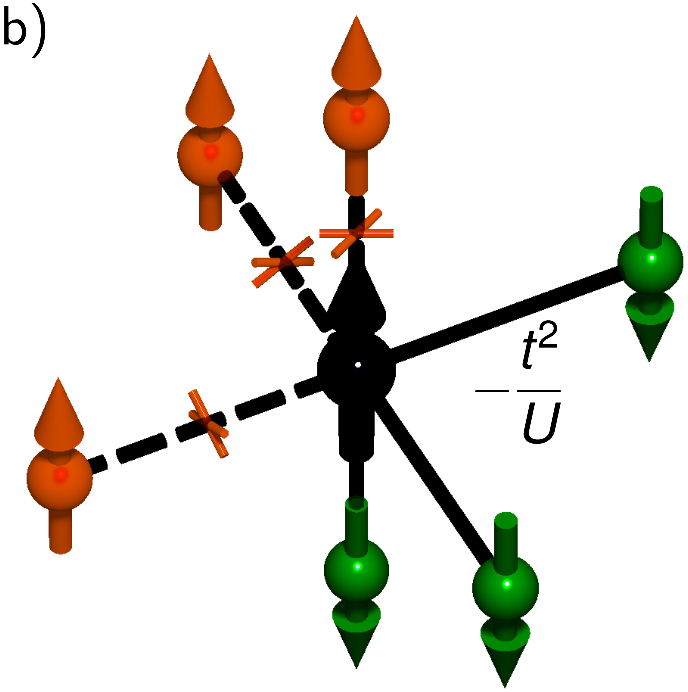
# Enhanced double occupancy: a signature of AF order

Illustration of mechanism for enhanced double occupancy (at strong coupling):

(a)




(b)




AF state:

electron can hop to all
$Z = 6$ next neighbors

$$E_{\mathrm{AF}} = -\frac{Z\,t^2}{U}$$

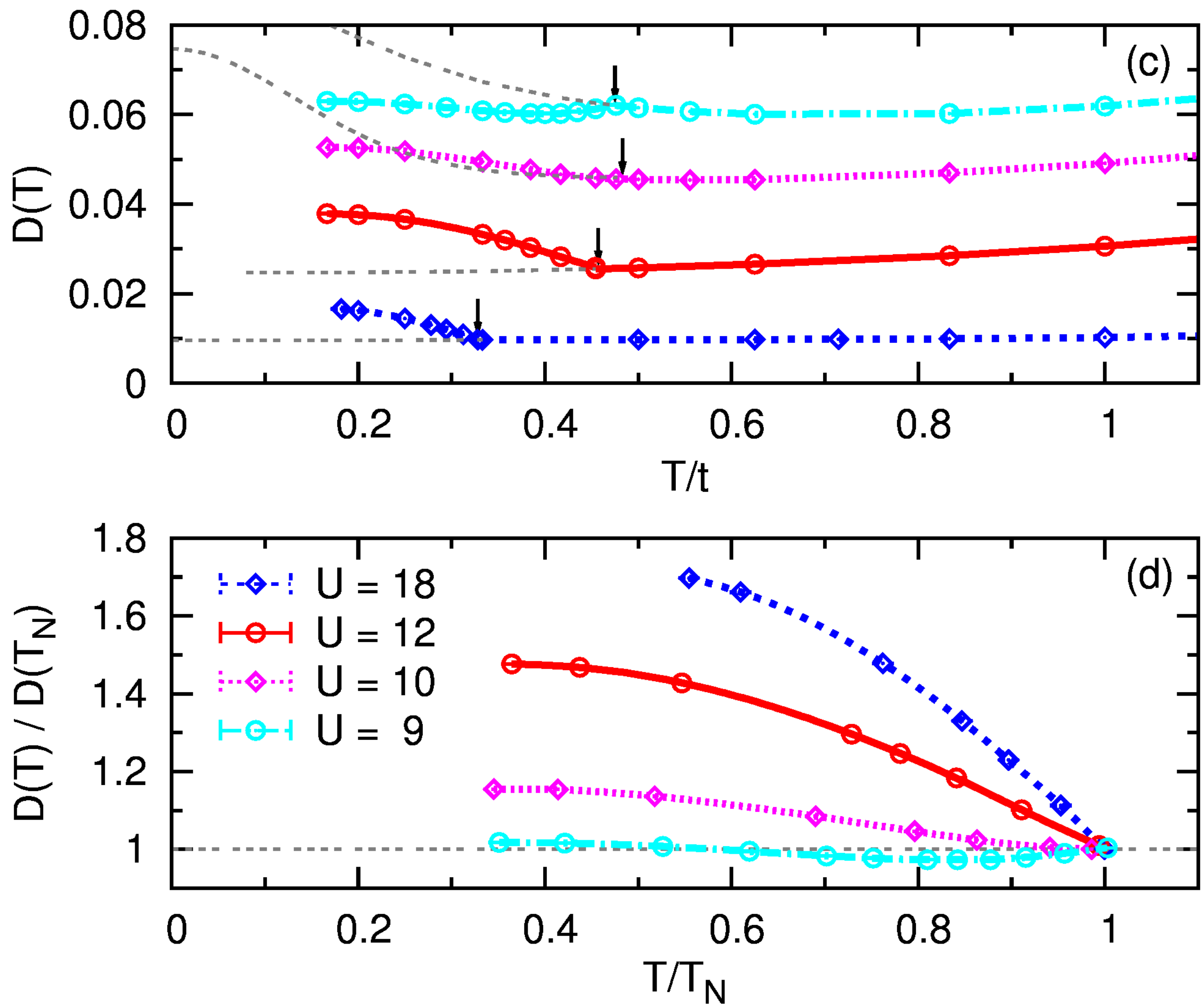
Paramagnetic state:

