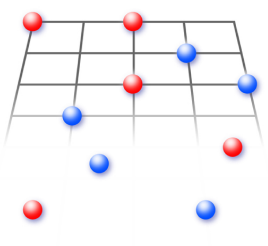
Quantum Monte Carlo simulations of ultracold fermions on optical lattices within dynamical mean-field theory

Nils Blümer and Elena Gorelik

Gutenberg University Mainz, Germany



Transregional Collaborative Research Centre SFB / TRR 49

Condensed matter systems with variable many-body interactions

Frankfurt / Kaiserslautern / Mainz

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Outline

Introduction: SCES, cold atoms on lattices

Approaches for correlated lattice Fermi systems, multigrid HF-QMC

Paramagnetic Mott transitions in 3-flavor mixtures

[E. V. Gorelik and N. Blümer, Phys. Rev. A **80**, 051602(R) (2009)]

Néel transition of lattice fermions in a harmonic trap (RDMFT)

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

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Effect of nonlocal correlations? Comparisons with direct QMC

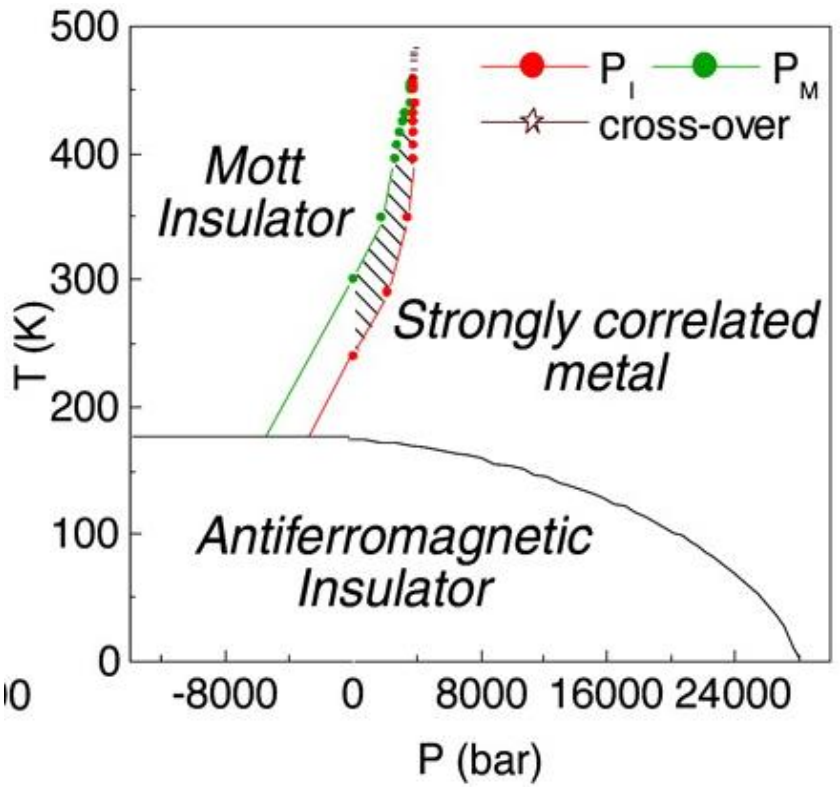
[ongoing collaboration with T. Paiva and R. Scalettar]

Summary and outlook

Introduction: Systems with strong electronic/fermionic correlations

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

Phase diagram



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

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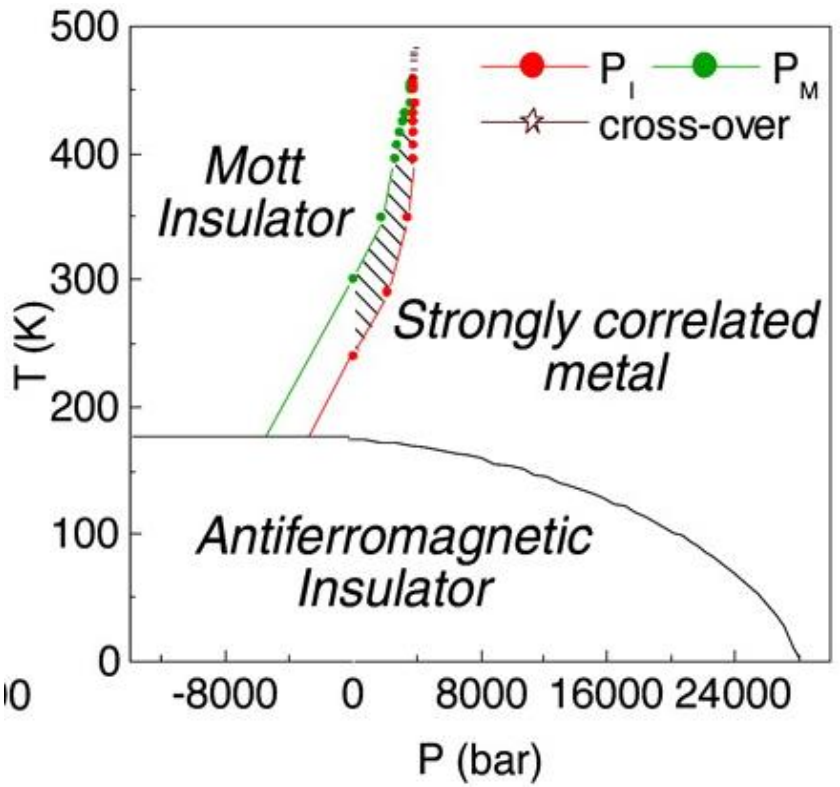

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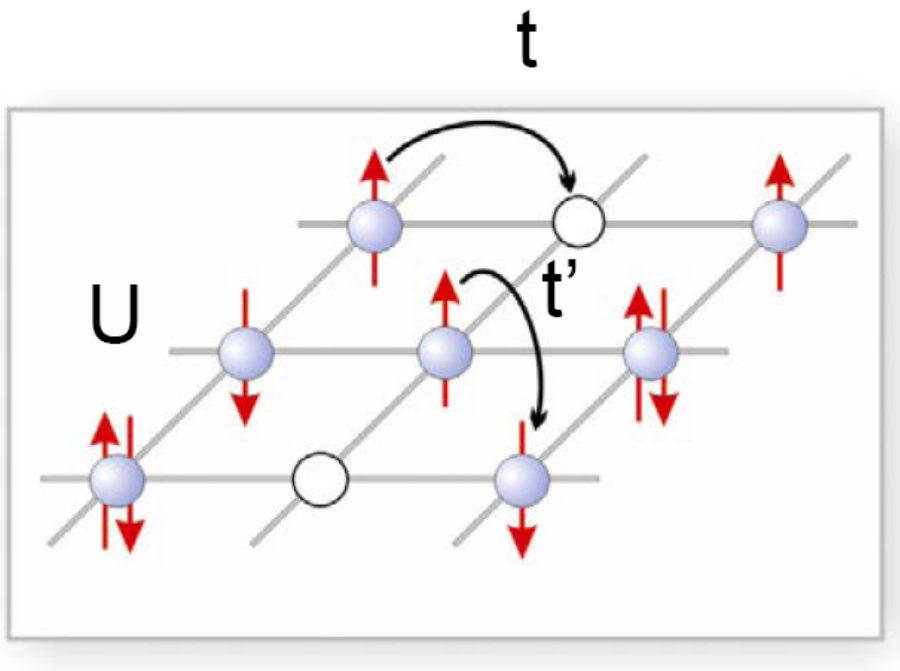

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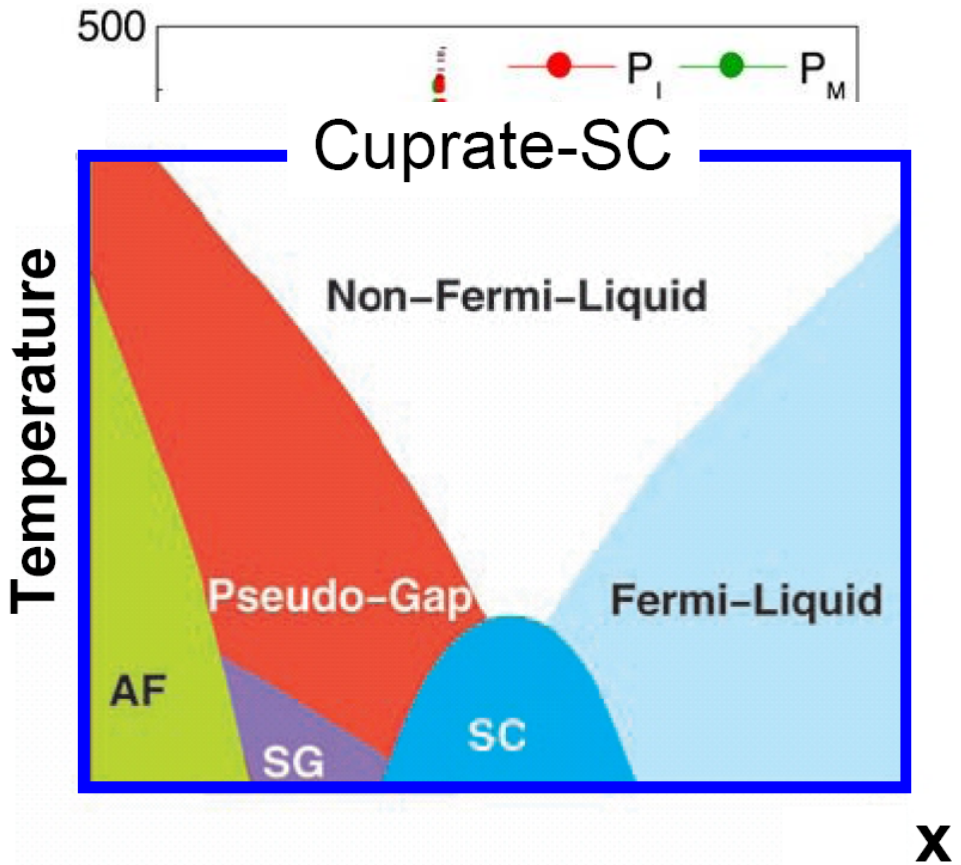
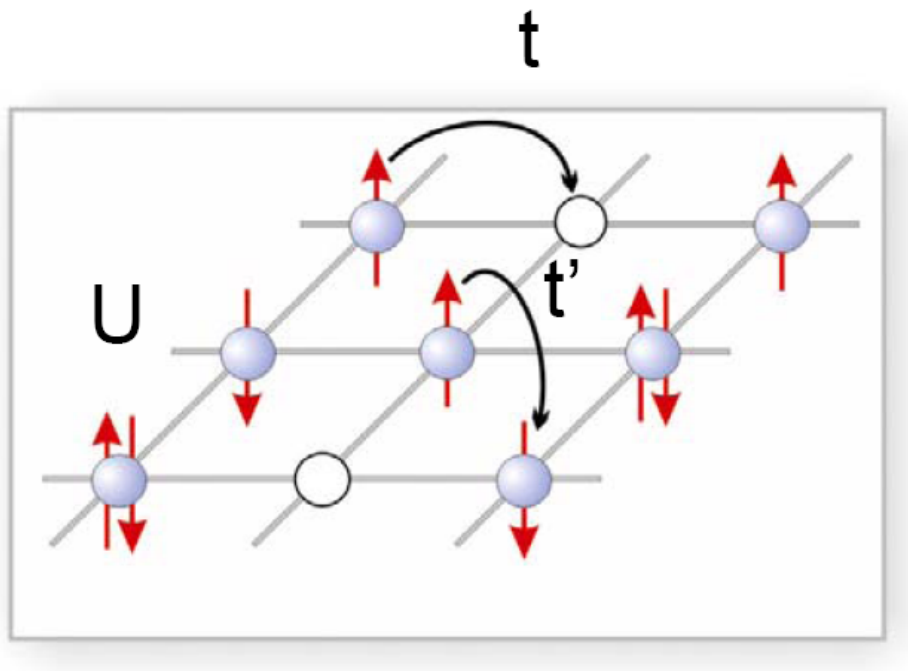


Mott metal-insulator transition and AF: generic physics of 1-band Hubbard model



Are AF and Mott phases essential for superconductivity?

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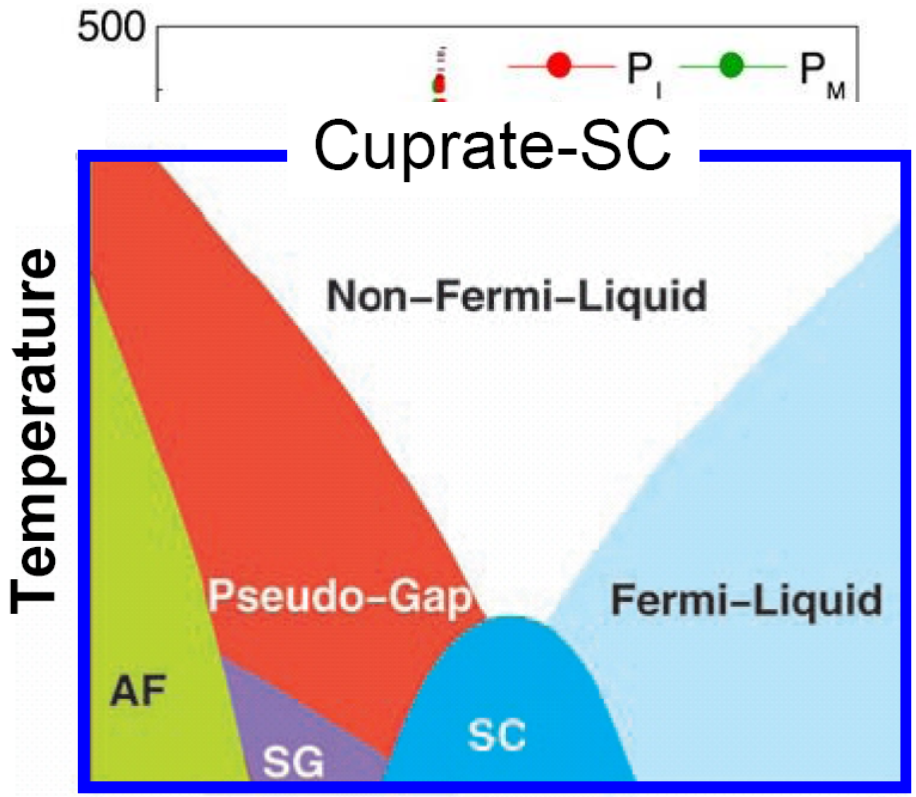

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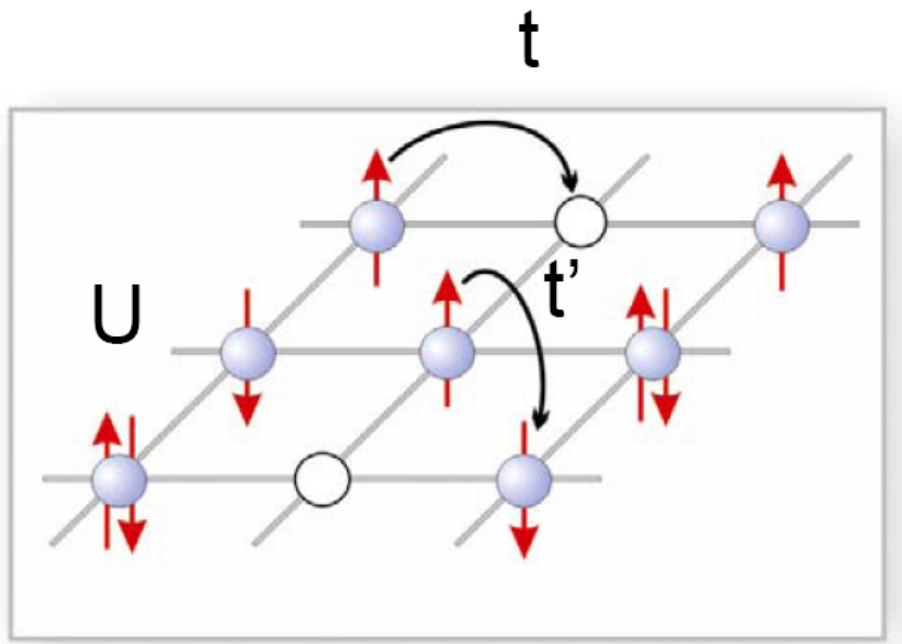


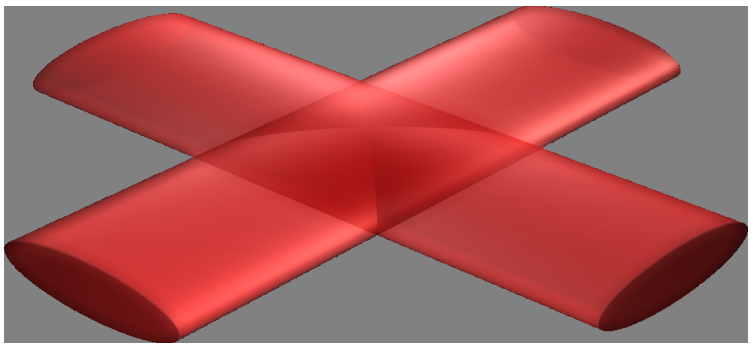
Are AF and Mott phases essential for superconductivity?

Claim: cold atoms $\rightsquigarrow$ quantum simulators

Correlated ultracold quantum gases on optical lattices: basics

Experimental systems: small dilute clouds of about 10^6 ultracold atoms $\rightsquigarrow$ need trap

Optical dipole trap (2 beams)



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time-averaged
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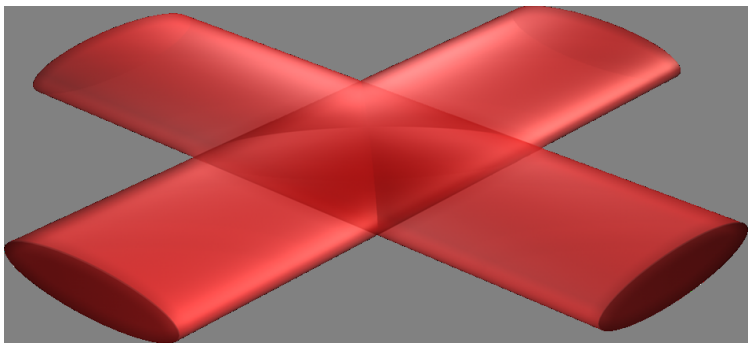

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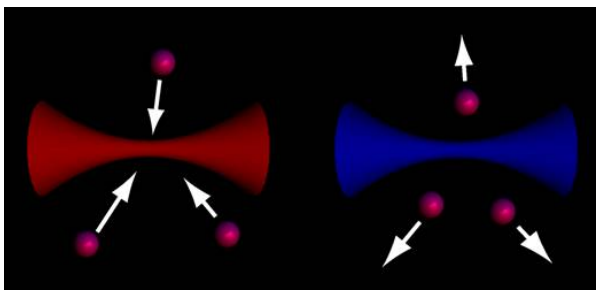
polarizability $\alpha(\omega_{\text{L}})$ changes sign at ω_0



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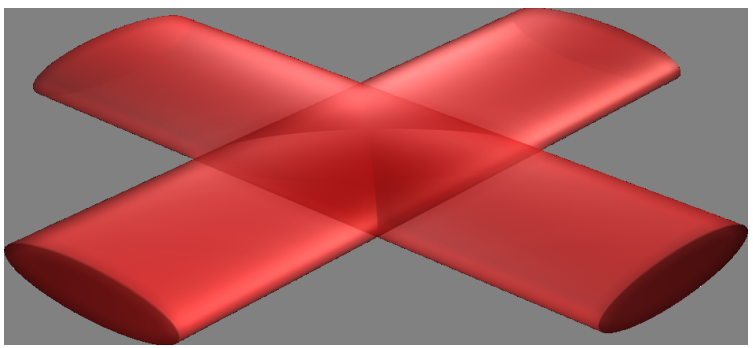

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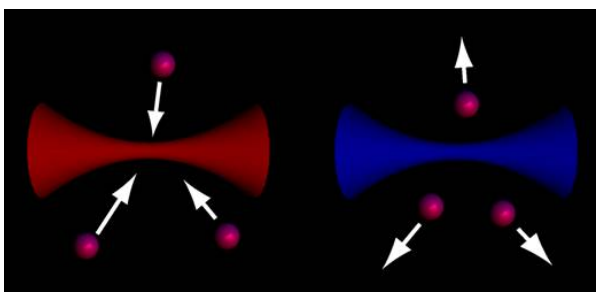
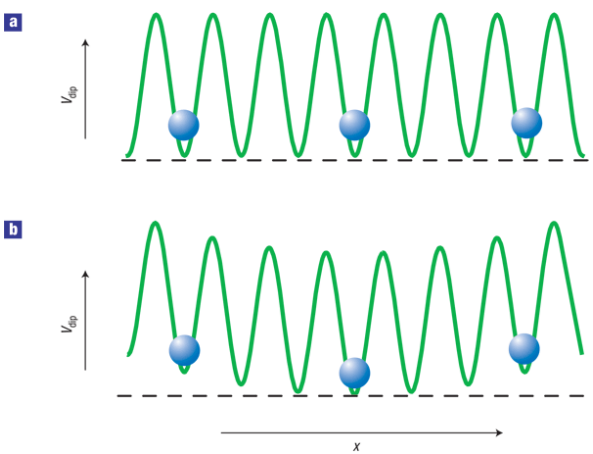


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



Beam profile: (anti) trapping

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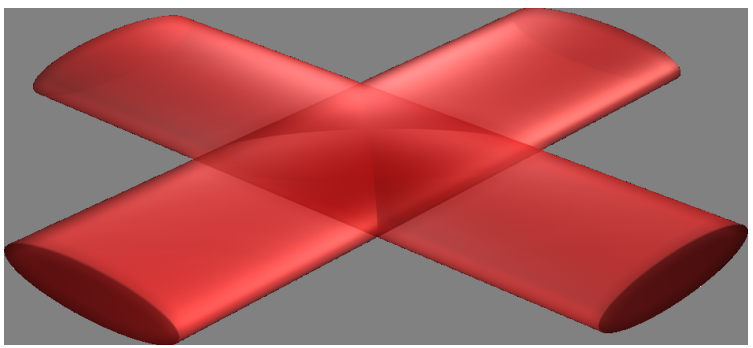