1/2 of the neighboring sites
are forbidden for hopping

$$E_{\mathrm{p}} = -\frac{Z\,t^2}{2U}$$

By $D = dE/dU$ (at $T = 0$), the argument implies $D_{\mathbf{AF}}/D_{\mathbf{p}} \overset{U\to\infty}{\longrightarrow} 2$.

# DMFT-QMC estimates of $D$ at half filling




AF $\Rightarrow$
enhanced $D$ at $U \gtrsim 10t$

arrows: Néel temperatures

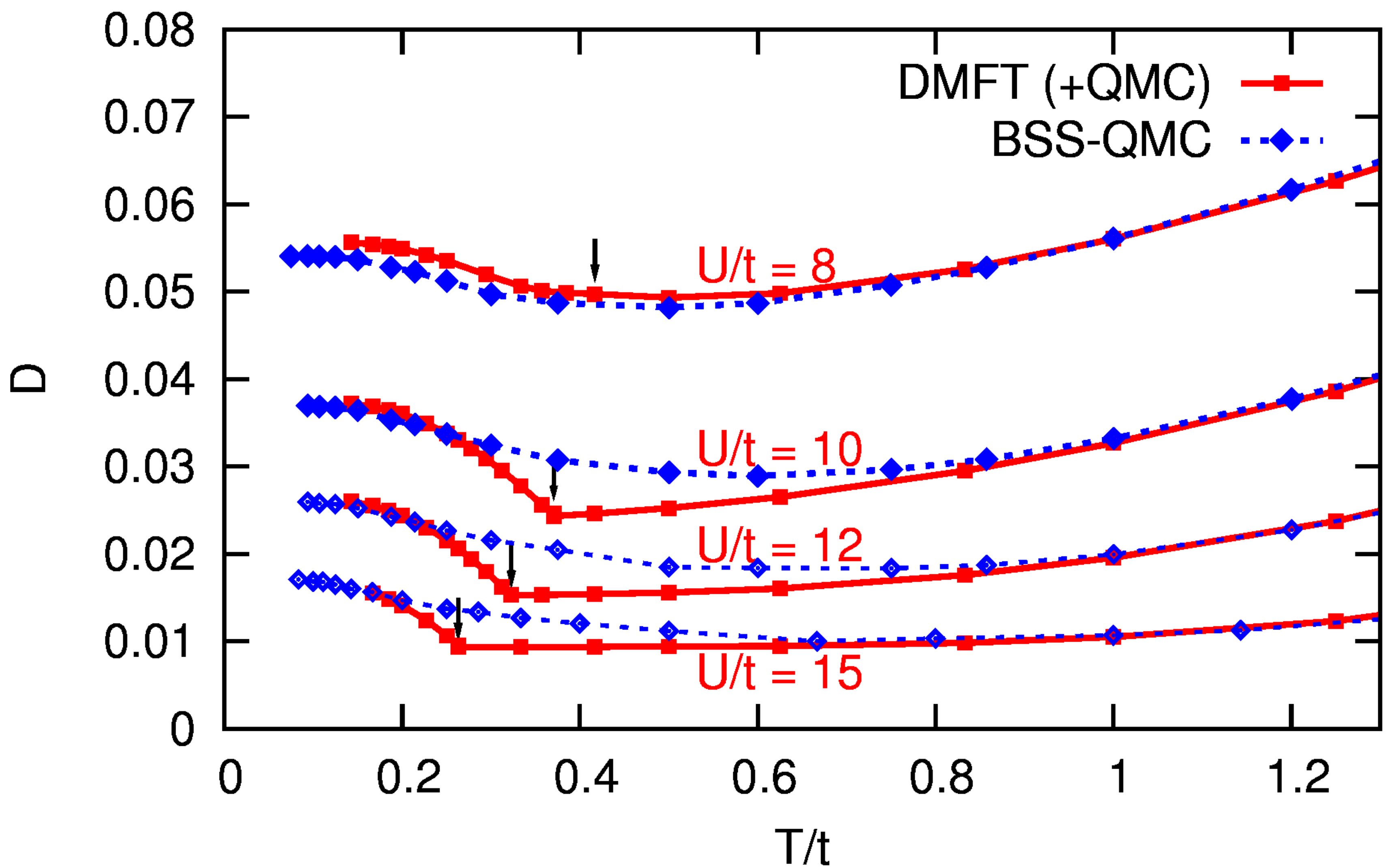
thin lines: metastable paramagnetic phase.

Data scaled to values of critical point:

relative enhancement
$D/D(T_N) \overset{U\to\infty}{\longrightarrow} 2$

Note: AF kills Pomeranchuk cooling [Werner, Parcollet, Georges, Hassan, PRL (2005)]!

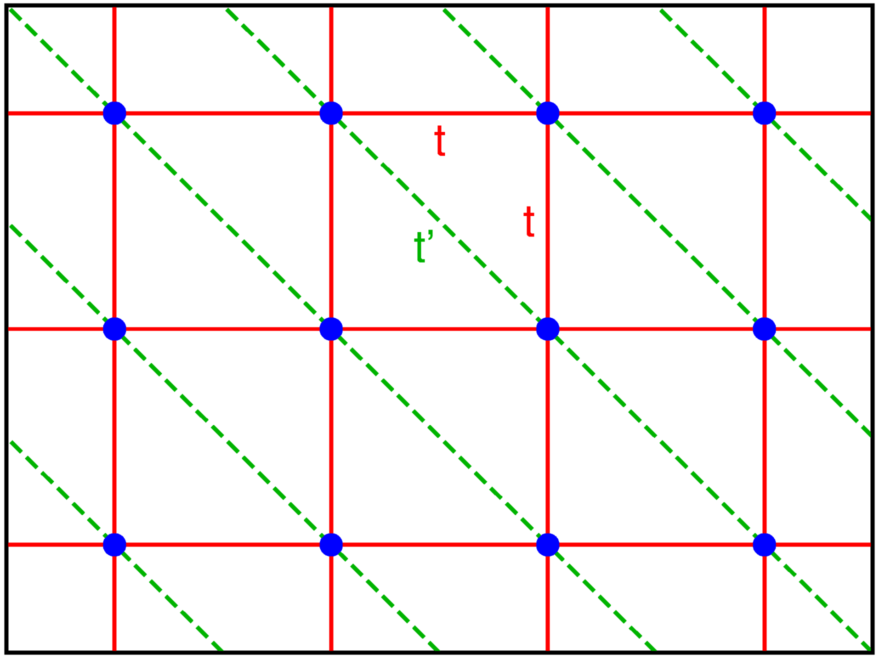
# How realistic is DMFT? Extreme test case: 2 dimensions (square)




Preliminary BSS-QMC data by Scalettar (UC Davis) and Paiva (Rio de Janeiro)

# Present study: controlled frustration in triangular lattices

Introduce frustration in controlled way as diagonal hopping in square lattice:



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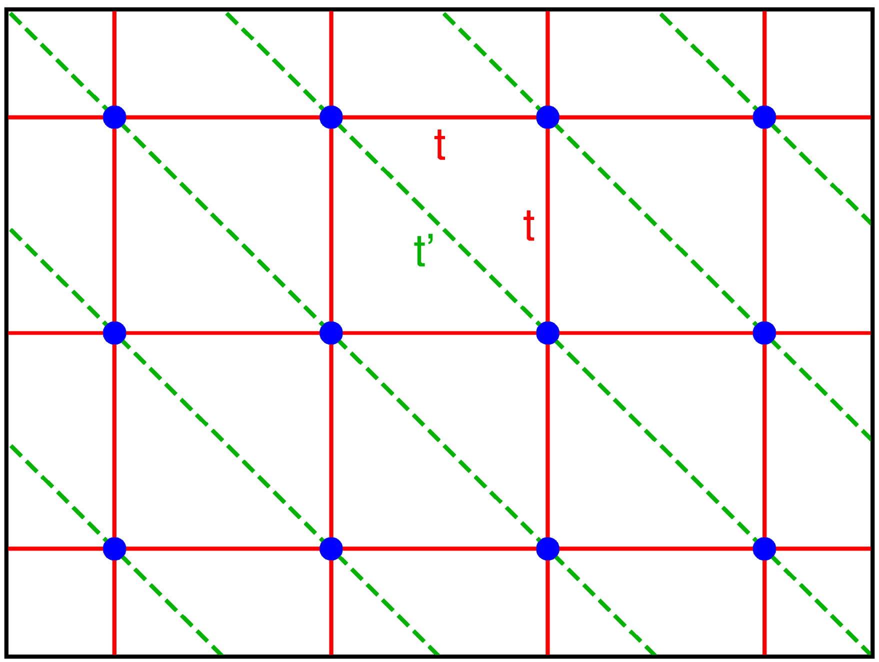
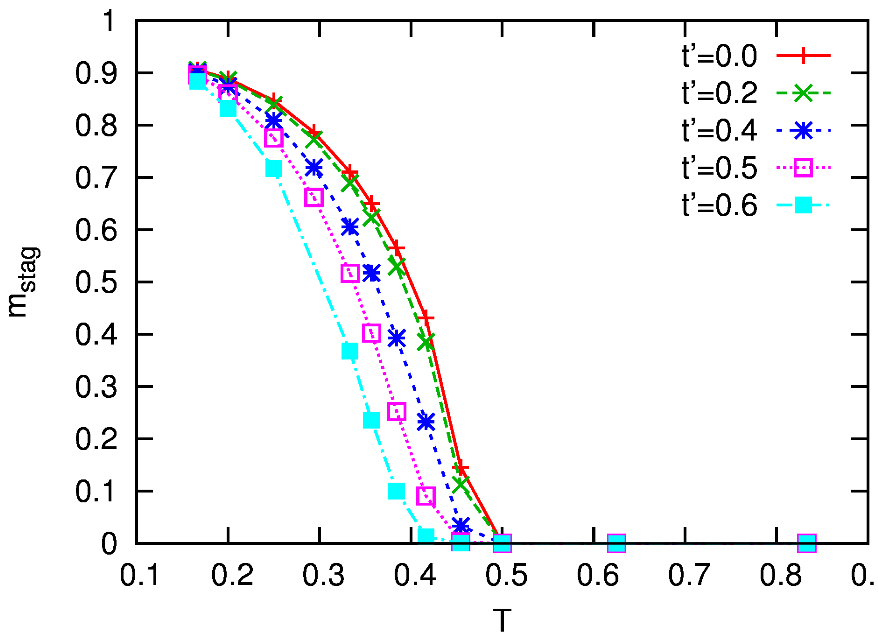
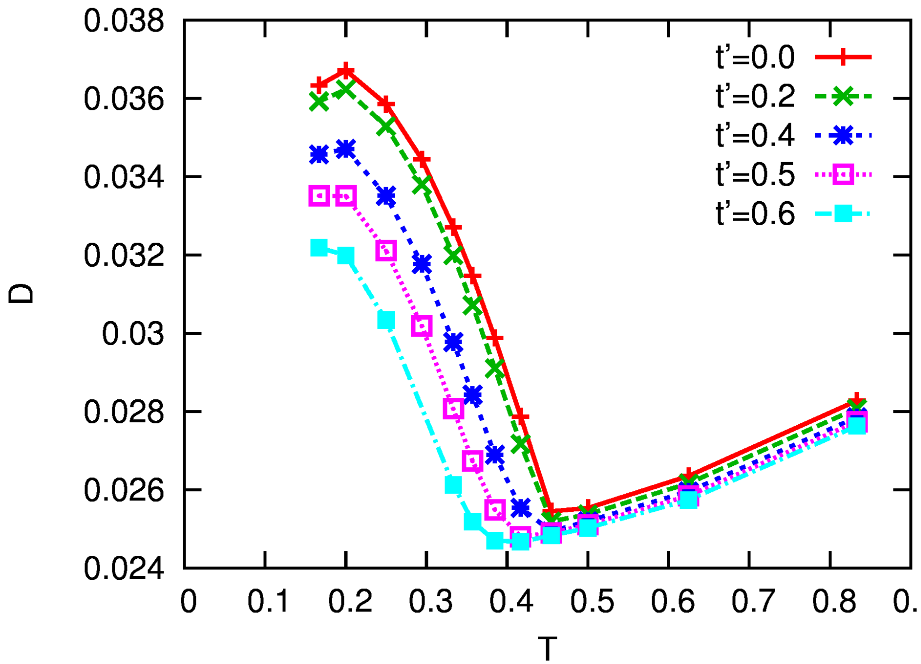



Double occupancy suppressed in AF phase before order breaks down

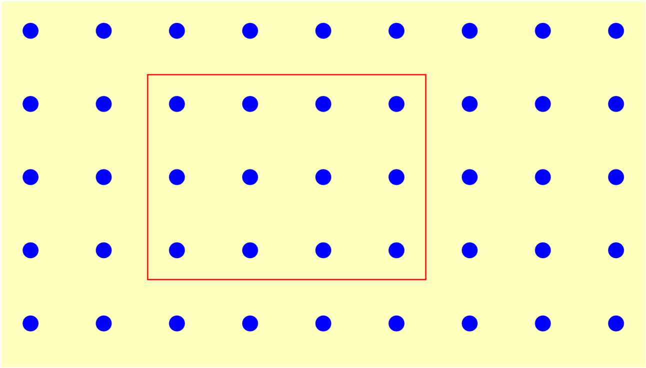


# Methods: approaches for Hubbard model

$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

- perturbative approaches (weak/strong)
- in 1 dimension: DMRG
- finite clusters: ED, QMC



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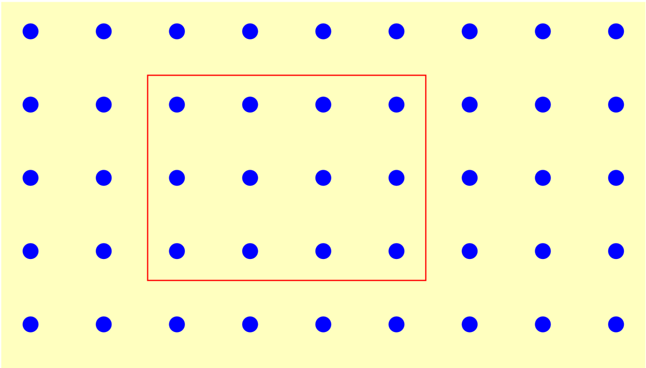
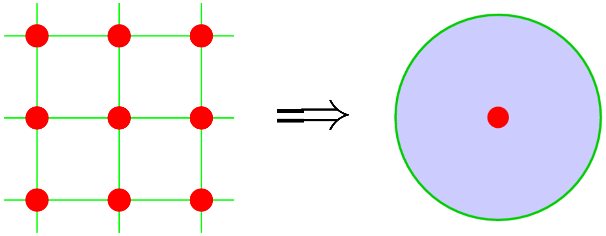