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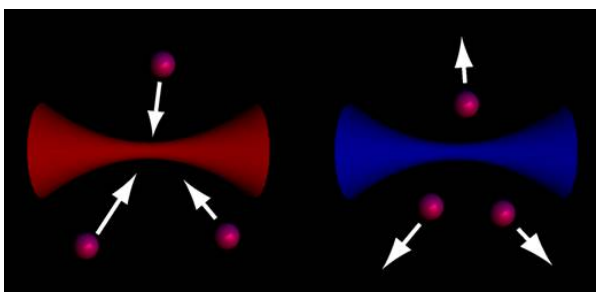

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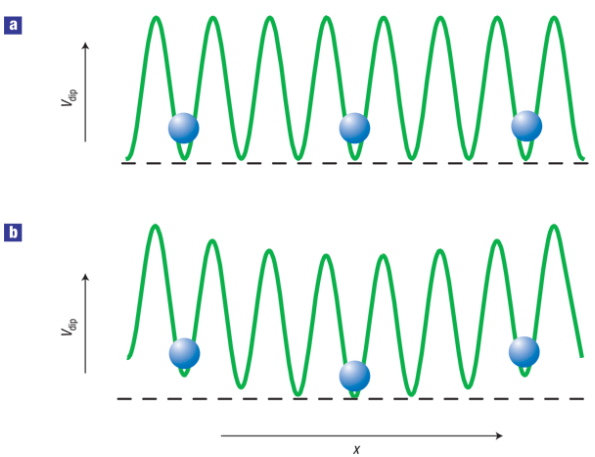


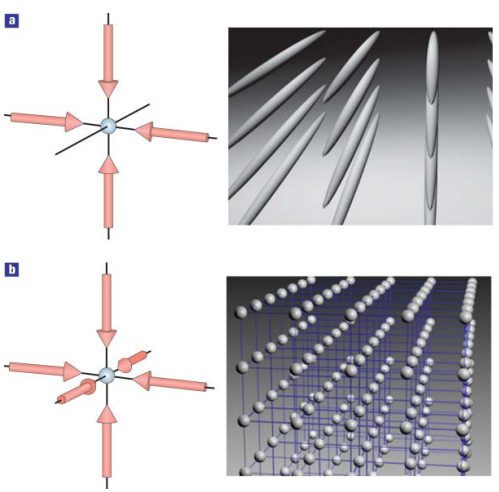
Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

2 pairs of lasers $\rightsquigarrow$ tubes

3 pairs of lasers $\rightsquigarrow$ 3D lattice

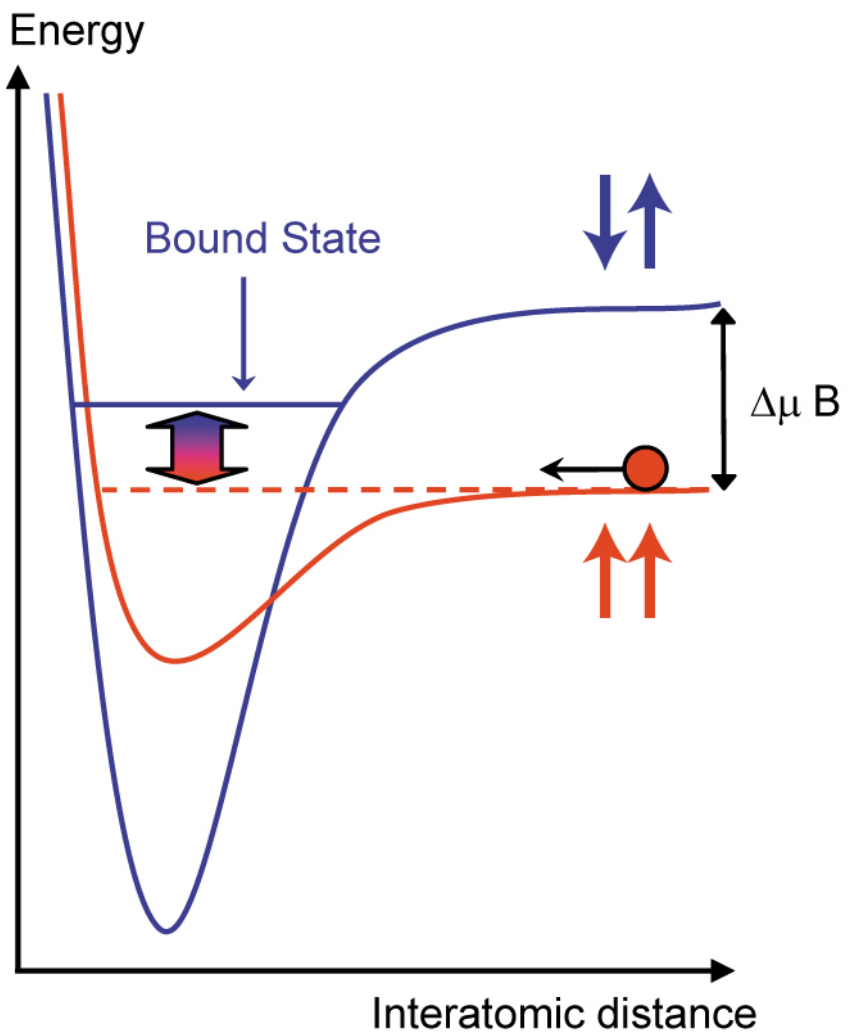
hopping t tunable by laser

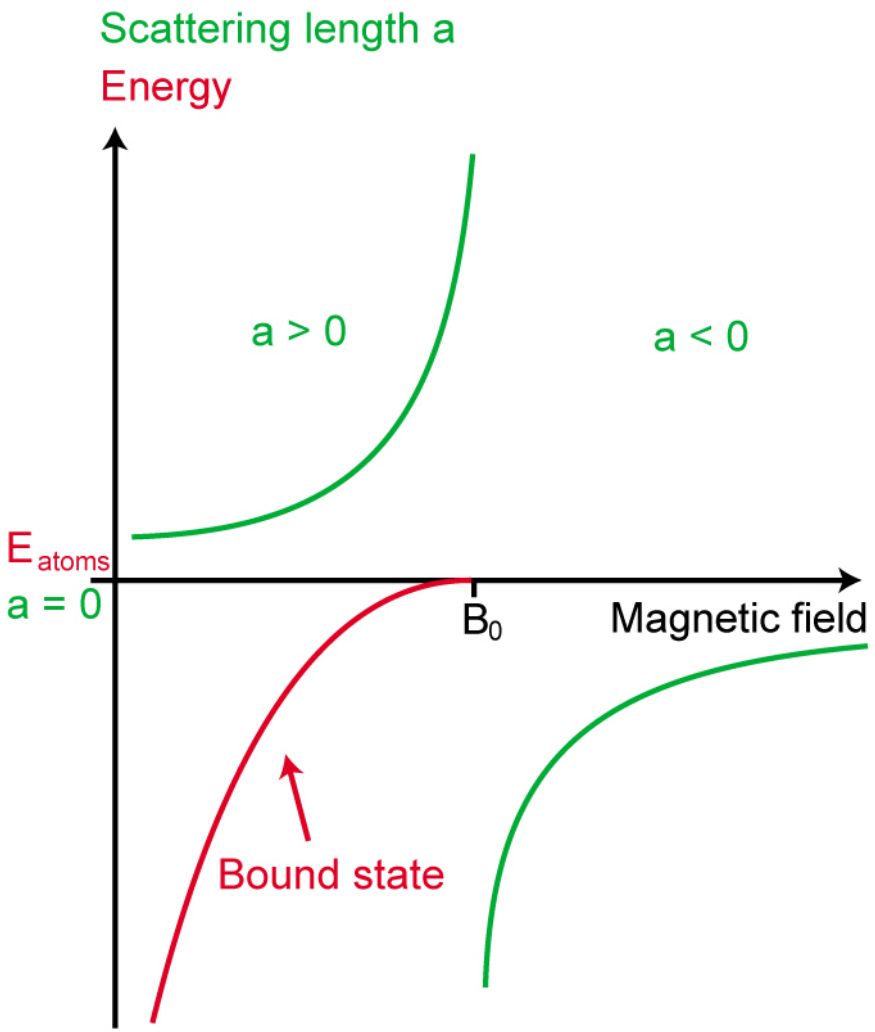


Interactions can be tuned via Feshbach resonances

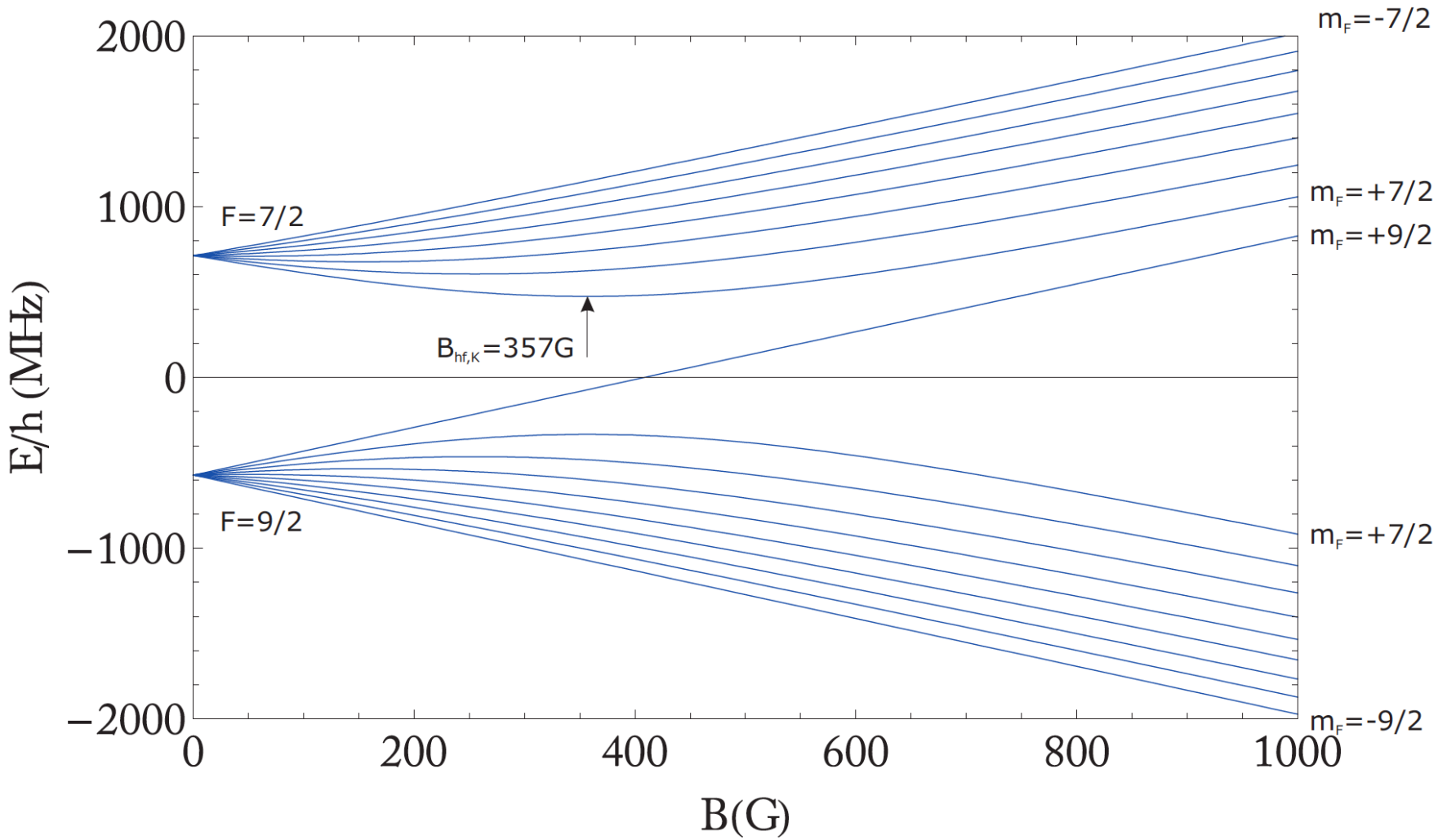
Interactions can be tuned via Feshbach resonances (here in magnetic field $\boldsymbol{B}$)

short ranged: characterized by scattering length a – both signs possible!





Large multiplets: reservoir of "flavors"



Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

[Tiecke, unpublished]

Main measurement technique: column density distribution, TOF

Send resonant parallel light through atomic cloud, detect by CCD

$\rightsquigarrow$ shadows $\propto$ column density (integrated over line of sight)

Use flavor sensitivity $\rightsquigarrow$ partial densities, "magnetization" profiles

In situ atomic (site) resolution only for 2-dimensional lattice systems:

large-aperture lens [Kuhr, Greiner], electron microscopy [Ott]

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switch off trap (and strong interactions), let atoms fall freely

assume $\hbar \boldsymbol{k}_i = m \boldsymbol{v}_i(0) \quad ; \quad \boldsymbol{r}_i(t) = \boldsymbol{r}_i(0) + \boldsymbol{v}_i(0) t - \frac{1}{2} g \hat{\boldsymbol{e}}_z t^2$

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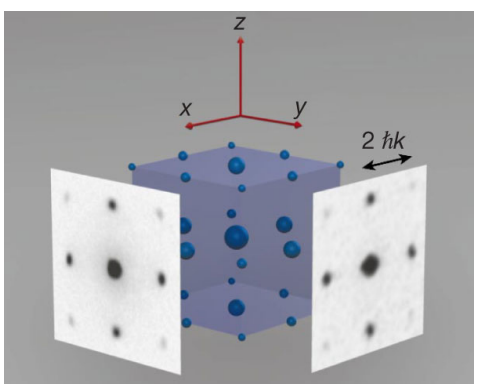
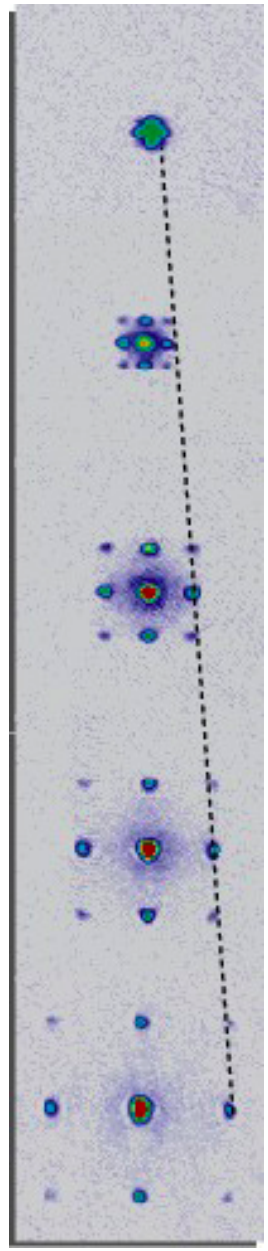
$\rightsquigarrow (\boldsymbol{r}_i(T) + \frac{1}{2} g \hat{\boldsymbol{e}}_z T^2) \frac{m}{\hbar T} \approx \boldsymbol{k}_i \quad$ for $T \sqrt{\langle \boldsymbol{v}^2 \rangle} \gg \sqrt{\langle r^2 \rangle}$

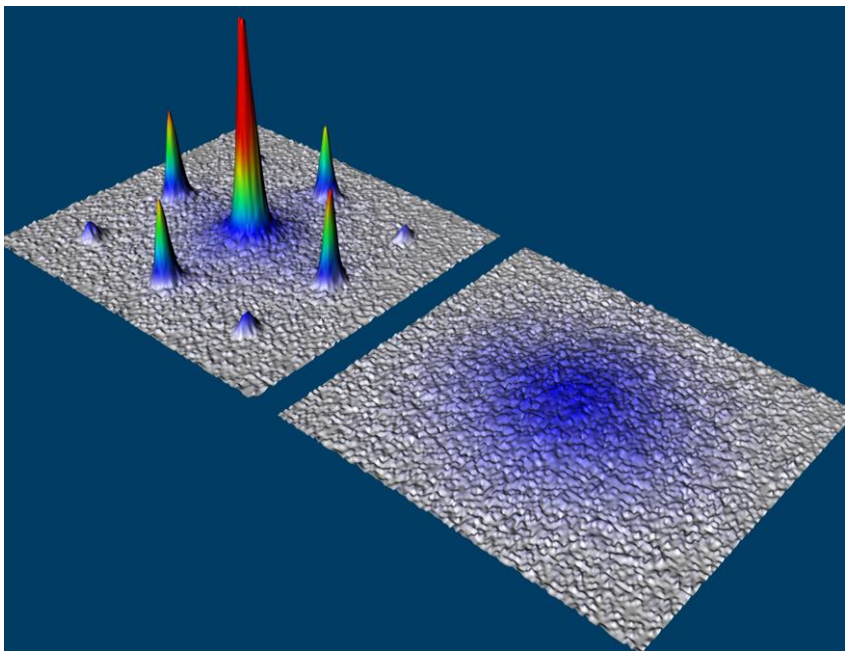




Correlated ultracold quantum gases on optical lattices: bosons

First evidence of strongly correlations in cold atoms: bosonic Mott transition

Time-of-flight image – $\boldsymbol{k}$ distribution



[Bloch group, 2002]

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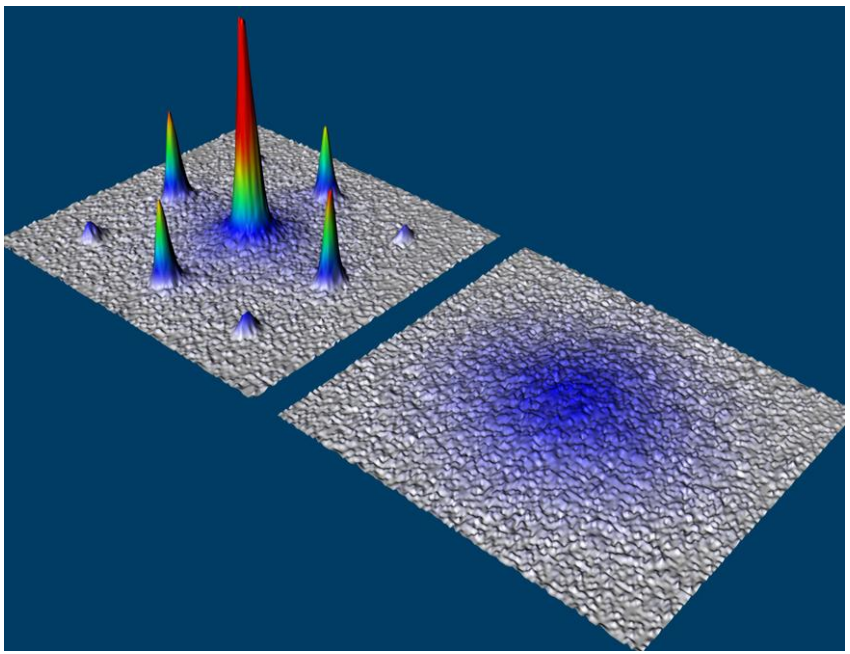
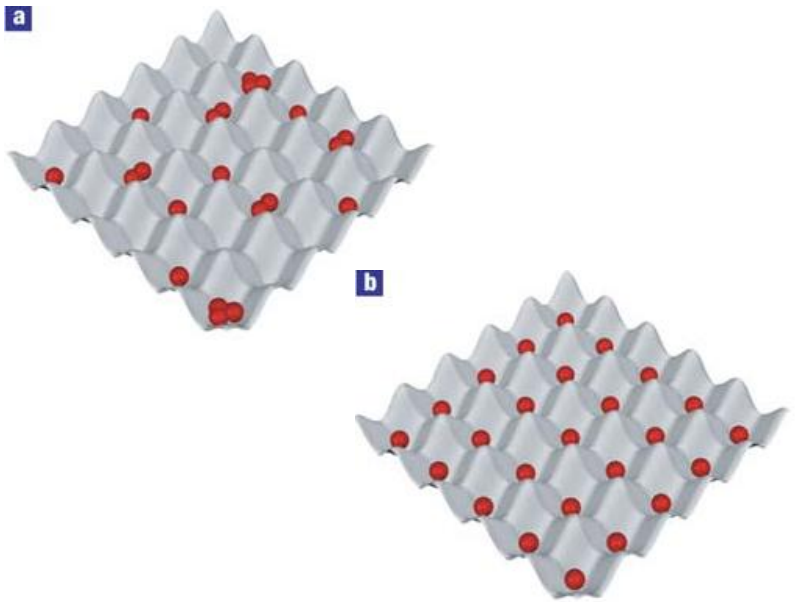


corresponding real-space picture



[Bloch group, 2002]

Superfluidity destroyed by density constraint at large U

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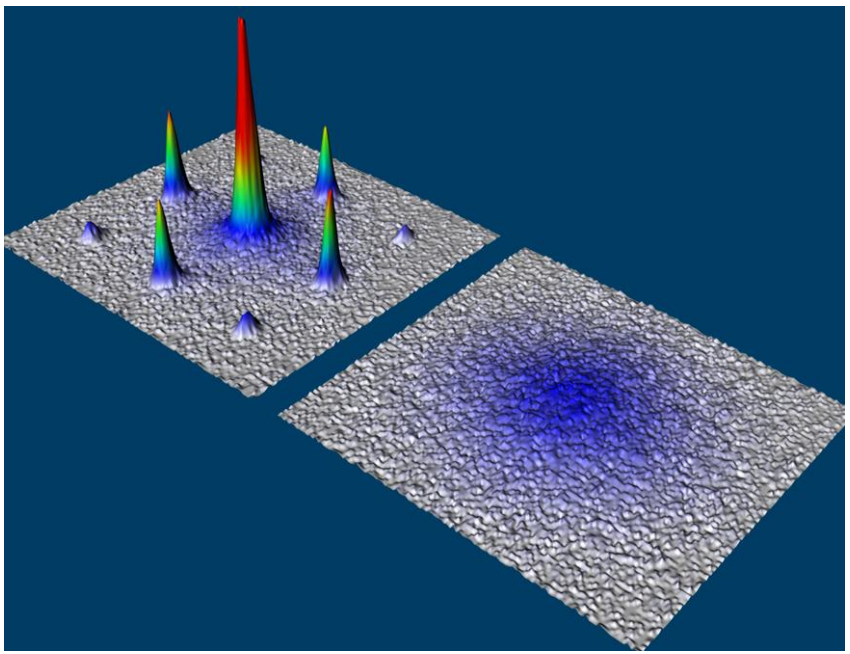

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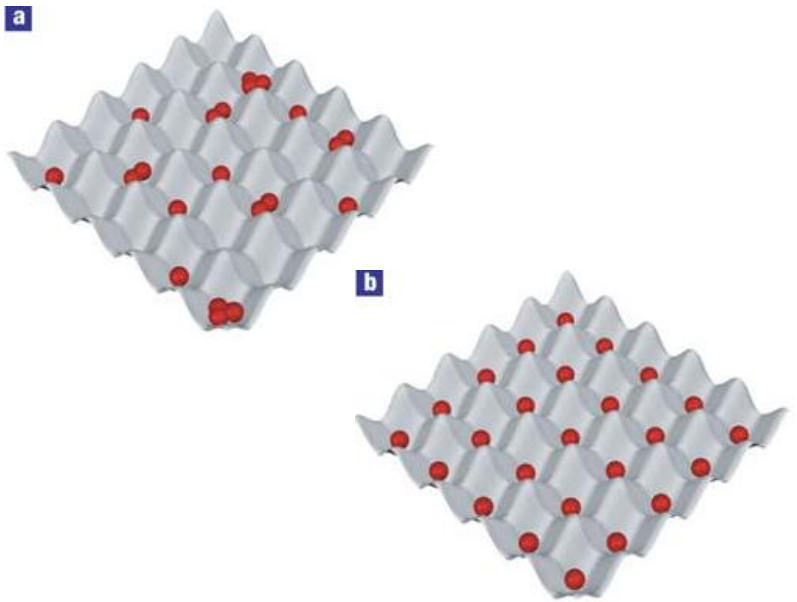
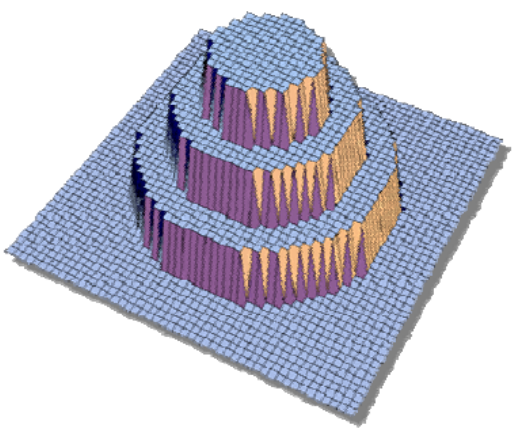
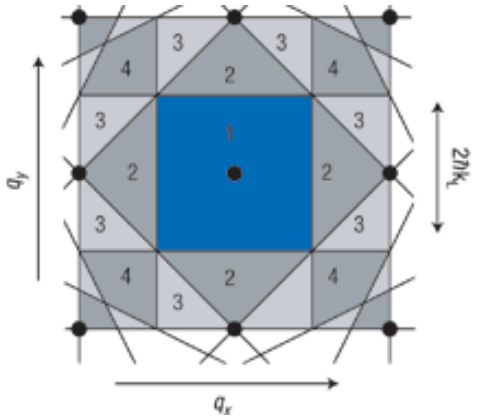


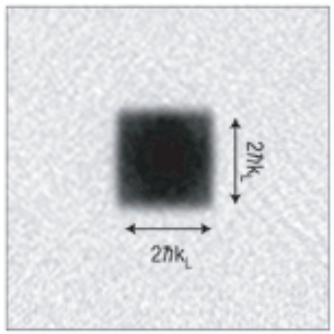


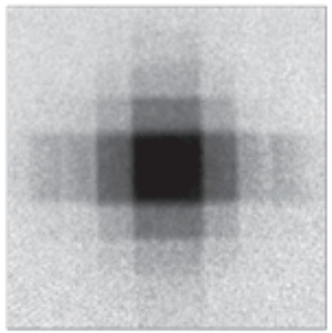
Superfluidity destroyed by density constraint at large U

Trapping potential $\rightsquigarrow$ wedding cake structure

Correlated ultracold quantum gases on optical lattices: fermions







1 species: band insulator for filled 1^{st} Brillouin zone:

[Köhl et al, PRL (2005)]

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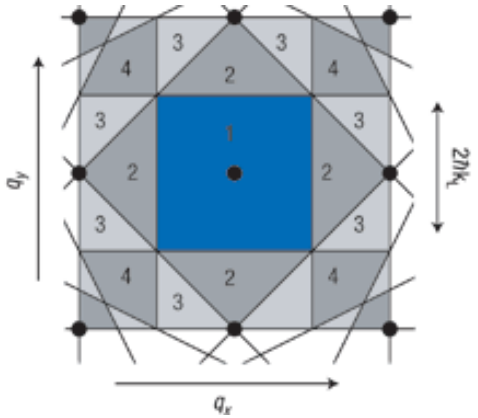

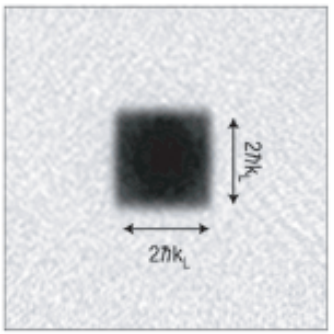

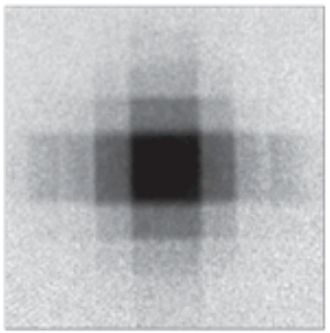

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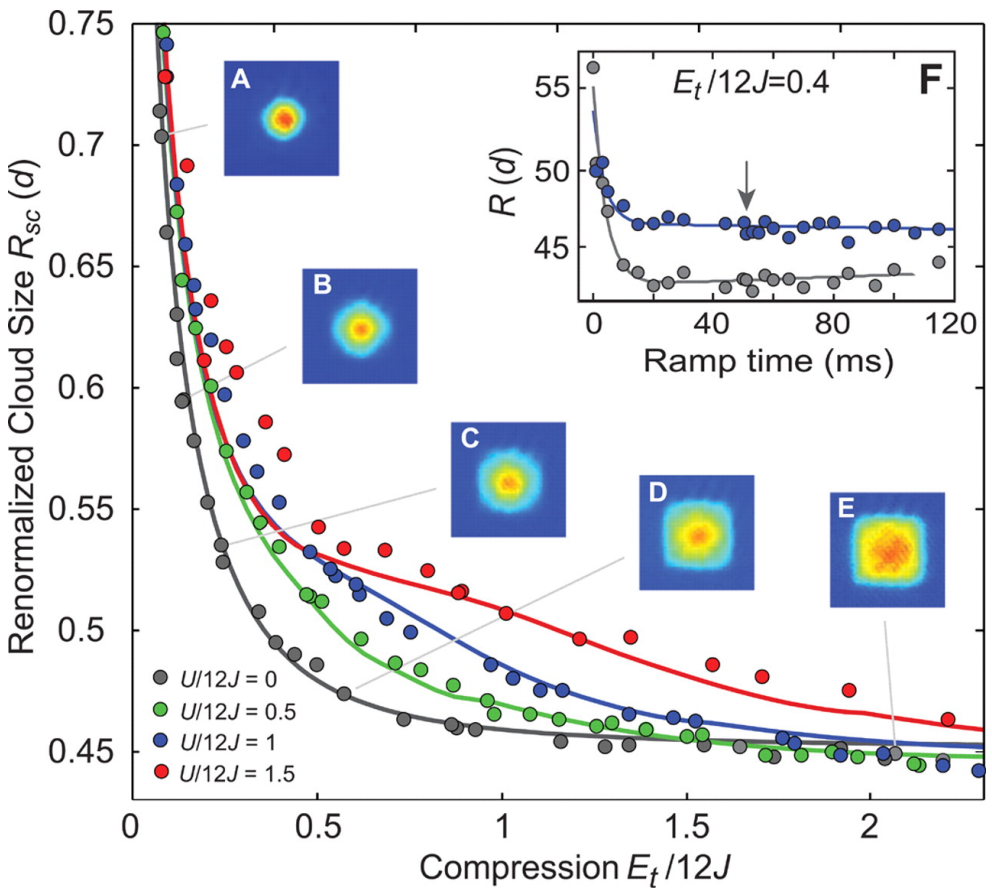
[Köhl et al, PRL (2005)]

Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

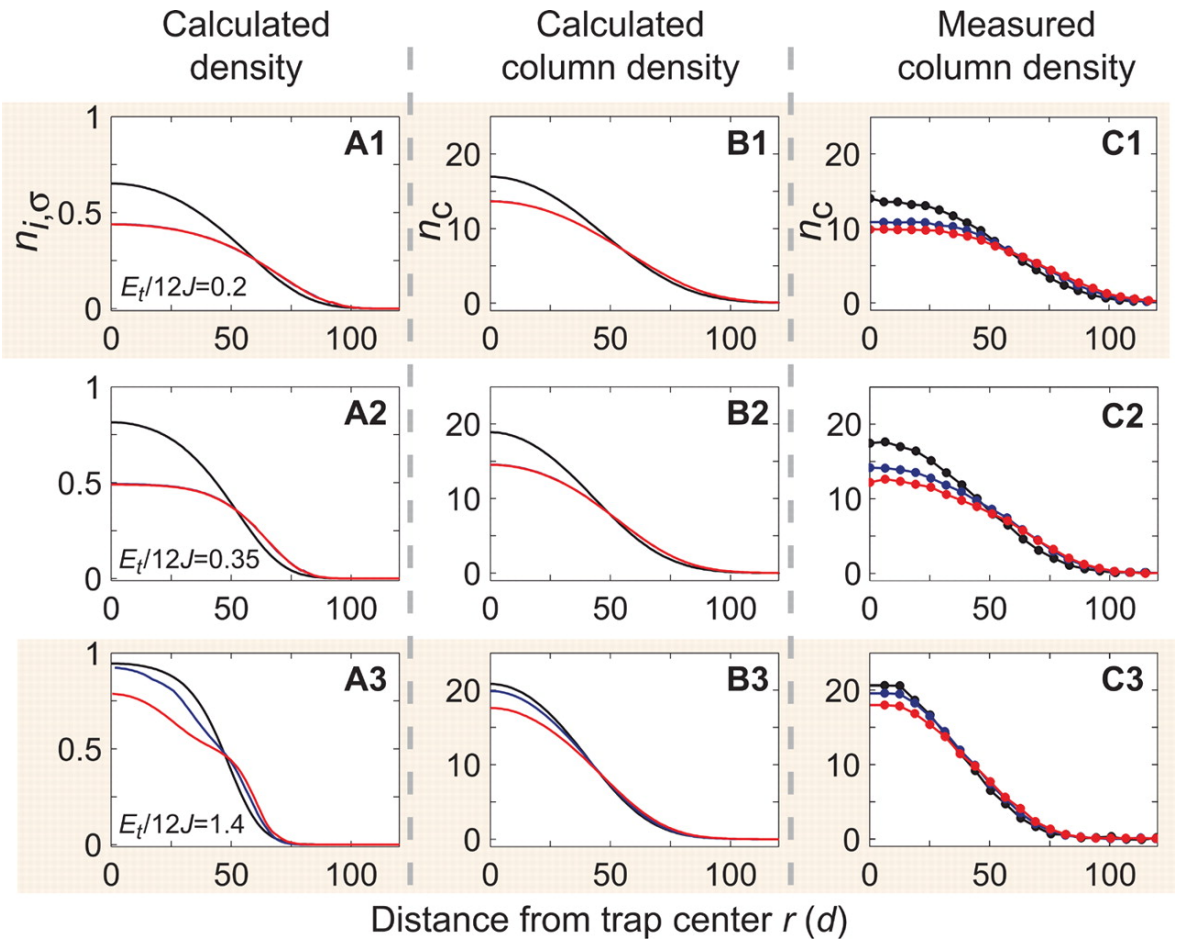
Detection method: measure cloud diameter vs. trap strength

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

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



Further MIT observables: column density, fraction of atoms with double occupations



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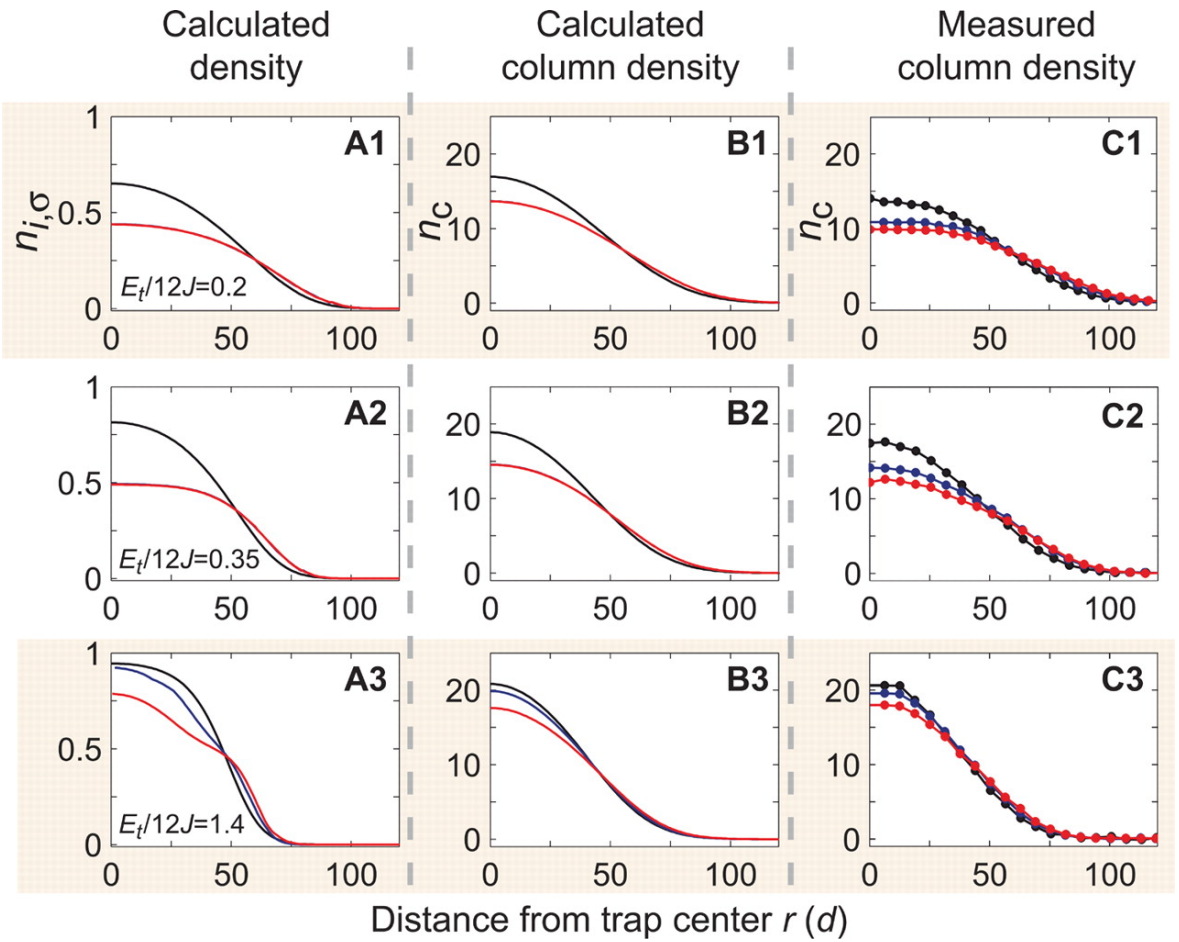

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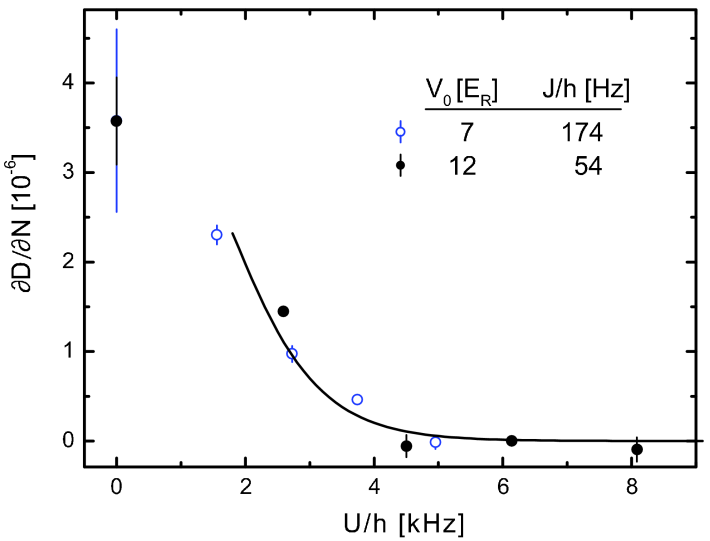

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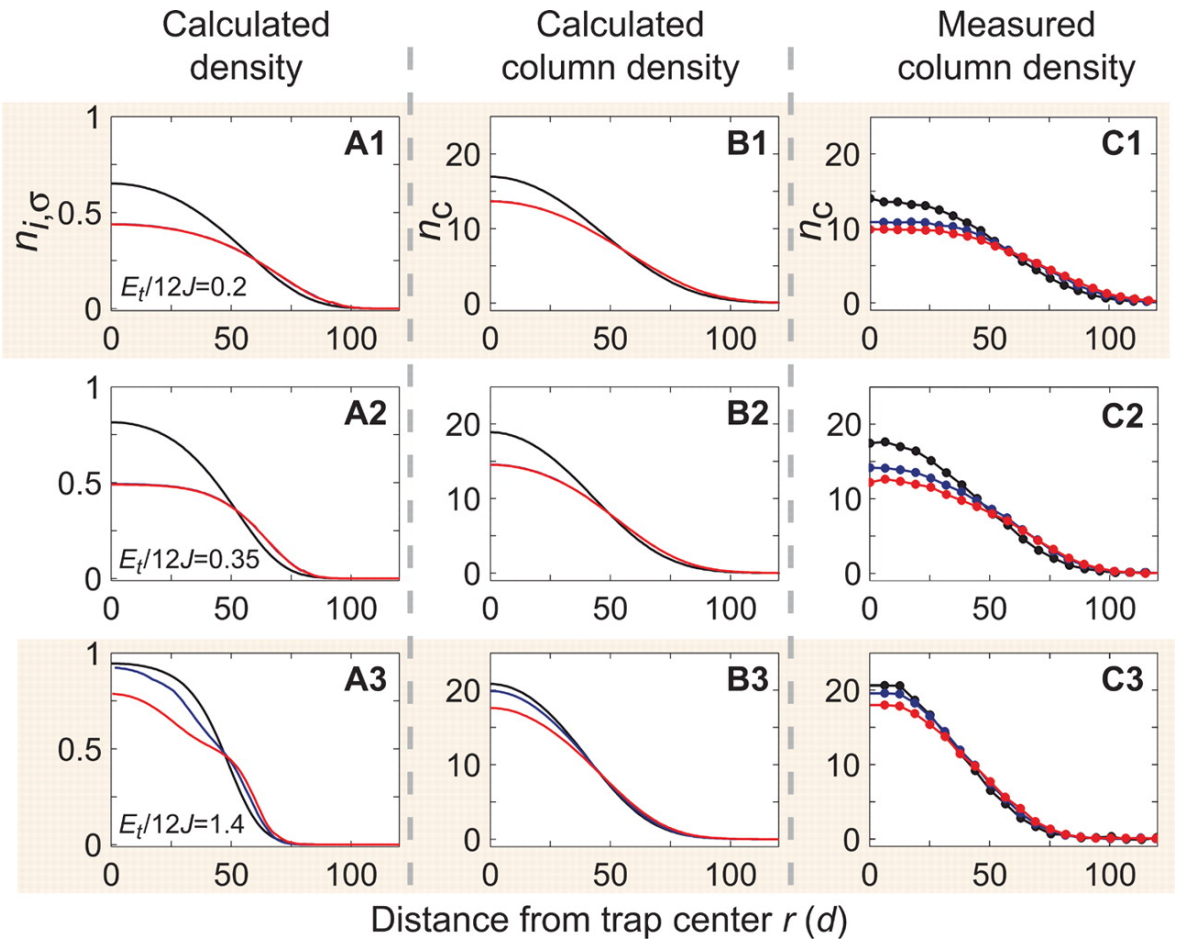
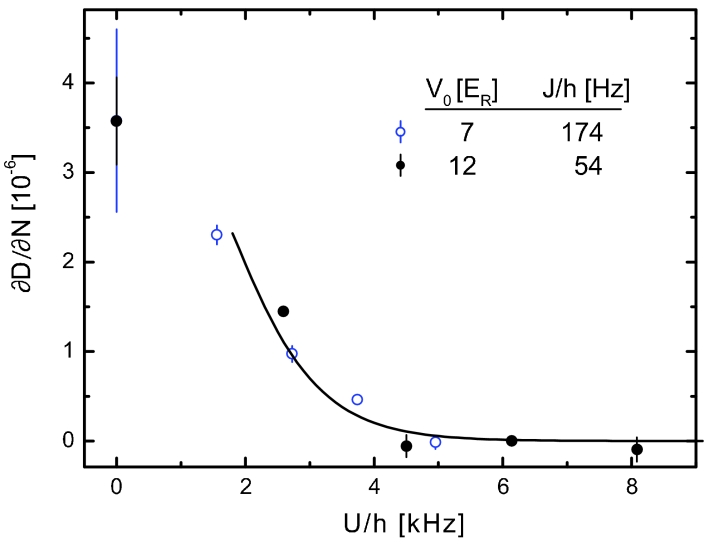


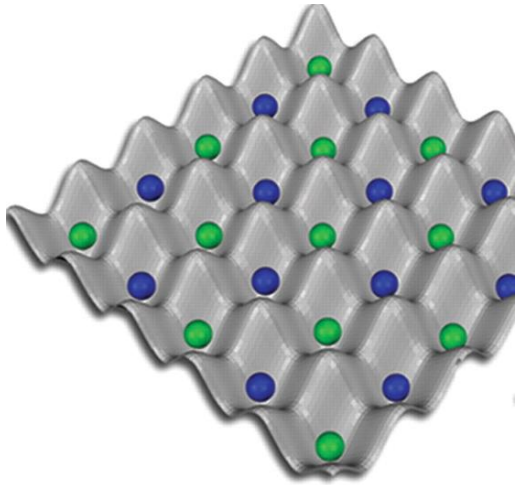
[Schneider et al, Science **322**, 1520 (2008)]



[Jördens et al., Nature (2008)]

Many other phenomena seen: superconductivity, vortices, BEC-BCS crossover, . . .