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k},\omega) \equiv \Sigma(\omega)$

[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit

+/− exact for coordination $Z \to \infty$



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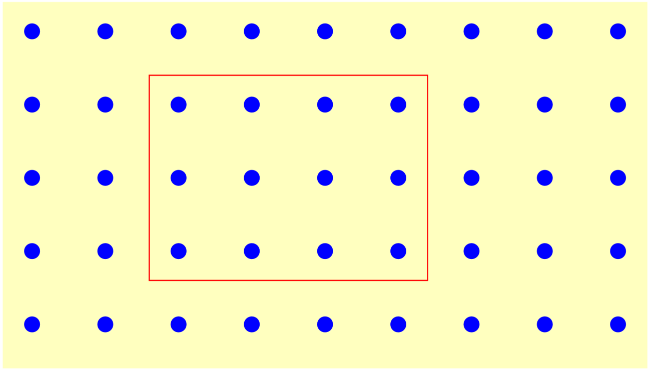

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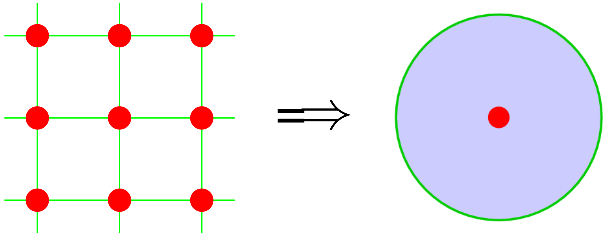
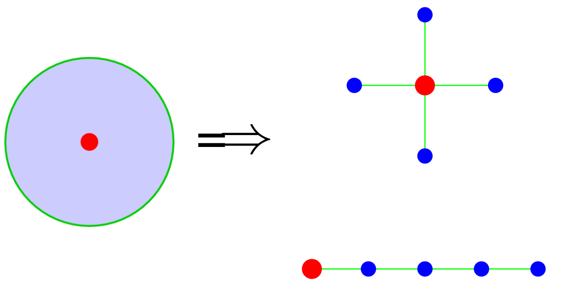


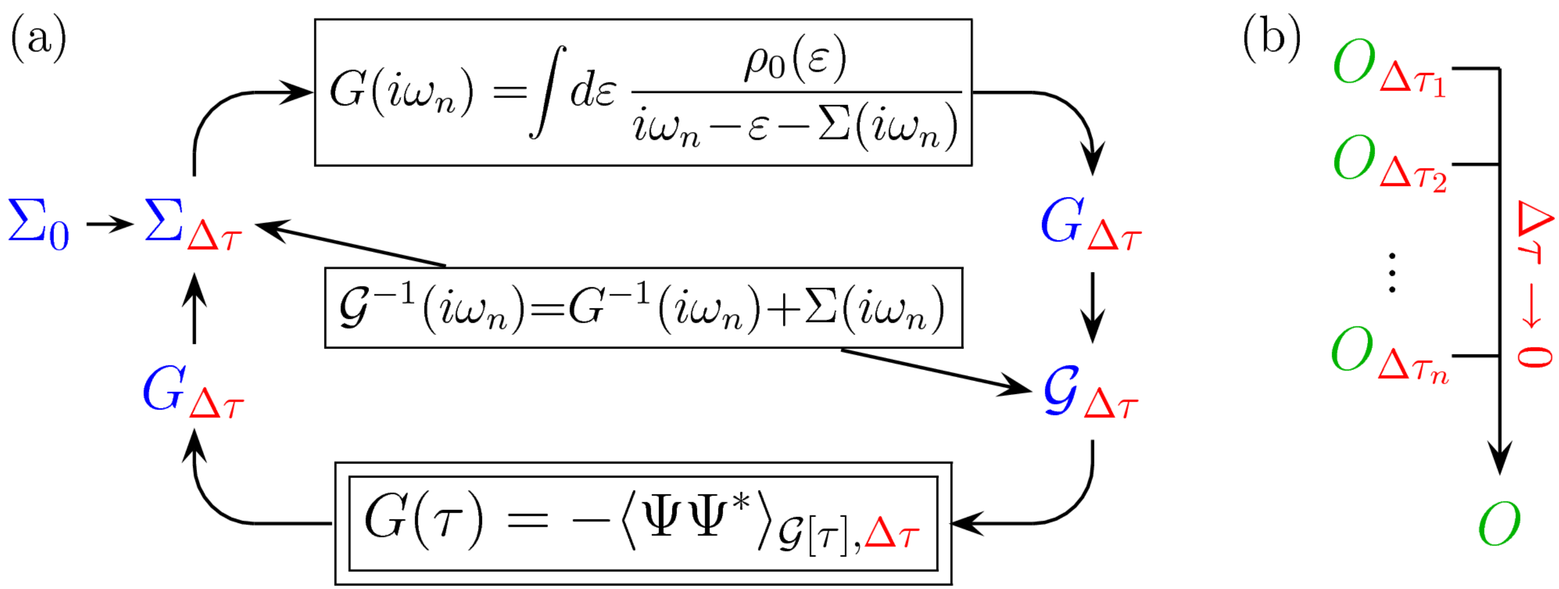
**DMFT impurity solver:**
- QMC (cost $\propto T^{-3}$)
- ED, DMRG, NRG . . .



# Multigrid Hirsch-Fye quantum Monte Carlo algorithm

State of the art: (a) conventional HF-QMC

(b) *a posteriori* extrapolation of selected observables



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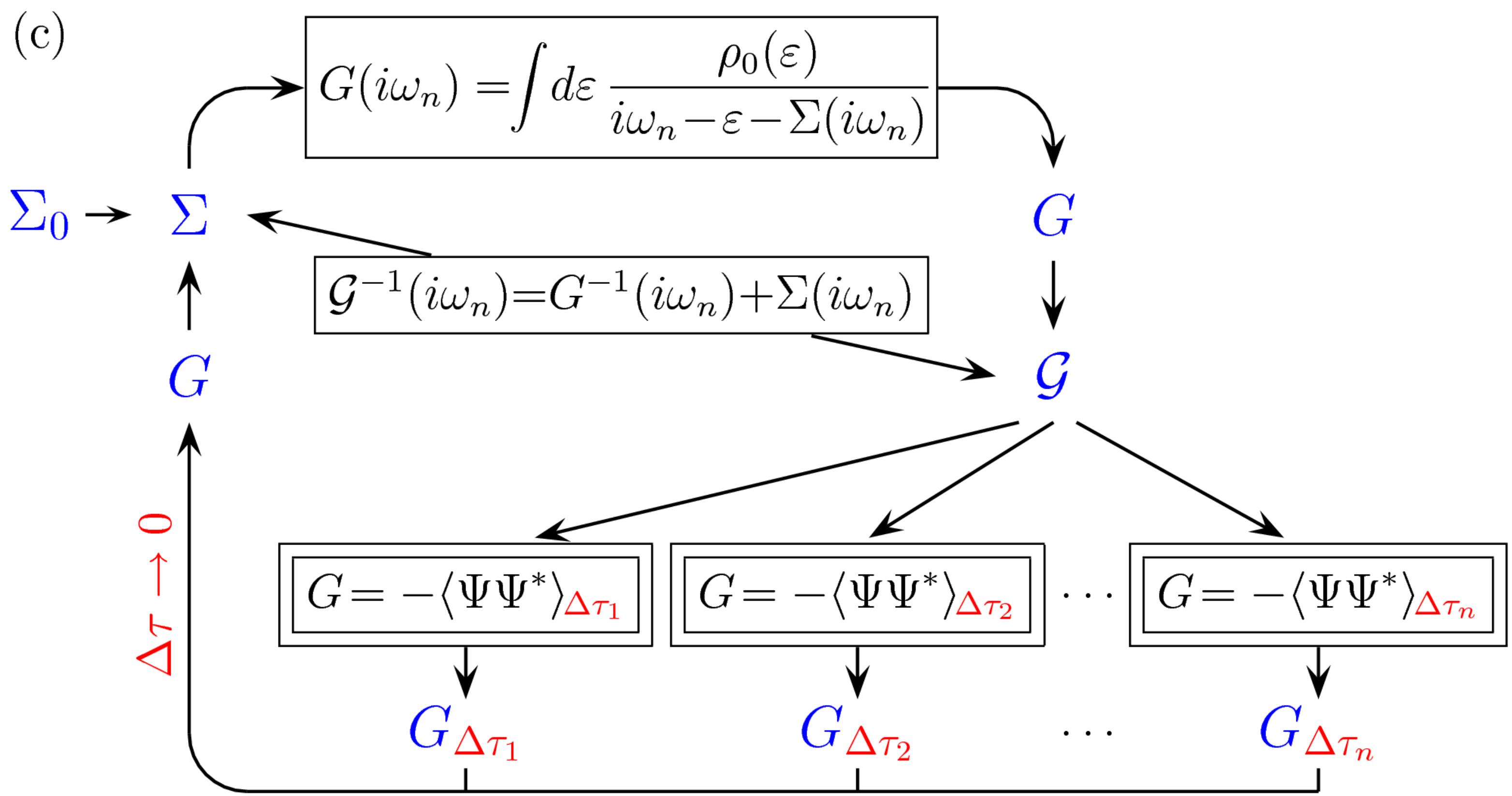
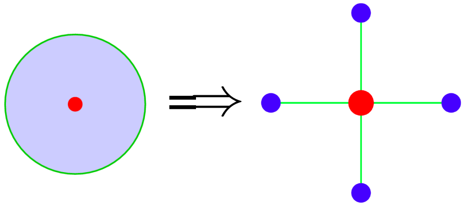



(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ quasi CT-QMC algorithm [NB, arXiv:0801.1222, PRA(2009)]