Next grand challenges:



Antiferromagnetism (staggered order) in ultracold fermions

Problems:

(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of order parameter is not straightforward

Realization of quantum magnetism: prerequisite for quantum simulation!

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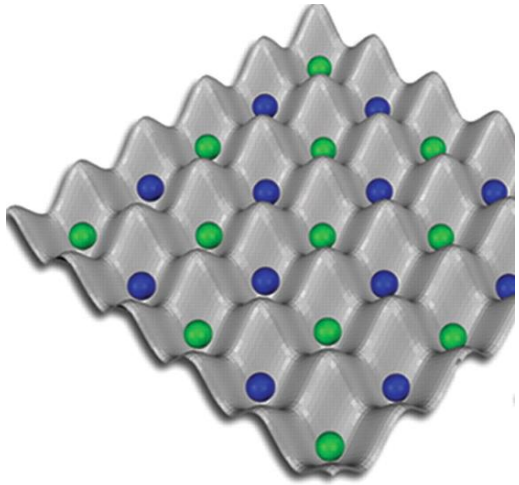

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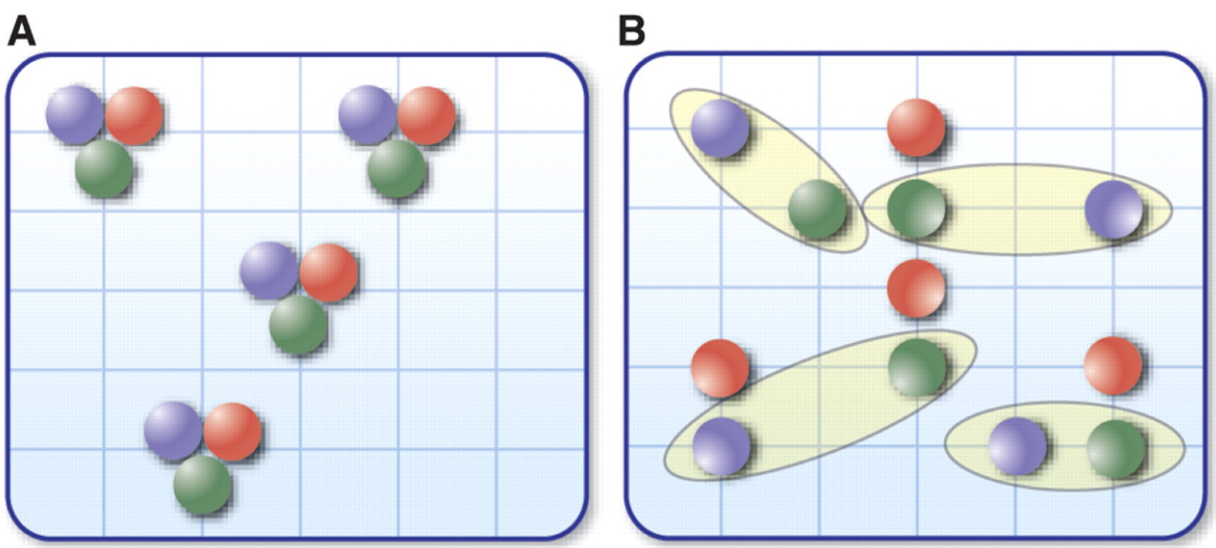
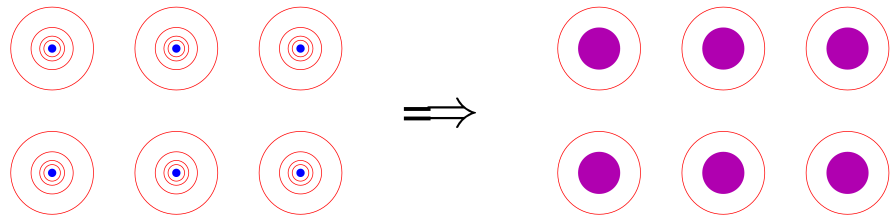
Multiflavor phenomena, e.g. trions versus color superconductivity



Approaches for correlated lattice Fermi systems

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_i V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

reduction to valence electrons



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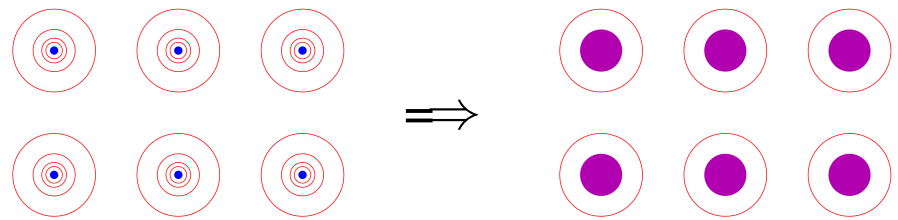

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occupation number formalism | Wannier orbitals

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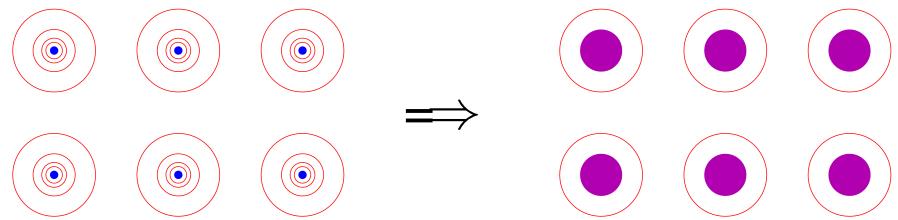

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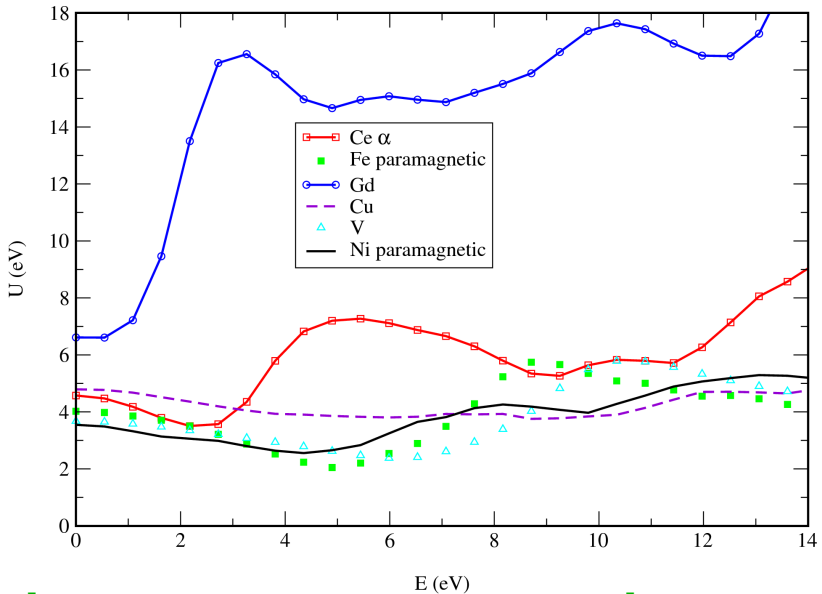
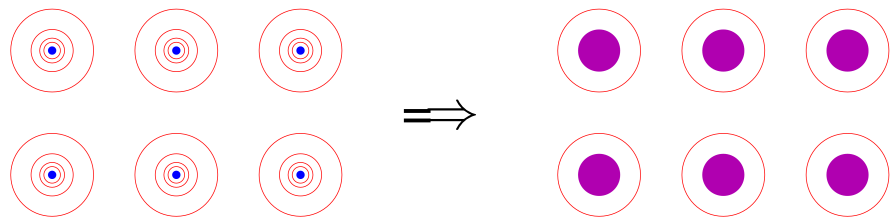
elated lattice Fermi systems



[Aryasetiawan et al., PRB 2006]

$$+ \sum_i V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

trons ↓



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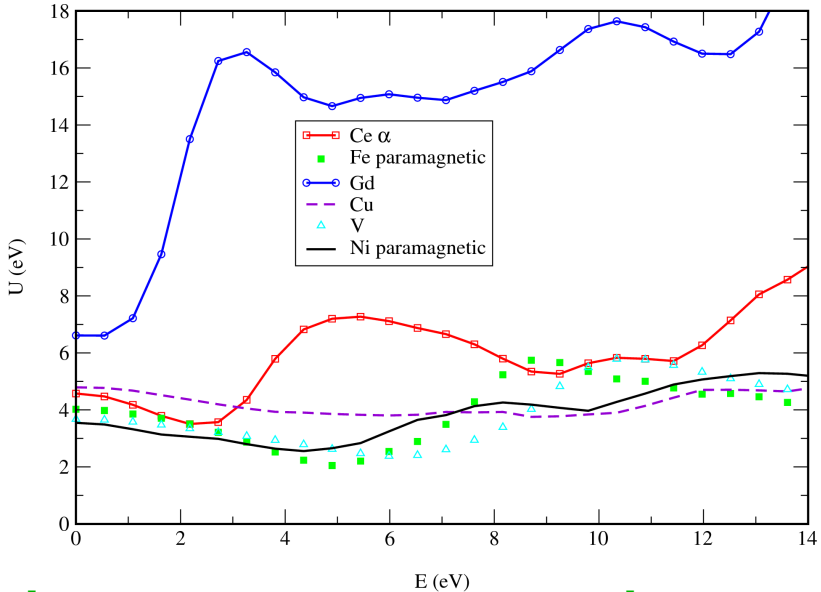

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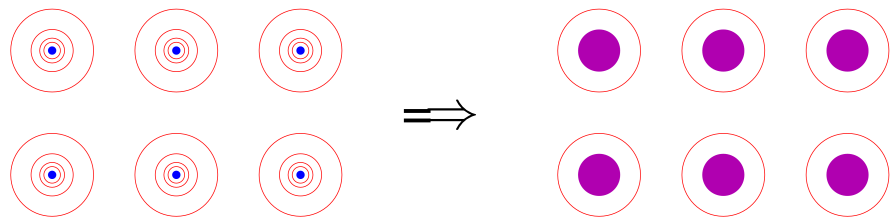

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Note: no core states in quantum gas case!

Approaches for Hubbard-type models

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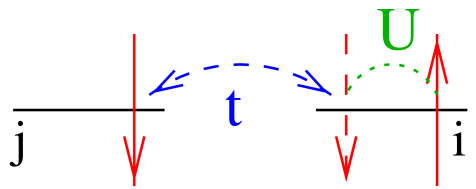
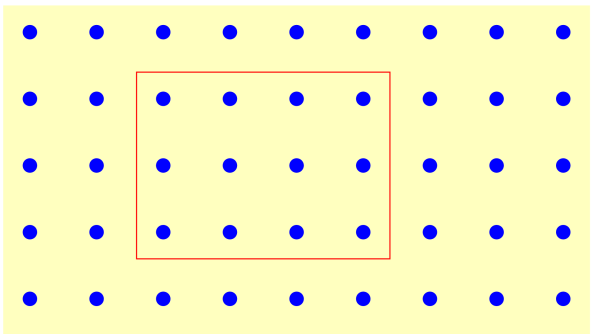


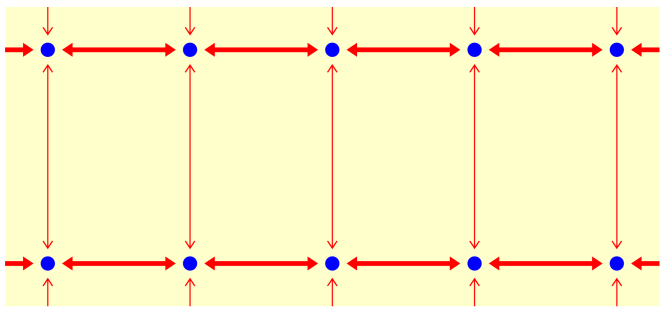
Perturbation theory

- $U \to 0$: Hartree-Fock
  2^{nd} order PT, . . .
- $t/U \to 0$ (for $n = 1$)
  $\rightsquigarrow$ Heisenberg model

finite clusters: ED, QMC



$d \to 1$: Bethe ansatz, DMRG



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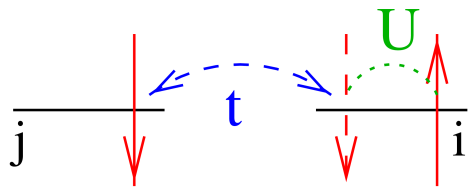

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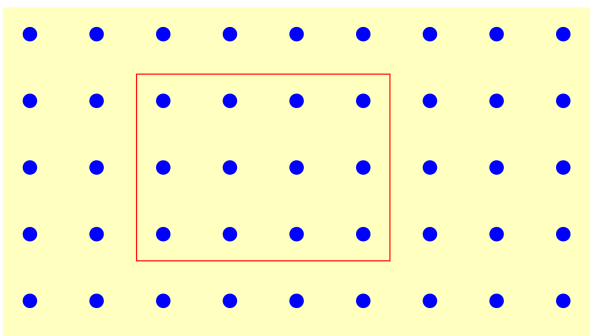

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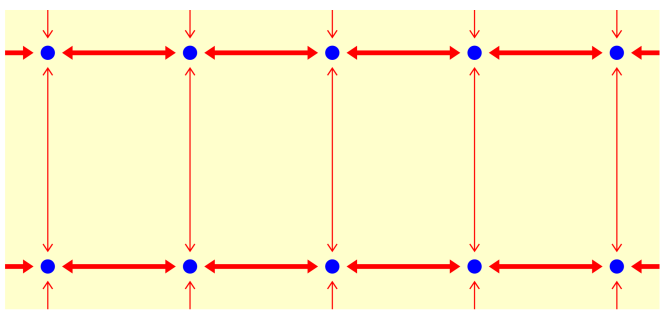


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

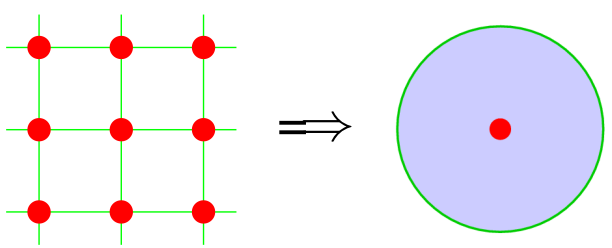
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

\+ non-perturbative $\rightsquigarrow$ valid at MIT

\+ dynamical on-site correlations preserved

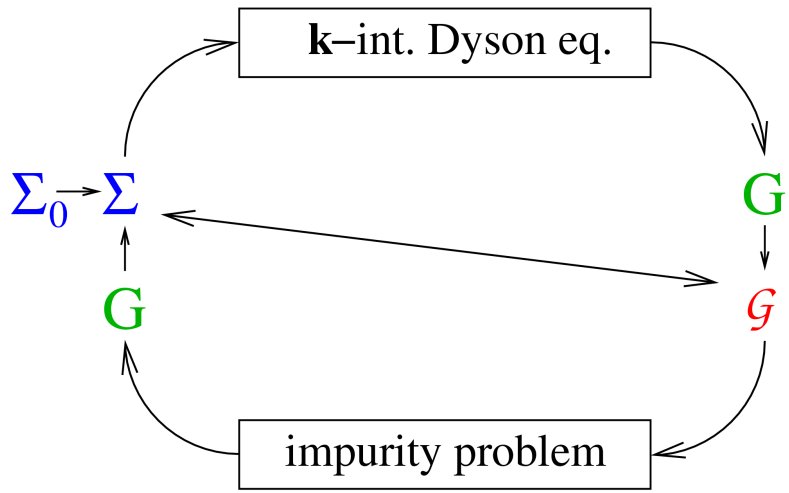
\+ in thermodynamic limit

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



Iterative solution of DMFT equations

0. Initialize self-energy
1. Solve Dyson equation
2. Solve single impurity Anderson model (SIAM)



$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu \boldsymbol{k}}$

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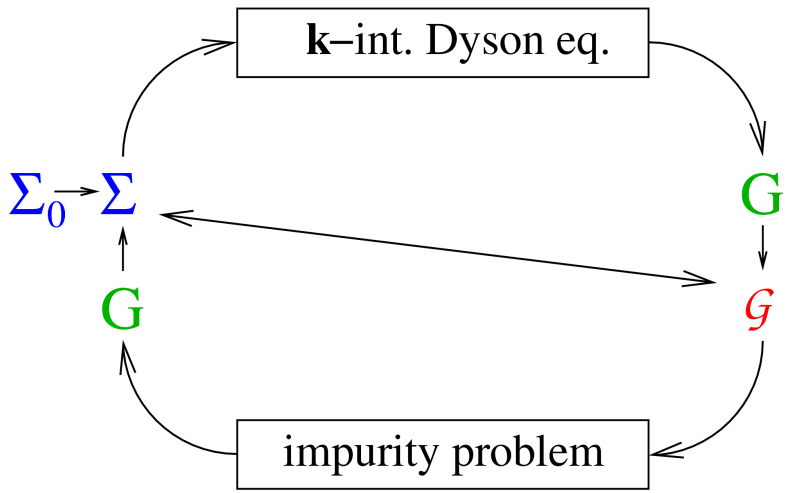
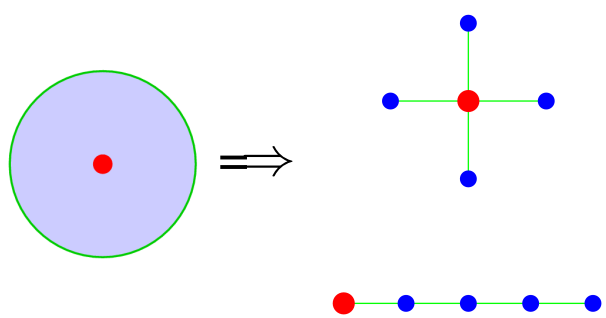


⟵ DOS / t_{ij} / $\varepsilon_{\nu \boldsymbol{k}}$

⟵ local interactions

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

Green function G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

$$G_\sigma(\tau_2 - \tau_1) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\, \mathcal{D}[\psi^*]\ \psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\ \exp\Big[\mathcal{A}_0 - U \sum_{\sigma\sigma'} \int_0^\beta d\tau\, \psi^*_\sigma \psi_\sigma \psi^*_{\sigma'} \psi_{\sigma'}\Big]$$

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(ii) Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} \approx \left[e^{-\Delta\tau \hat{T}} e^{-\Delta\tau \hat{V}}\right]^\Lambda$

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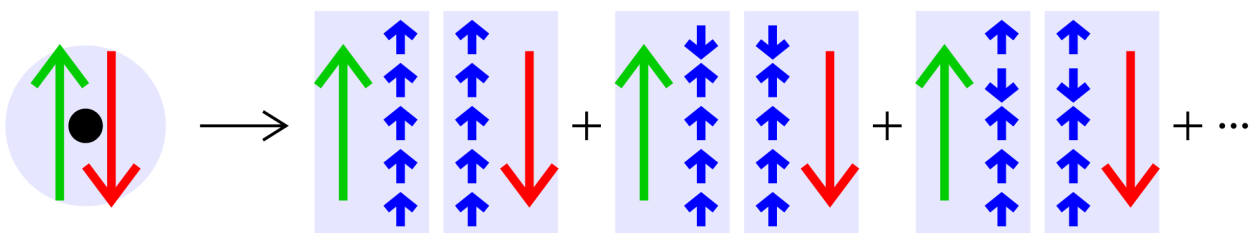
(iii) Hubbard-Stratonovich transformation



Wick theorem:

$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

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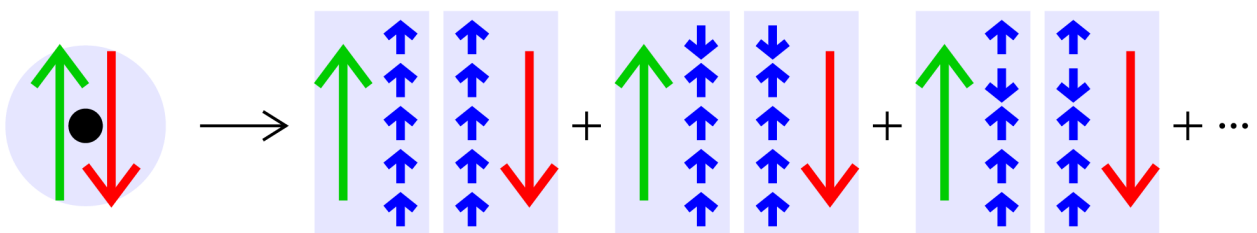

Wick theorem:

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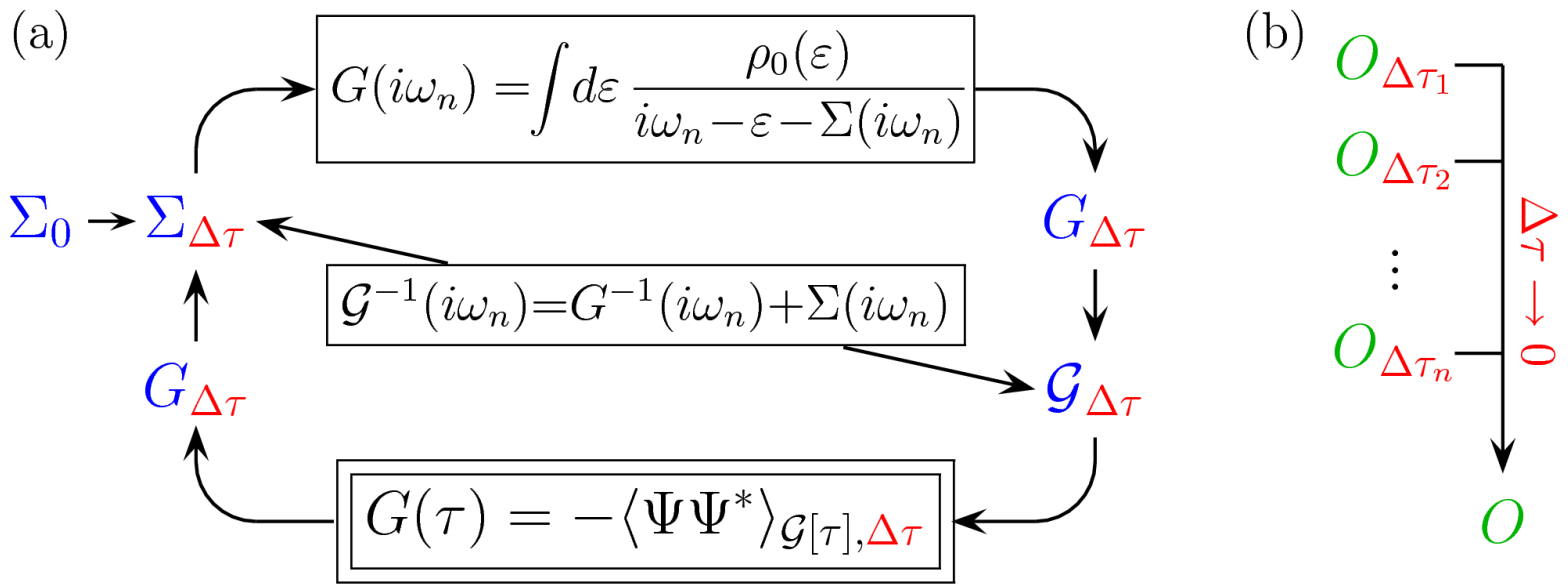
(iv) MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

\+ numerically exact, + no sign problem, (density-type interactions) − effort scales as T^{-3}

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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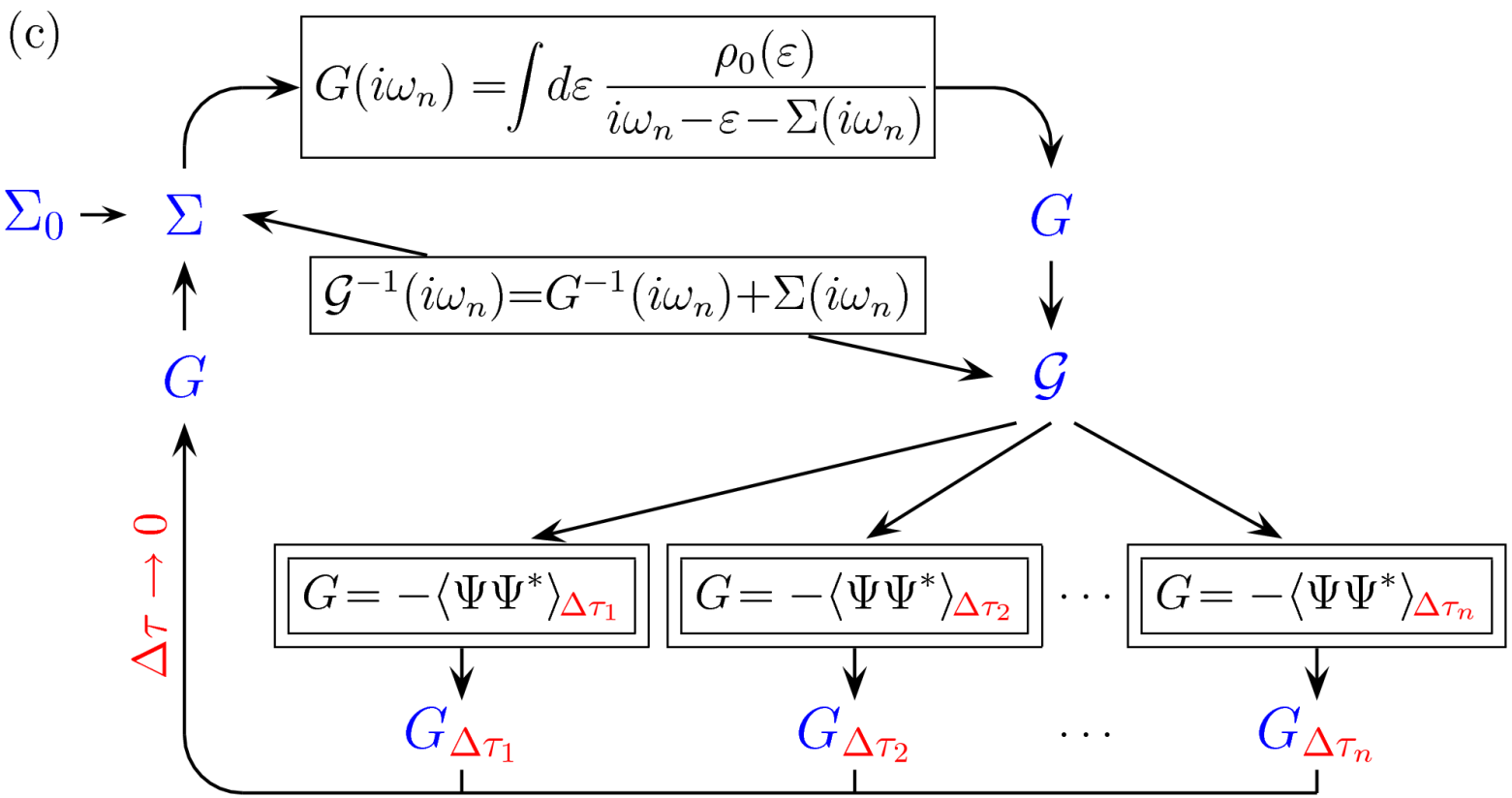
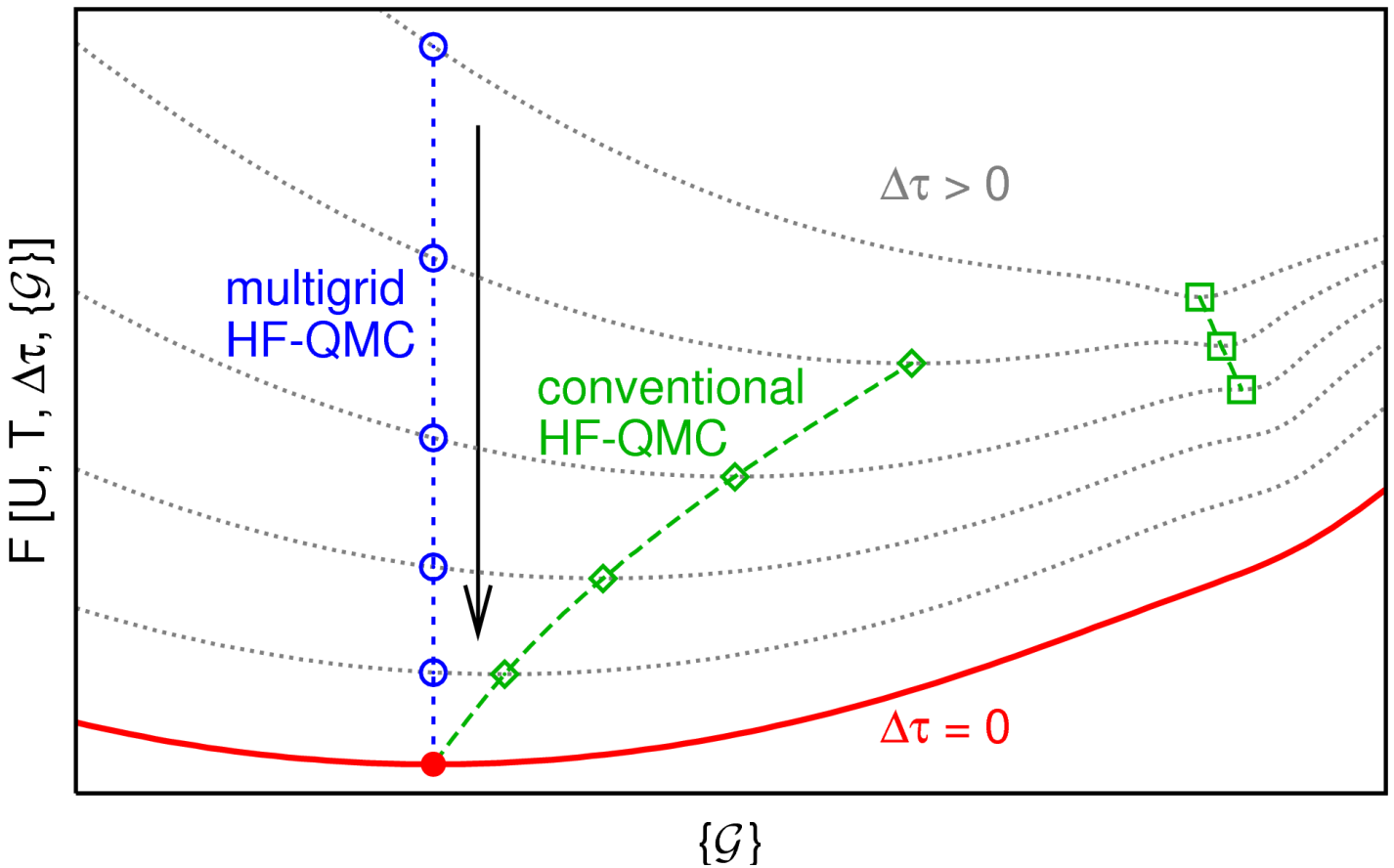


(c) Multigrid HF-QMC: internal elimination of Trotter error

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

Schematic comparison via generalized Ginzburg-Landau functionals



Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

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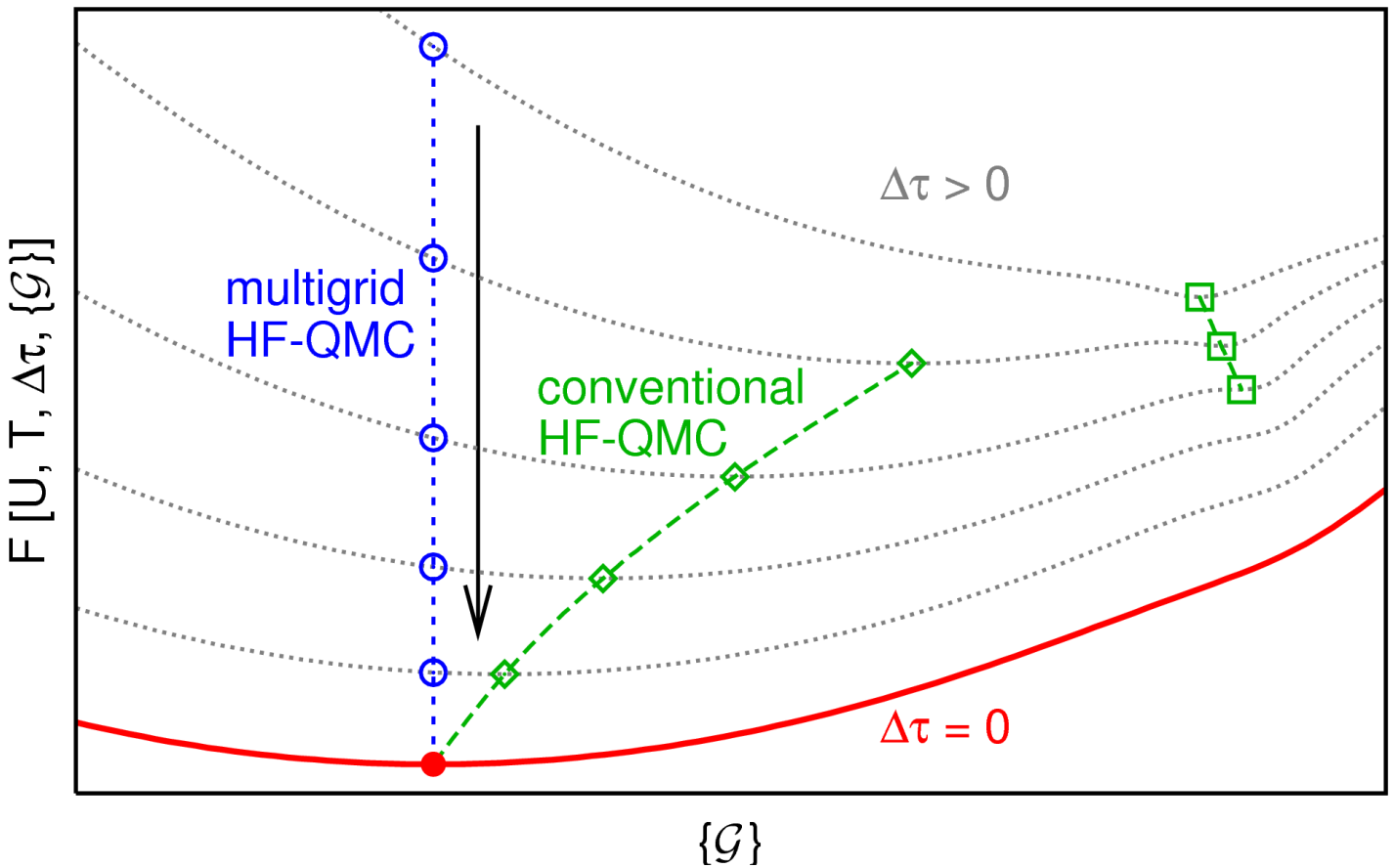

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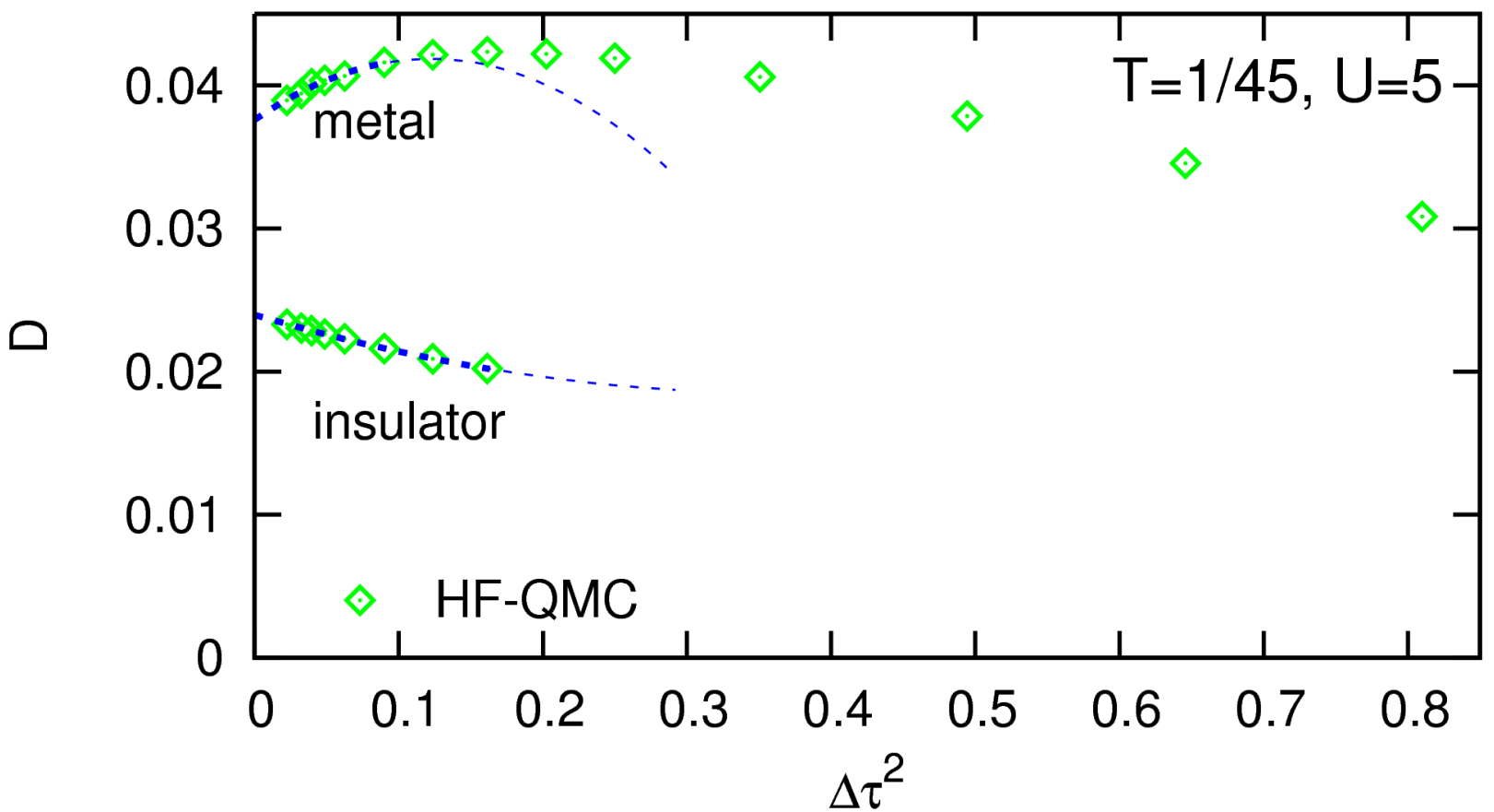
Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

Implementation: Green function extrapolation, hierarchy of frequency scales

Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$

very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

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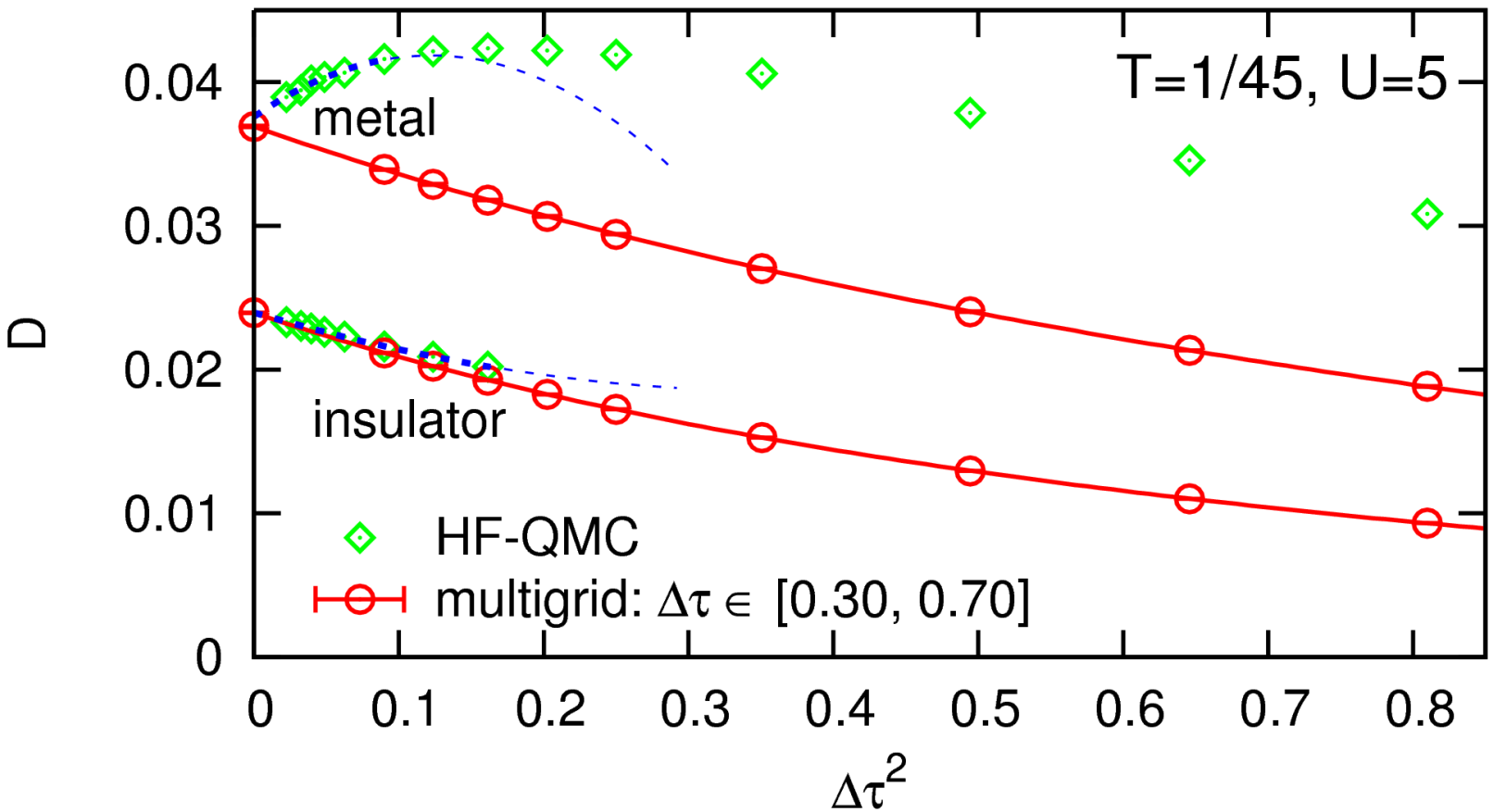