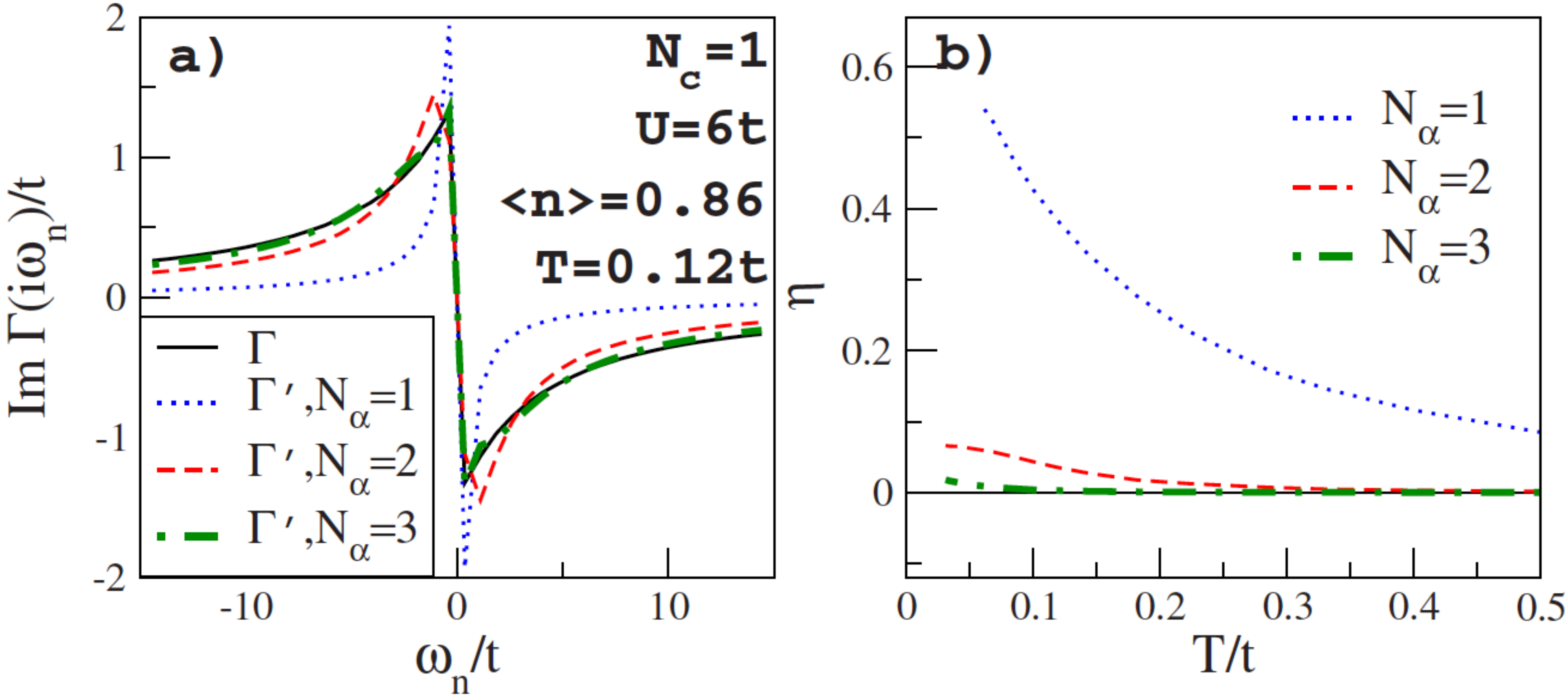
# Project: unbiased QMC impurity solver with linear scaling in $1/T$

Recent proposal: • map impurity model to Hamiltonian,



i.e. fit hybridization function $$\Gamma'(i\omega_n) = \sum_{\alpha=1}^{N_\alpha} \frac{|V_\alpha|^2}{i\omega_n - \epsilon_\alpha}$$

• treat with BSS-QMC algorithm [Blankenbecler, Scalapino, Sugar (1981)] (instead of ED)