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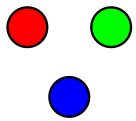
very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

Multigrid HF-QMC: vastly larger useful range of $\Delta\tau$

Paramagnetic Mott transitions in 3-flavor mixtures



3 flavors: simplest case beyond electronic systems

1^{st} approximation: all flavors equivalent, bulk system

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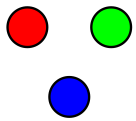

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  Color superconductivity
  Trionic phase
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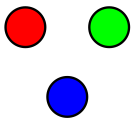

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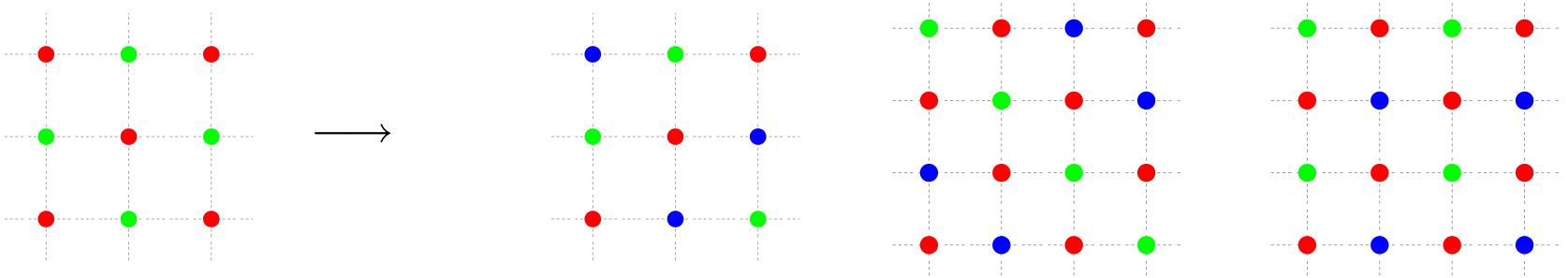

2 spins/flavors

3 spins/flavors

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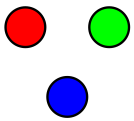

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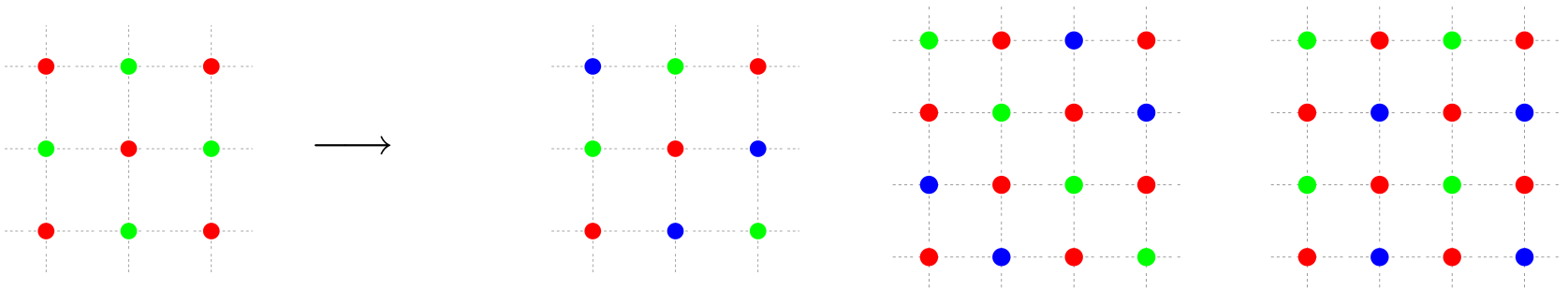
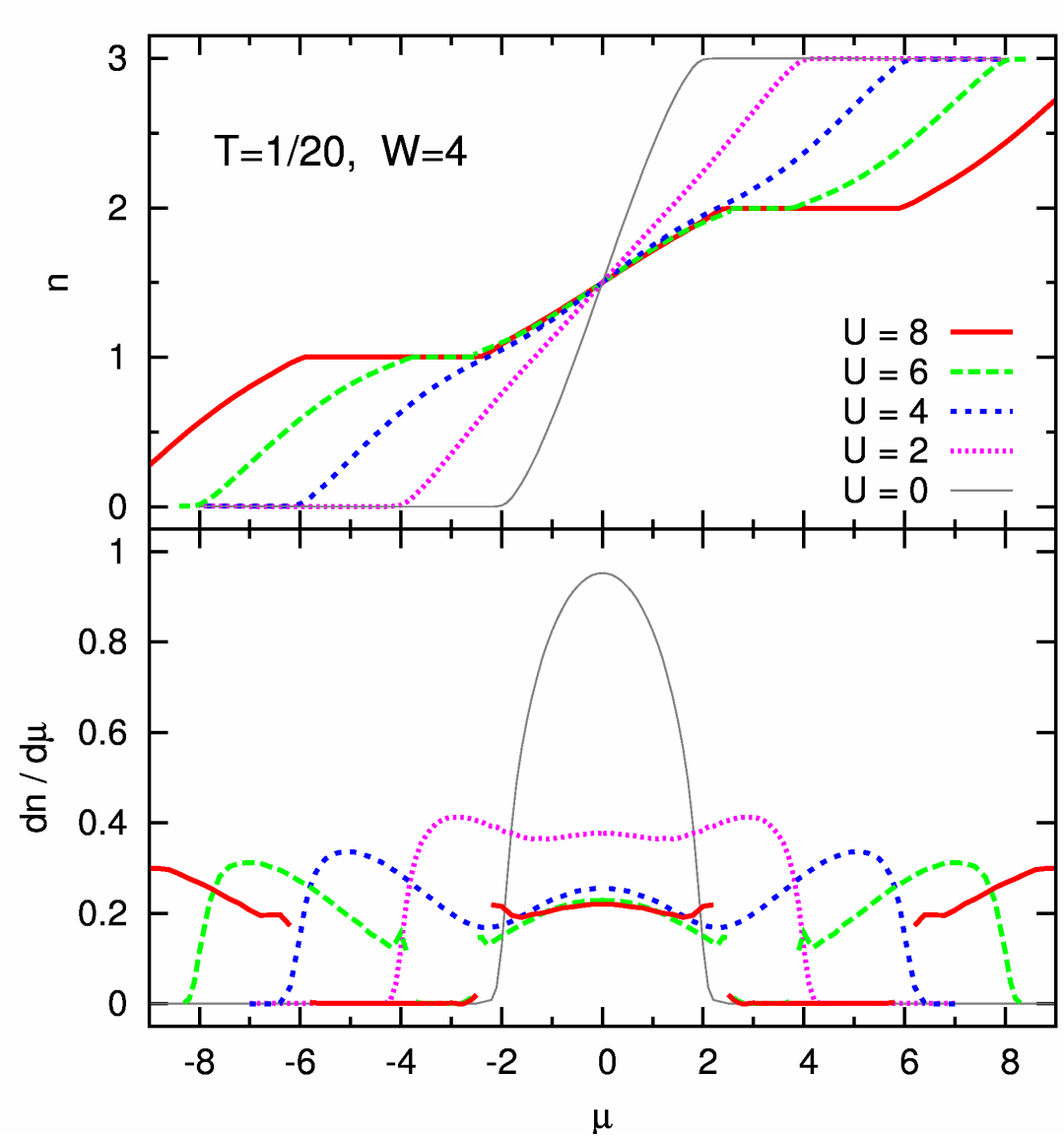


2 spins/flavors

3 spins/flavors

Most "electron-like": $U > 0$, paramagnetic phase

Results at low T: particle density n and compressibility $\kappa = \frac{dn}{d\mu}$ (vs. μ)



HF-QMC, Bethe DOS ($W = 4$)

Plateaus at integer filling ($U \gtrsim 5.5$)

$\rightsquigarrow$ incompressible Mott phases

[E. Gorelik, N. Blümer, PRA(2009)]

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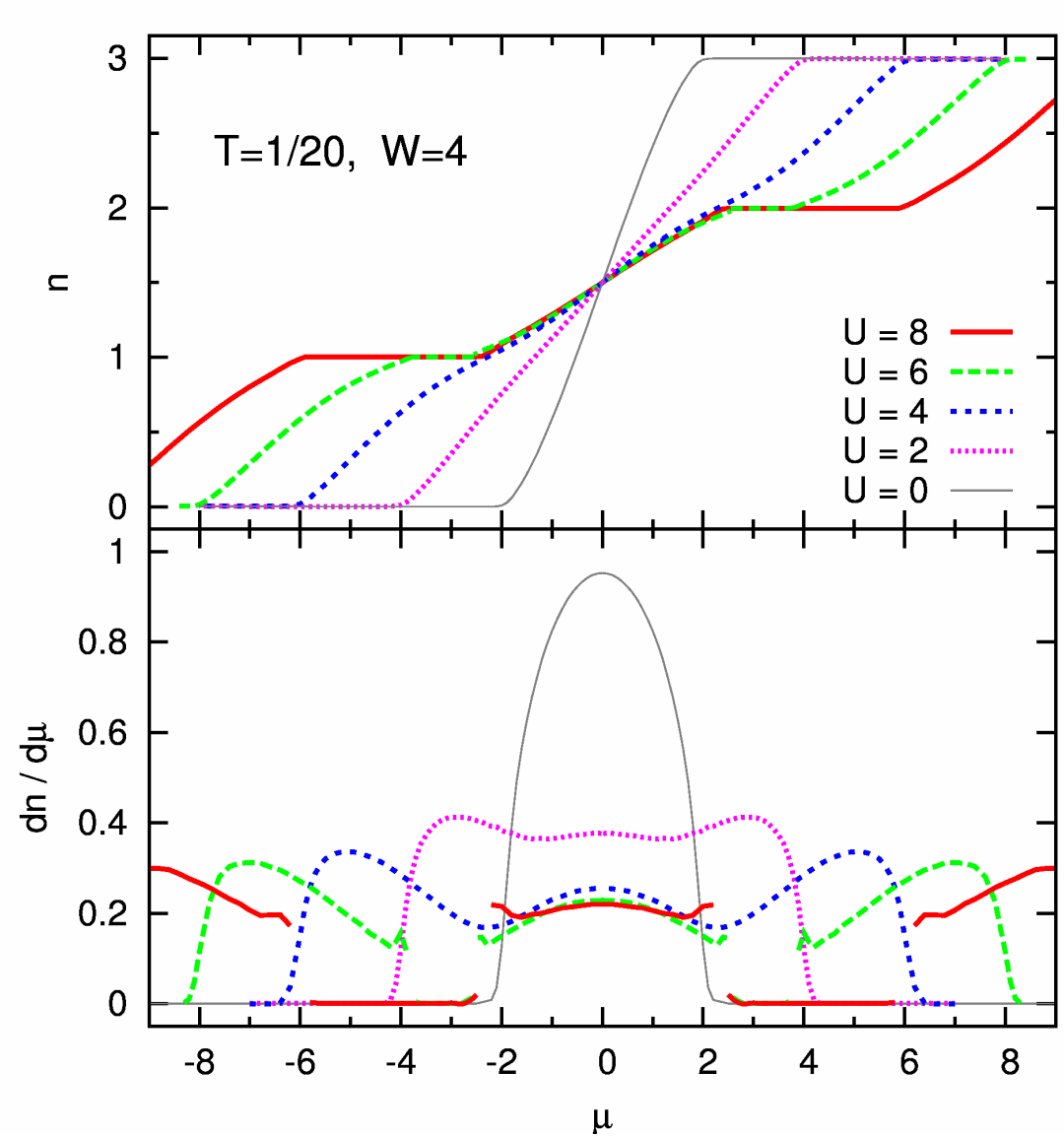

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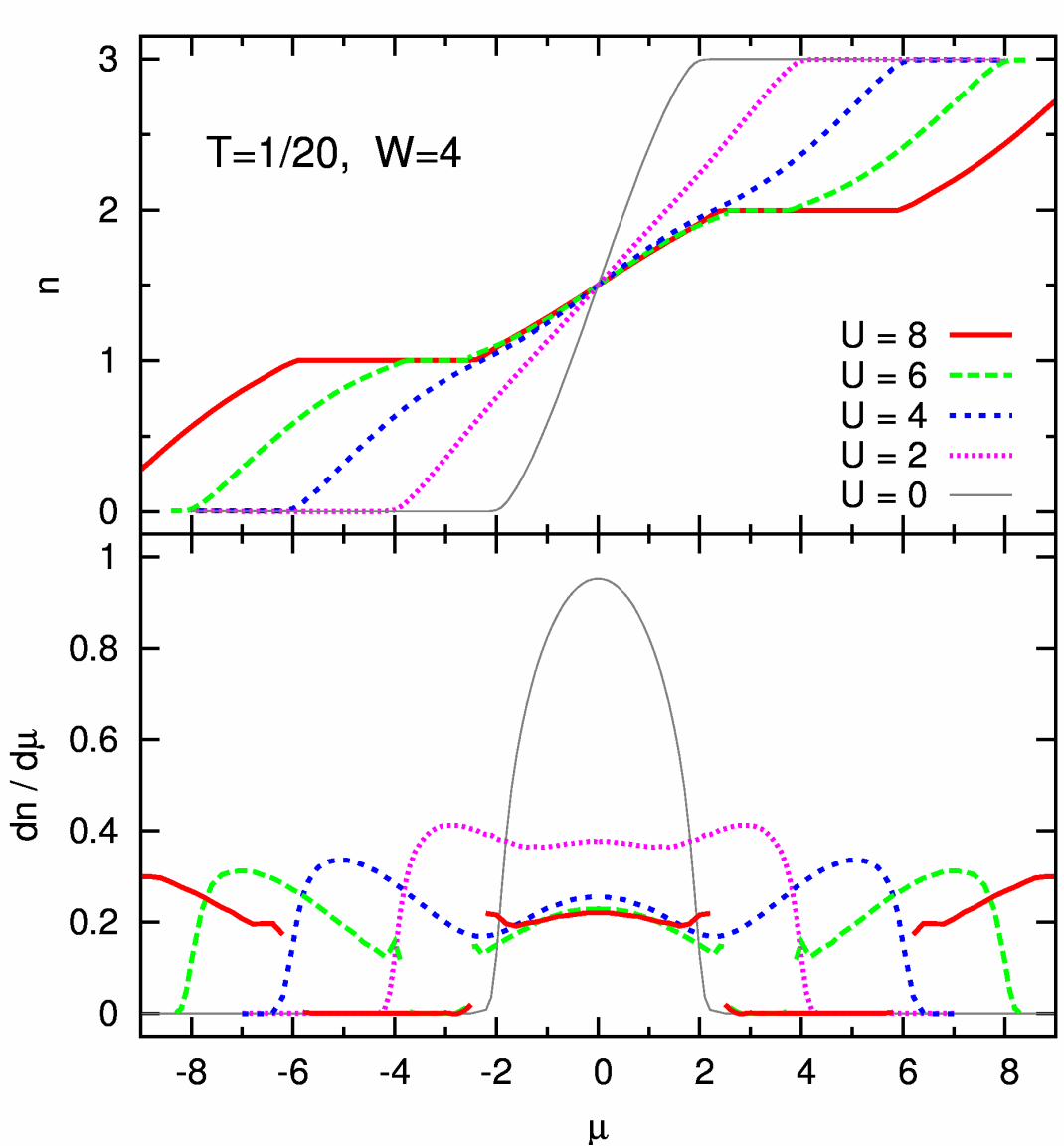

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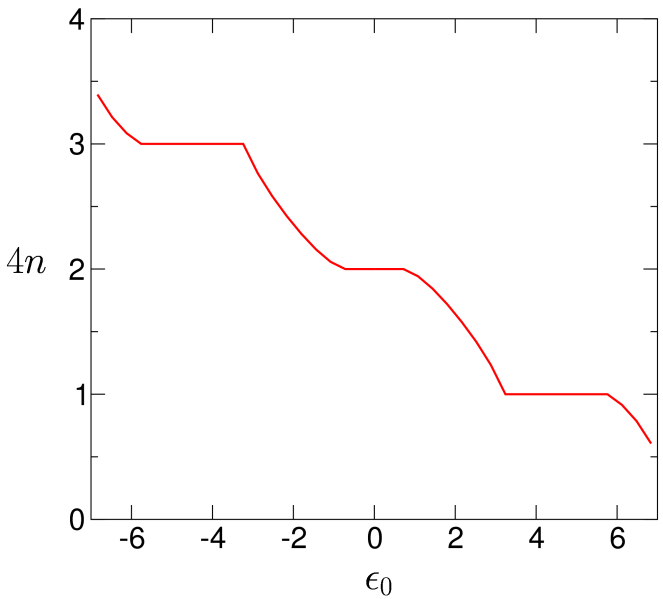
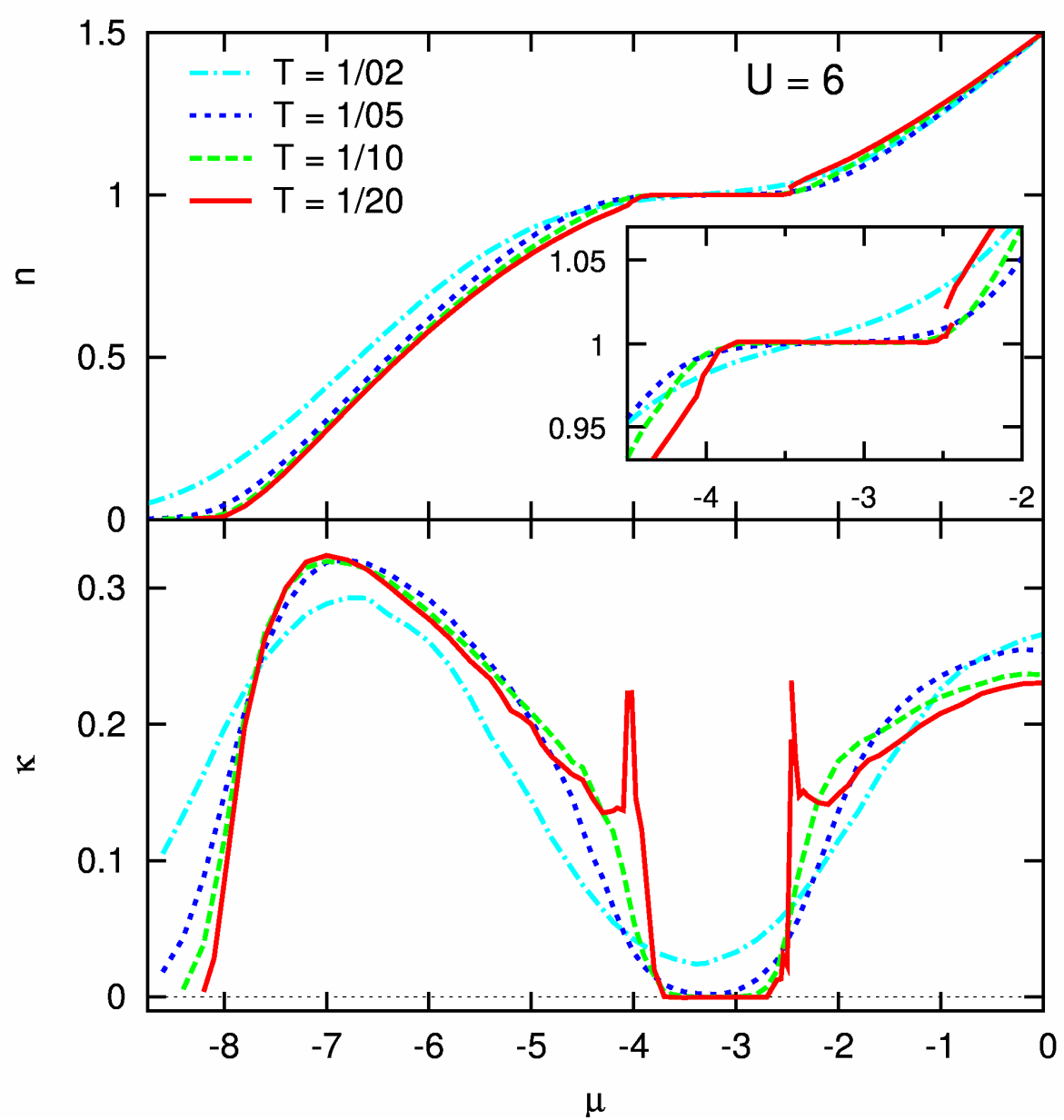
Contrast with SU(4) system:



[Florens, Georges, PRB **70**, 035114 (2004)]

T dependence of density n and compressibility κ



Multigrid HF-QMC results

Critical temperature $T^* \approx 1/20$

not shown: hysteresis at $T = 1/30$

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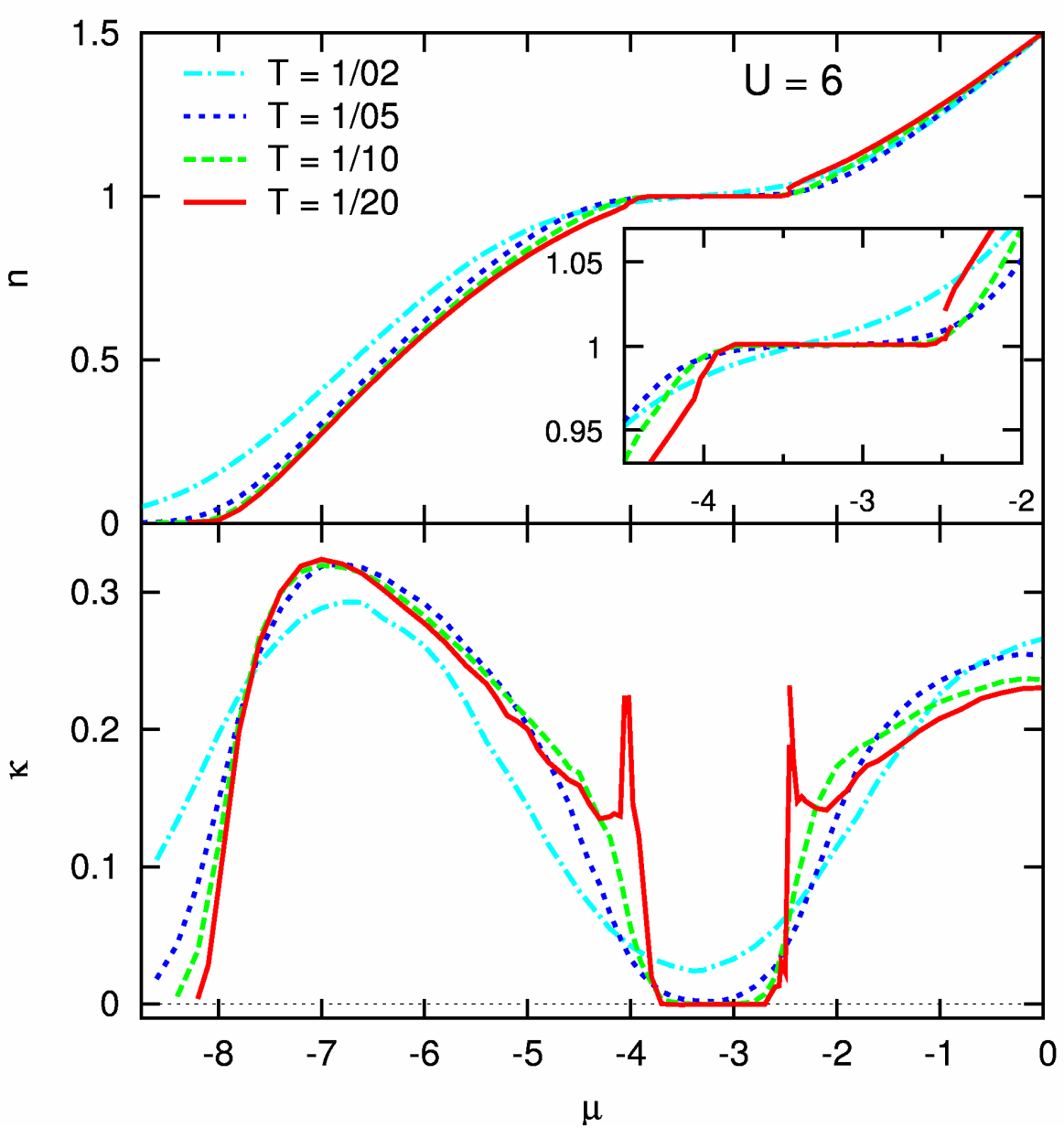

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Critical temperature $T^* \approx 1/20$

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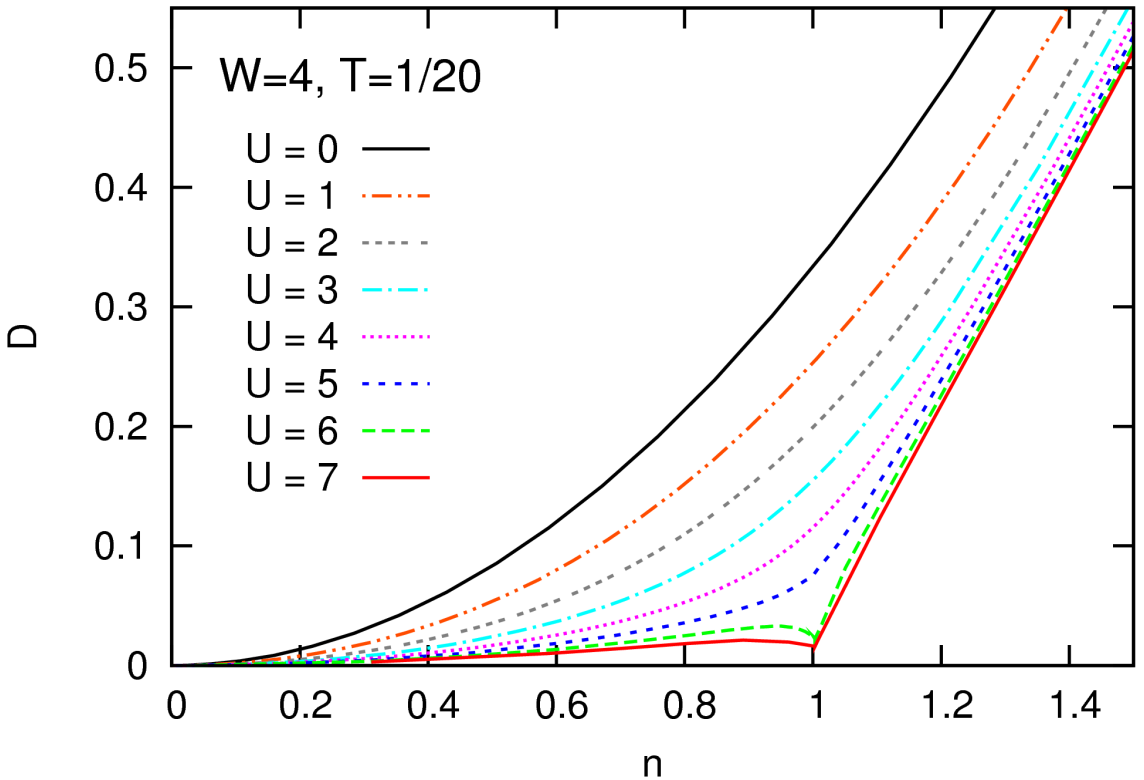
Important for experiments:

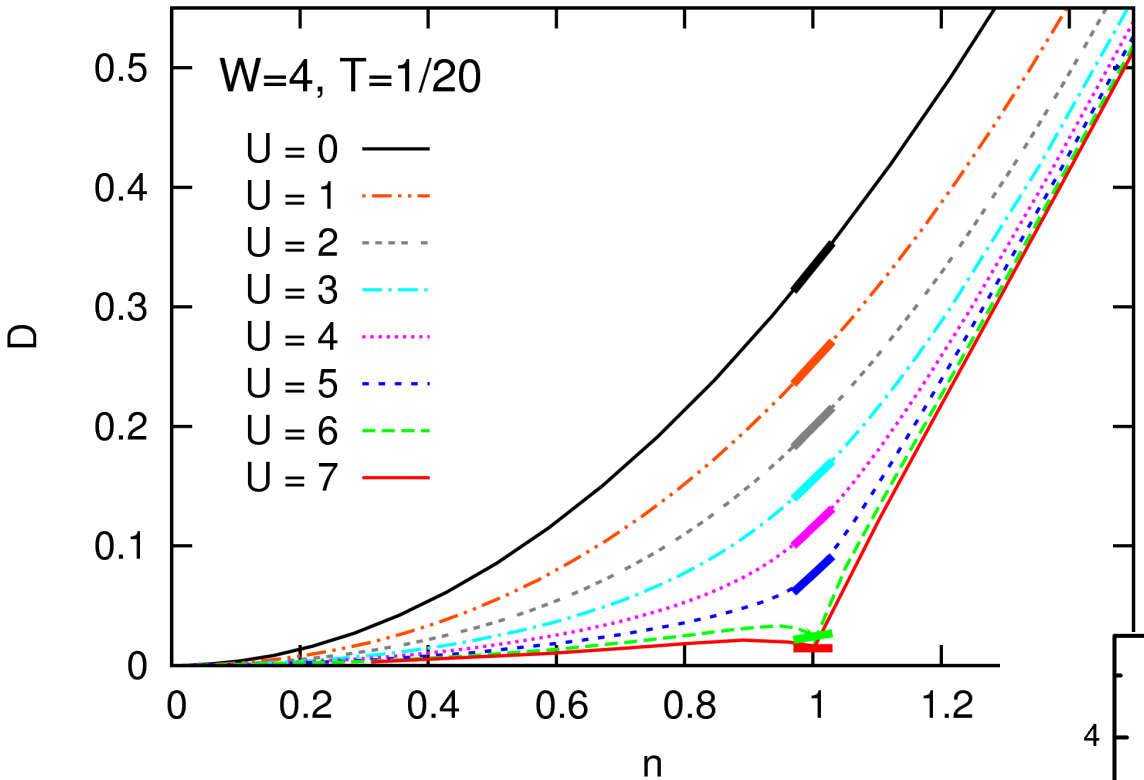
Signatures of Mott transition persist to high temperatures:

nearly complete suppression of κ (at $n \approx 1$) up to $T \approx 1/5$.



3-spin/flavor system:

Pair occupancy vs. density



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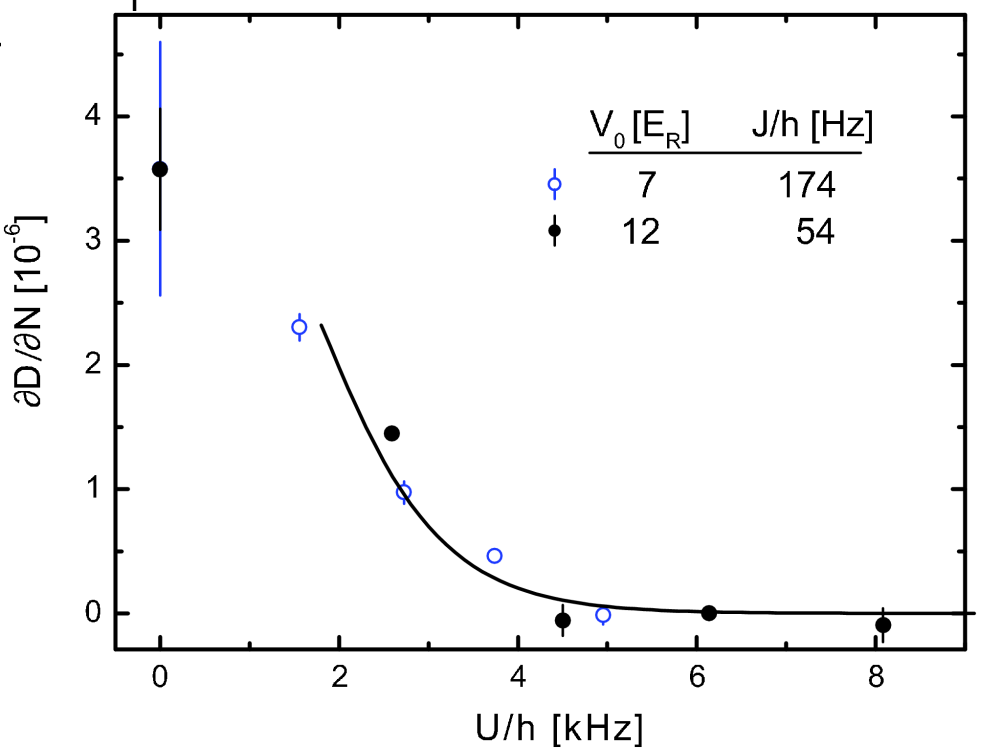
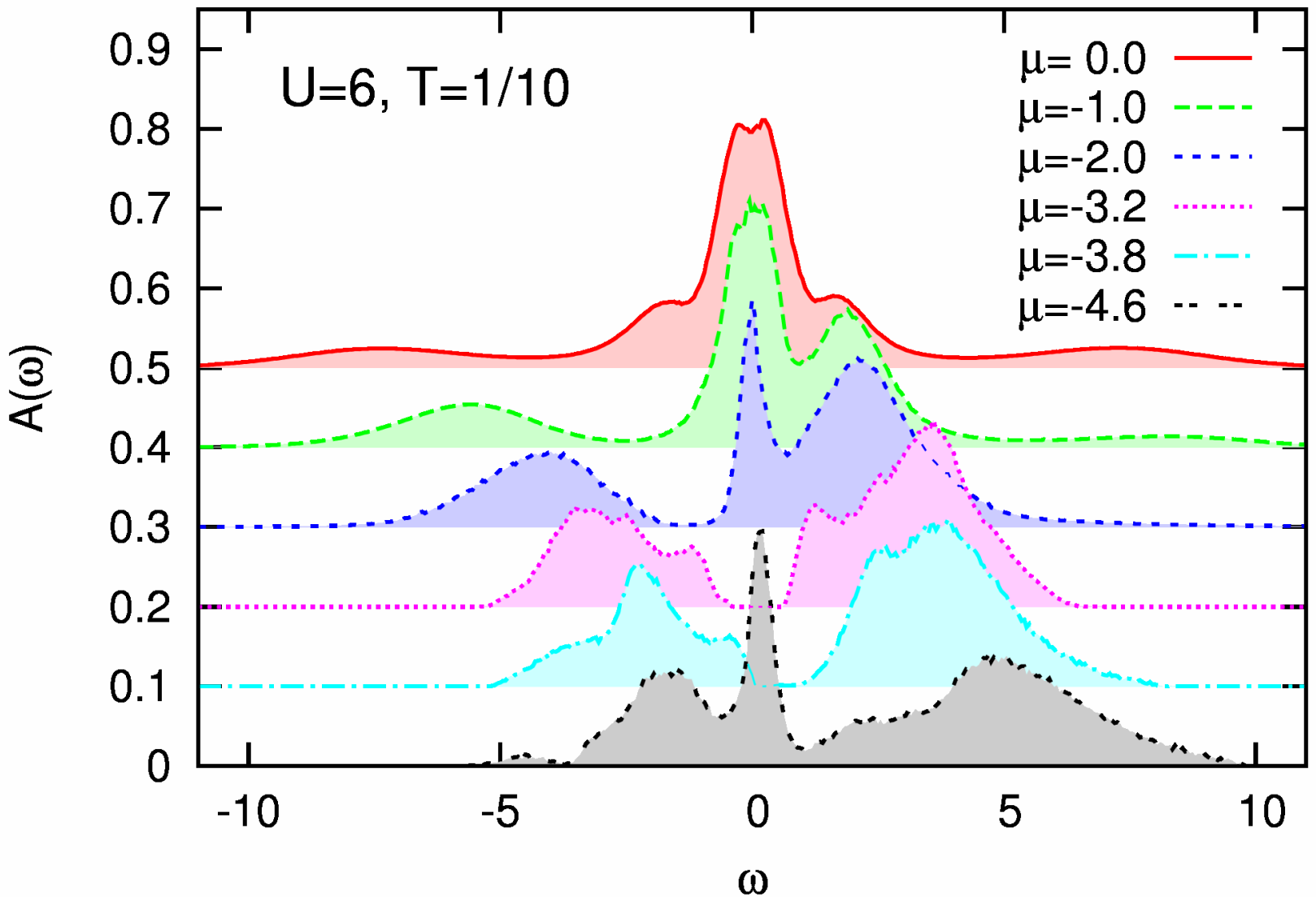


Experiment: 2-spin system

Transition to an incompressible phase

[Jördens et al., Nature (2008)]

Local spectral function



RAPID COMMUNICATIONS

PHYSICAL REVIEW A **80**, 051602(R) (2009)

Mott transitions in ternary flavor mixtures of ultracold fermions on optical lattices

E. V. Gorelik and N. Blümer
Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany
(Received 7 May 2009; revised manuscript received 9 July 2009; published 11 November 2009)

RAPID COMMUNICATIONS

PHYSICAL REVIEW A **81**, 021603(R) (2010)

Three-component fermionic atoms with repulsive interaction in optical lattices

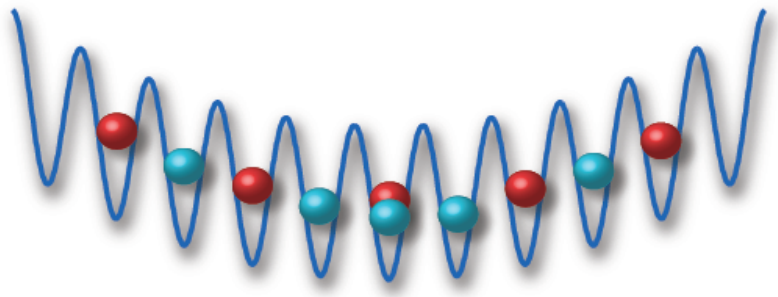
Shin-ya Miyatake,[1] Kensuke Inaba,[2] and Sei-ichiro Suga[1,3]
[1]*Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan*
[2]*NTT Basic Research Laboratories, NTT Corporation, Atsugi 243-0198, Japan, and CREST, JST, Chiyoda-ku, Tokyo 102-0075, Japan*
[3]*Department of Materials Science and Chemistry, University of Hyogo, Himeji 671-2280, Japan*
(Received 4 December 2009; published 17 February 2010)

- MIT at integer filling (same authors, Physica C)
- inequivalent flavors
- ordering at half filling

Antiferromagnetic order at finite T in an optical trap

Now include trapping potential, e.g.: $V_i = V r_i^2$

$$H = -\sum_{(ij),\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} \; + \; U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} \; + \; \sum_{i,\sigma} V_i \, n_{i\sigma}$$



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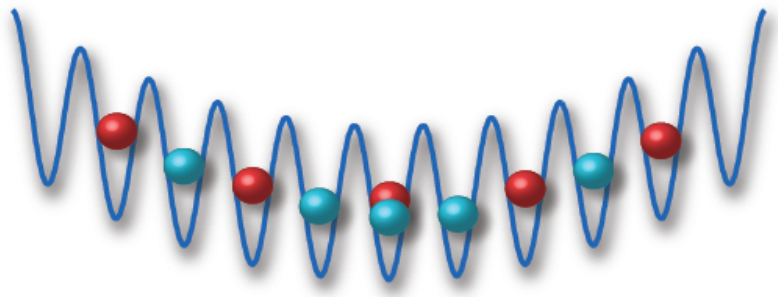

Real-space DMFT: use local self-energy in inhomogeneous system

$\rightsquigarrow$ N single-site impurities, coupled by modified lattice Dyson equation:

$$\Big[G_\sigma(i\omega_n)\Big]^{-1}_{ij} = \big(\mu_\sigma + i\omega_n\big)\delta_{ij} - t_{ij} - \big(V_i + \Sigma_{i\sigma}(i\omega_n)\big)\delta_{ij} \equiv z_i(i\omega_n)\,\delta_{ij} - t_{ij}$$

[M. Snoek, I. Titvinidze, C. Toke, K. Byczuk, and W. Hofstetter, New Journal of Physics (2008); R. Helmes, T. A. Costi, and A. Rosch, PRL (2008)]

Also: inhomogeneous DMFT (for Falicov-Kimball model) [Freericks]

RDMFT algorithm

0) Choose $\Sigma_i(i\omega_n) \rightsquigarrow z_i(i\omega_n)$

1) For each ω_n evaluate lattice Dyson equation ($z_i \equiv z_i(i\omega_n)$):

Example: 1d chain with open bc

$$\begin{pmatrix} G_{-2,-2} & G_{-2,-1} & G_{-2,0} & G_{-2,1} & G_{-2,2} \\ G_{-1,-2} & G_{-1,-1} & G_{-1,0} & G_{-1,1} & G_{-1,2} \\ G_{0,-2} & G_{0,-1} & G_{0,0} & G_{0,1} & G_{0,2} \\ G_{1,-2} & G_{1,-1} & G_{1,0} & G_{1,1} & G_{1,2} \\ G_{2,-2} & G_{2,-1} & G_{2,0} & G_{2,1} & G_{2,2} \end{pmatrix} = \begin{pmatrix} z_{-2} & -t & 0 & 0 & 0 \\ -t & z_{-1} & -t & 0 & 0 \\ 0 & -t & z_0 & -t & 0 \\ 0 & 0 & -t & z_1 & -t \\ 0 & 0 & 0 & -t & z_2 \end{pmatrix}^{-1}$$

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3) Solve impurity model ($\mathcal{G}_i$, U_i, V_i, μ, T) for each inequivalent site i

4) Compute new self-energy $\Sigma_i(i\omega_n) = \mathcal{G}_i^{-1}(i\omega_n) - G_{ii}^{-1} \quad \forall i, \omega_n$