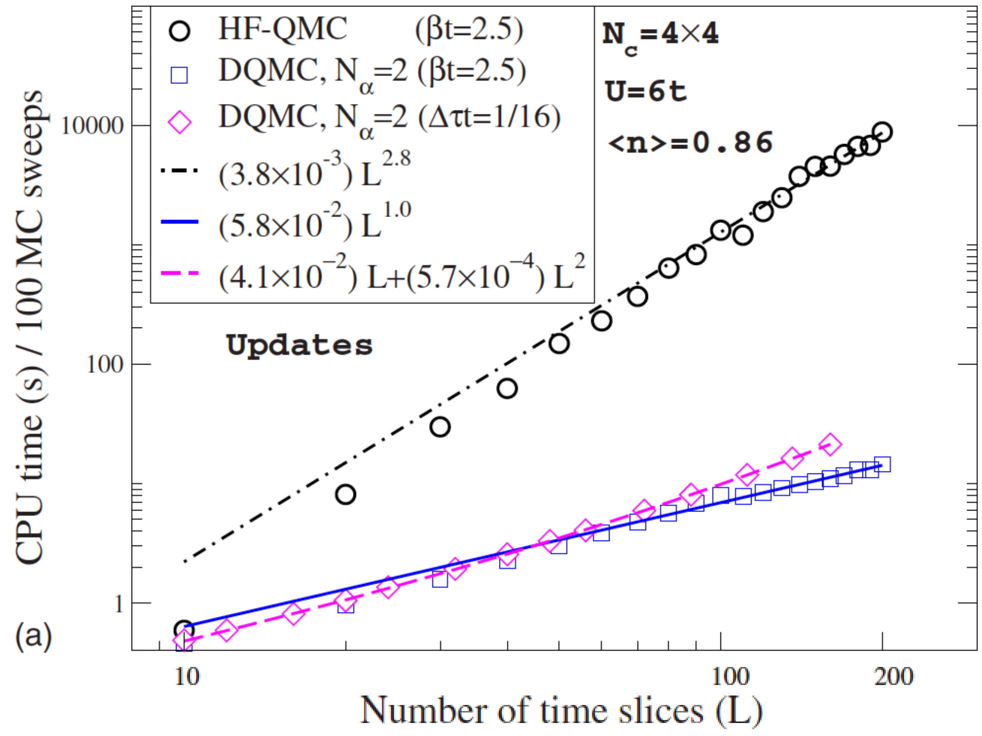



[Khatami, Lee, Bai, Scalettar, and Jarrell, PRE **81**, 056703 (2010)]

Advantage of existing hybrid scheme:
linear (instead of cubic) scaling in $1/T$

Problem: systematic errors from
Trotter and bath discretizations

Proposal: use multigrid approach
or direct continuous-time formulation
⇝ cheap and exact impurity solver



# Numerical challenges

- $10^9$ updates of small matrices: error propagation, cache optimization (QMC)
  Schömer, . . .
- spline interpolation of noisy data, FT, extrapolation (DMFT cycle, multigrid)
  Hanke-Bourgeois
- inverse problems: analytic continuation of spectra (QMC),
  fitting of hybridization function (hybrid)
  Hanke-Bourgeois, Meyer, Althaus, Decker, . . .
- inversion of large sparse matrices (RDMFT)
  Kühne
- massive parallelization using MPI and Open MP
  Schömer, Kühne, . . .
- data storage/organization: typically 100 GB in $10^4$ files per week
  (bio-informatics, meteorology)

# General method development: new initiative DFG-FG 1346

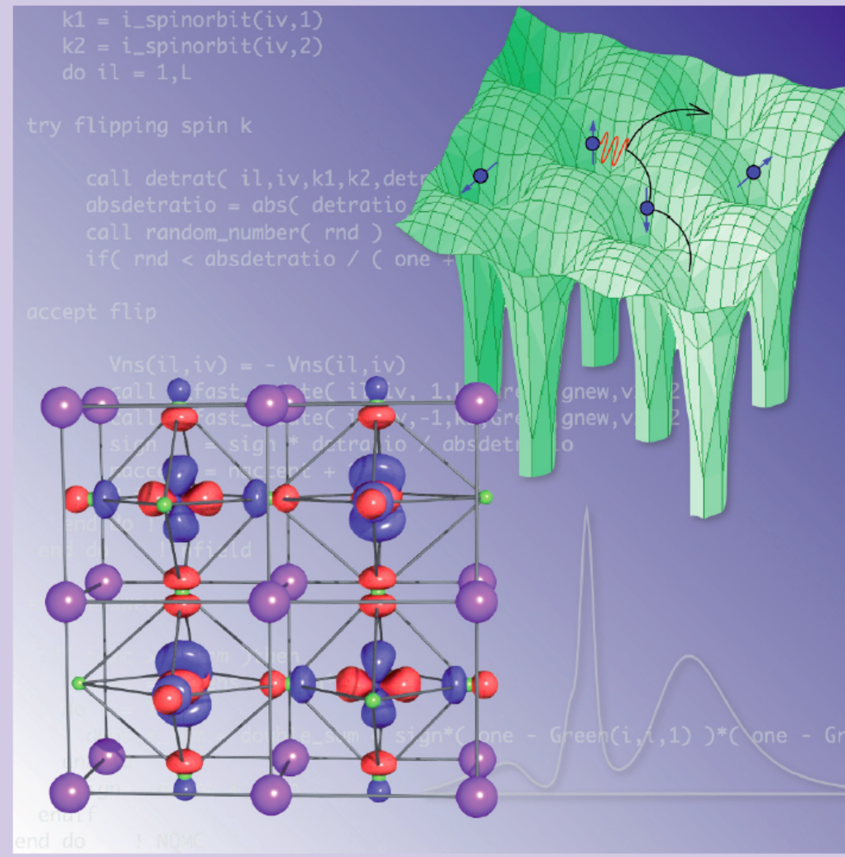
Theory group + 2 experimentalists (PES), started in July 2010

**P8: QMC impurity solvers (F. Assaad, N. Blümer, P. Werner)**

- most efficient QMC impurity solver for important problem classes?
- study impact of neglected interactions
- generalize CT-QMC solvers for frequency-dependent interactions
- eliminate systematic errors in BSS solver (linear in $1/T$) using multigrid approach

No other projects from Mainz

**FOR 1346: Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials**

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