Repeat steps 1) – 4) until convergence

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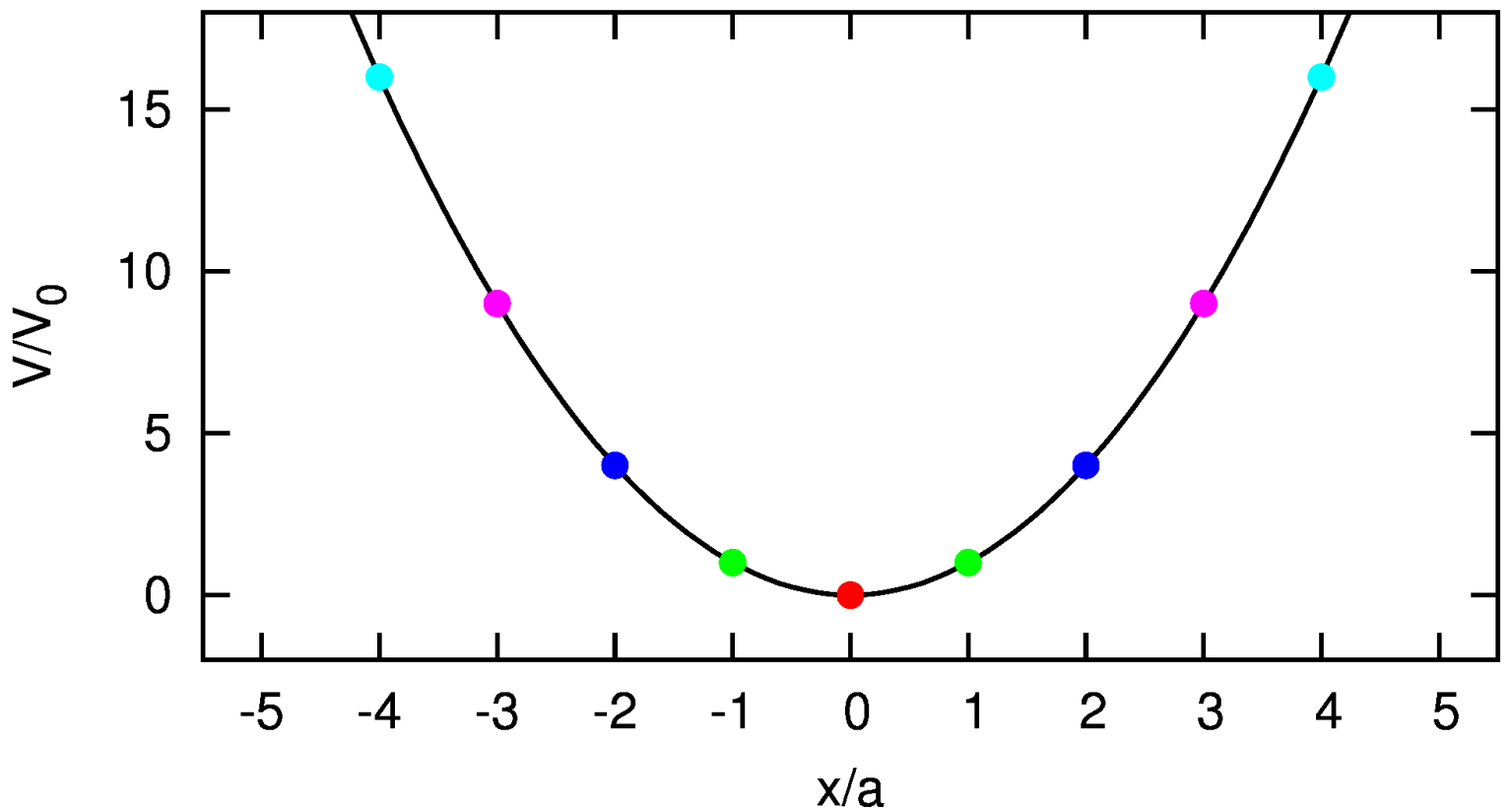
Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

All previous implementations: RDMFT+NRG

Simple approximation: "local density approximation (LDA)"

Approximate properties of each site by properties of homogeneous system with same effective chemical potential ($\rightsquigarrow$ standard DMFT)

Example: 1d chain



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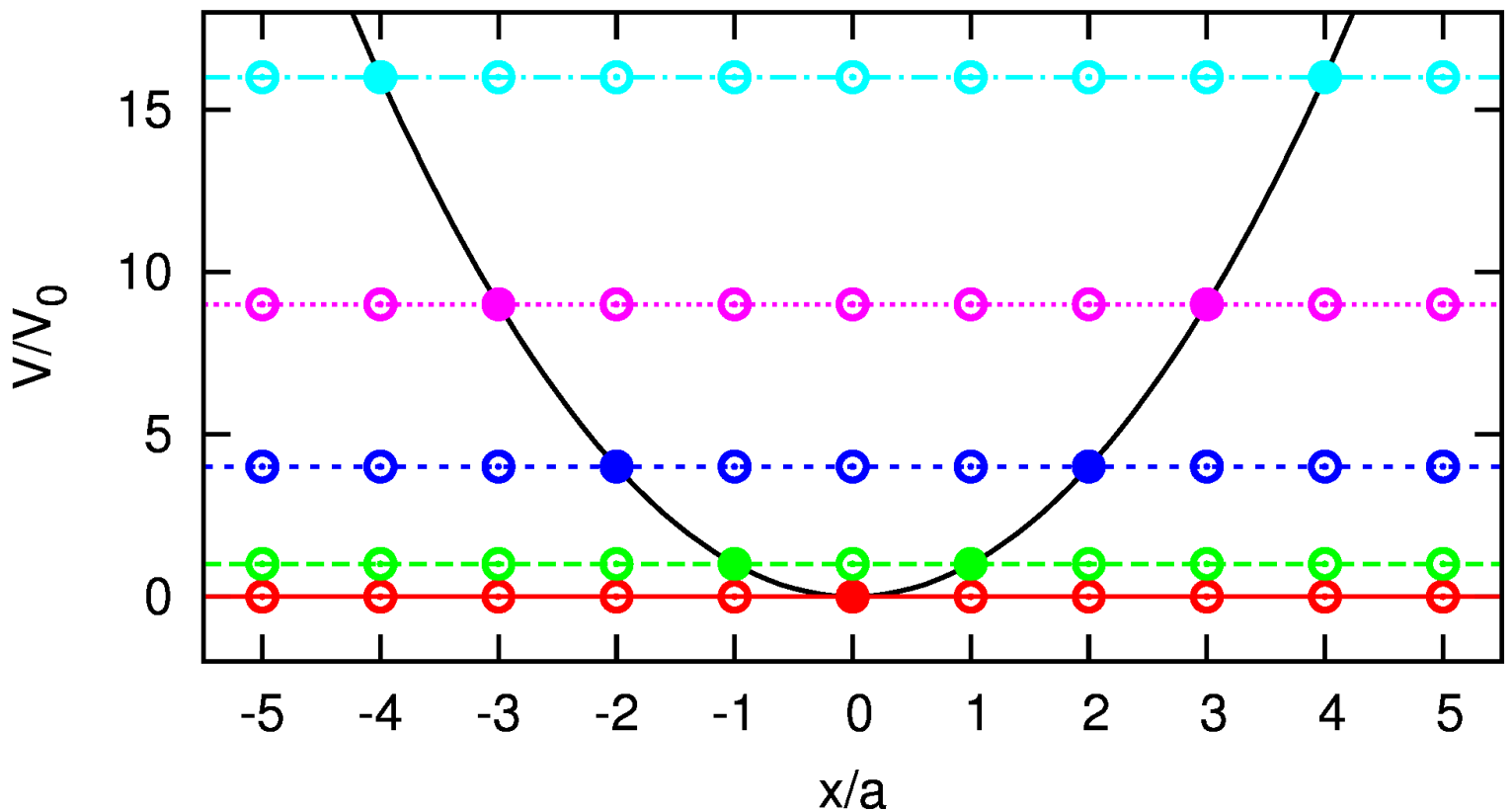


. . . will be used for comparison to RDMFT

RDMFT-NRG results in 2 dimensions ($T = 0$)

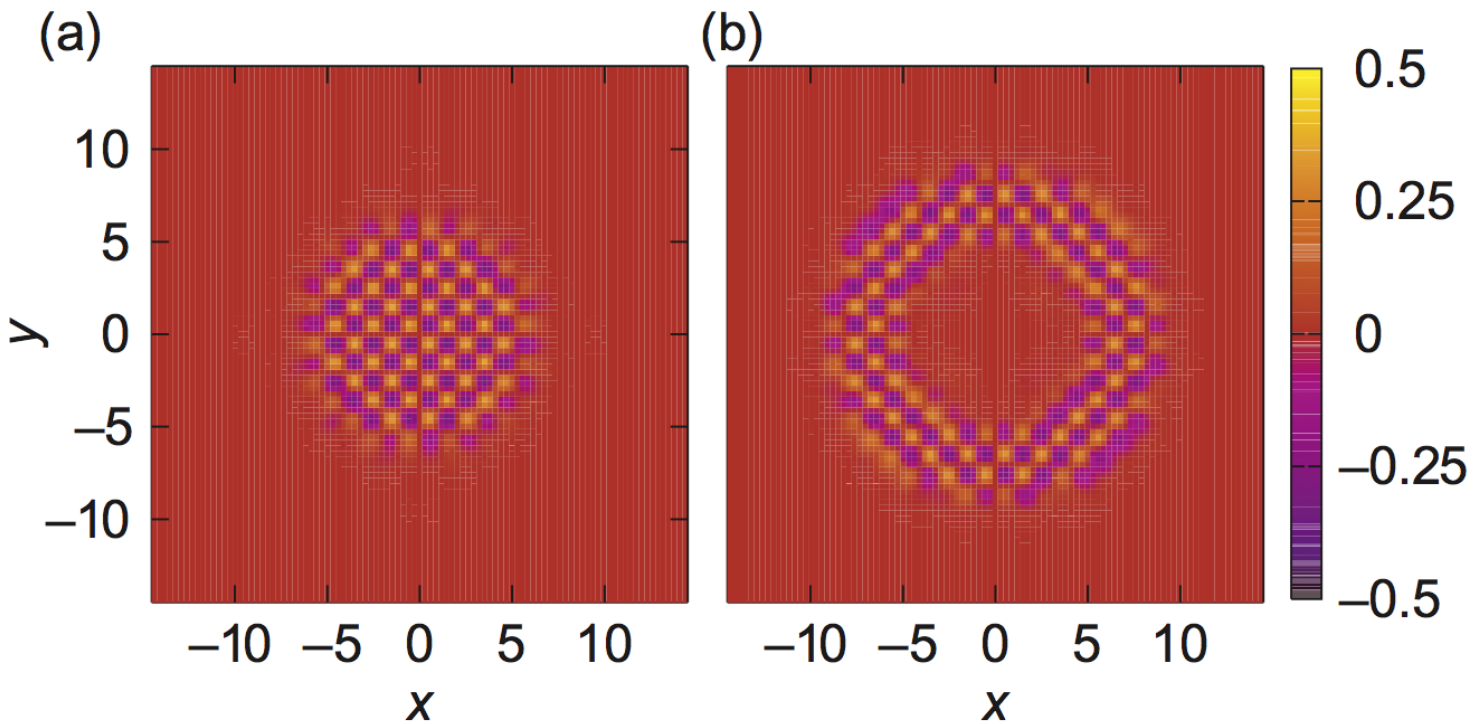
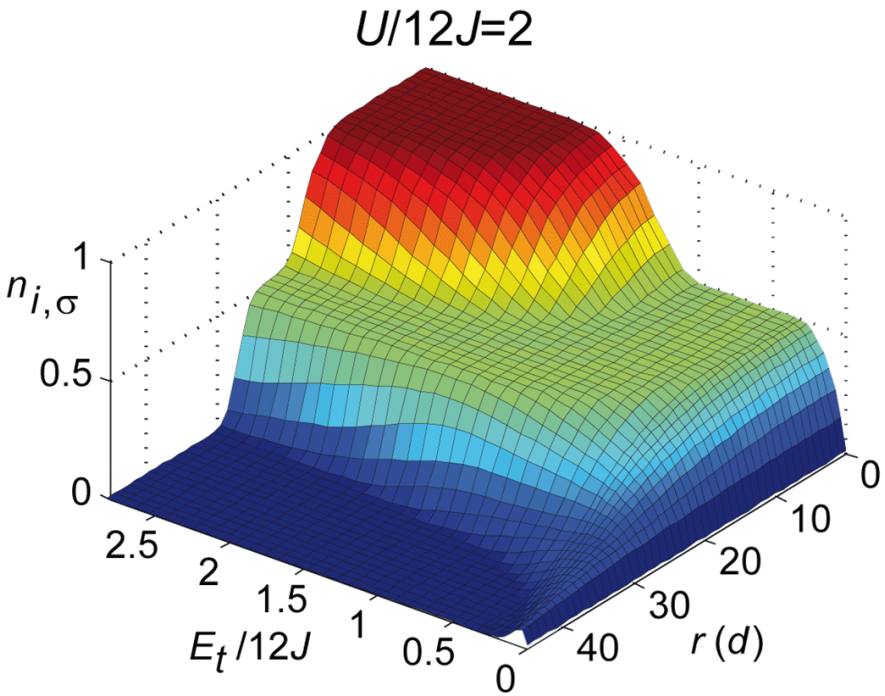


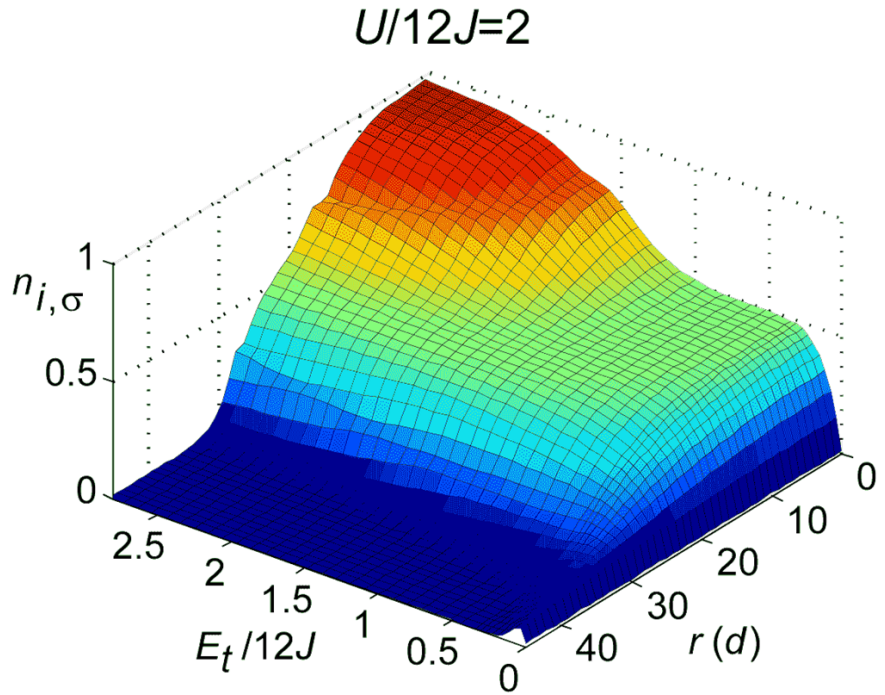
Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_\uparrow = \mu_\downarrow = 5$; (b) $V = 0.2$ and $\mu_\uparrow = \mu_\downarrow = 15$. Energies are expressed in units of the hopping parameter J.

[Snoek, Titvinidze, Töke, Byczuk, Hofstetter, NJP **10**, 093008 (2008)]

But: NRG problematic at elevated temperatures



$T = 0.07t$

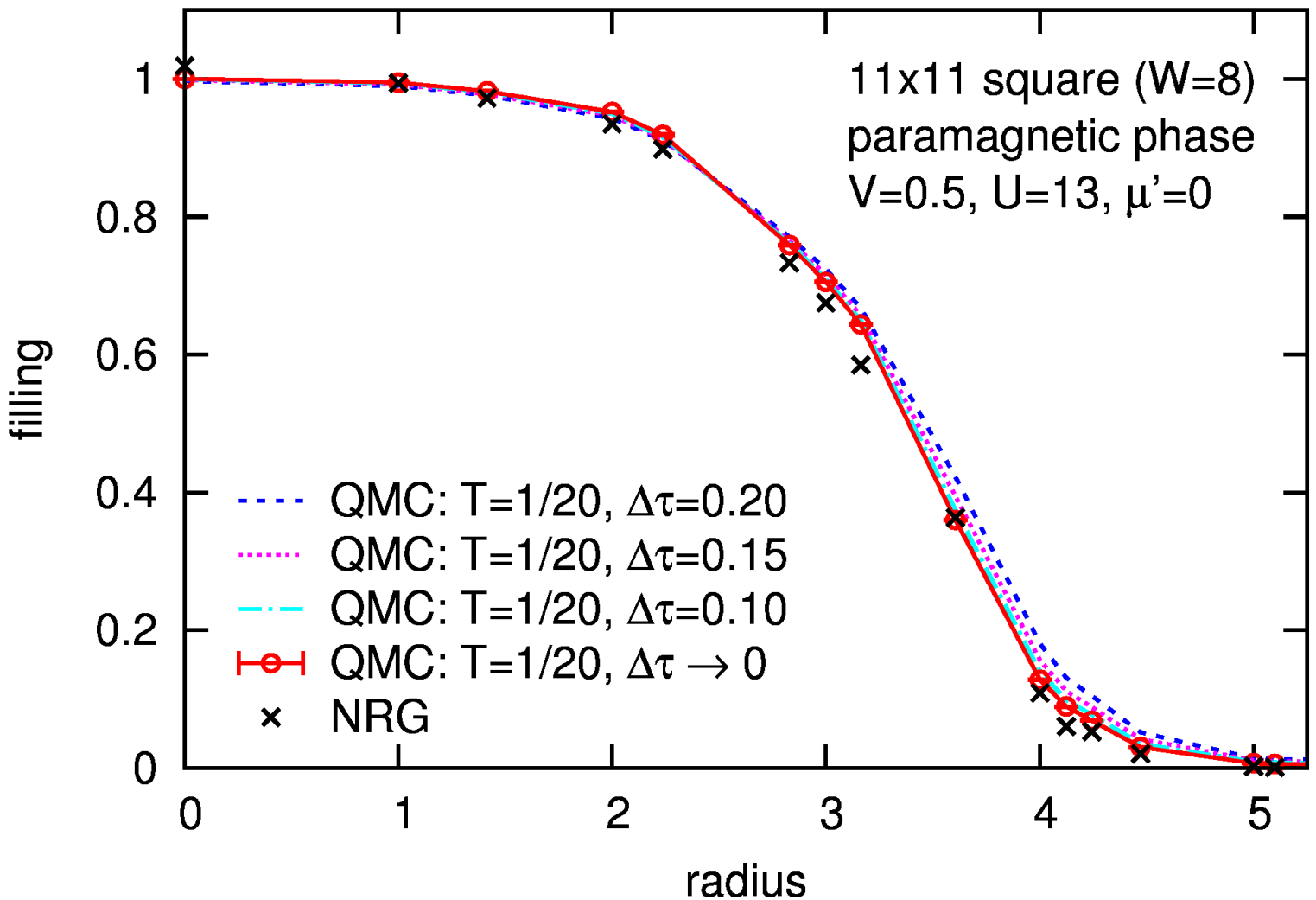


$T = 0.15t$

Additional plateau/kinks at $n_\sigma \approx 0.8$ for $T = 0.15t$ [Rosch group, courtesy of U. Schneider]

However: experimental temperatures are high $\rightsquigarrow$ advantage for QMC!

Real-space DMFT results for paramagnetic phase: QMC vs. NRG



Good agreement QMC ↔ NRG (at low/zero T) not shown: NRG worse for AF

[NRG data by I. Titvinidze (collaboration within SFB/TR 49)]

Simulations of 3D systems with $\mathcal{O}(10^5)$ particles

Naive full RDMFT simulation of experimental situation requires $M = 100^3$ lattice

Scaling: QMC CPU time $\propto M$

Green function memory $\propto M^2$

Green function inversion time $\propto M^3$

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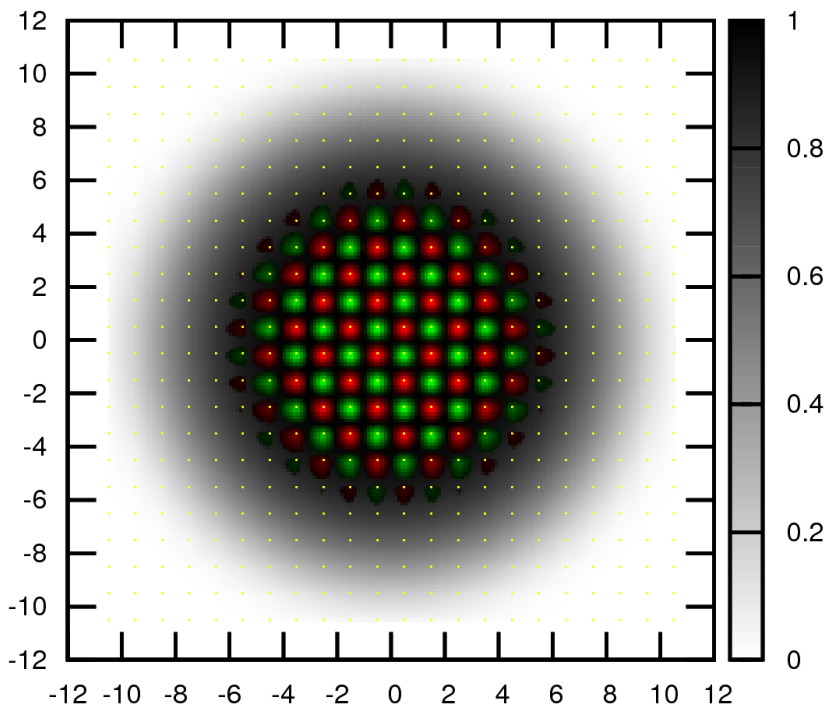
Practical (dense inversion, fully parallel): $\lesssim$ 10000 sites $\rightsquigarrow$ need smart strategies



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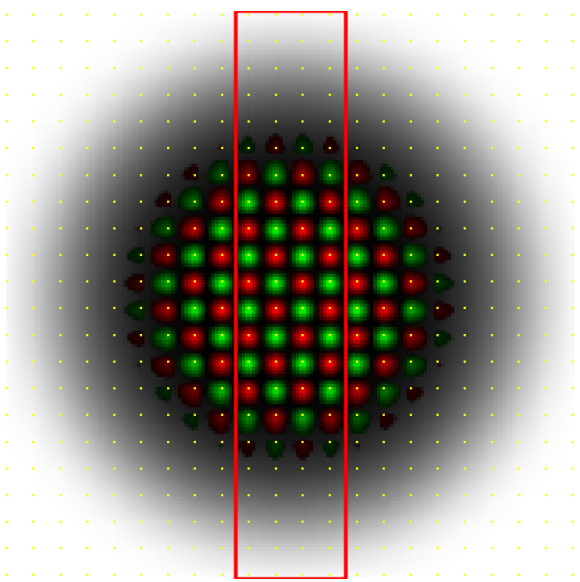

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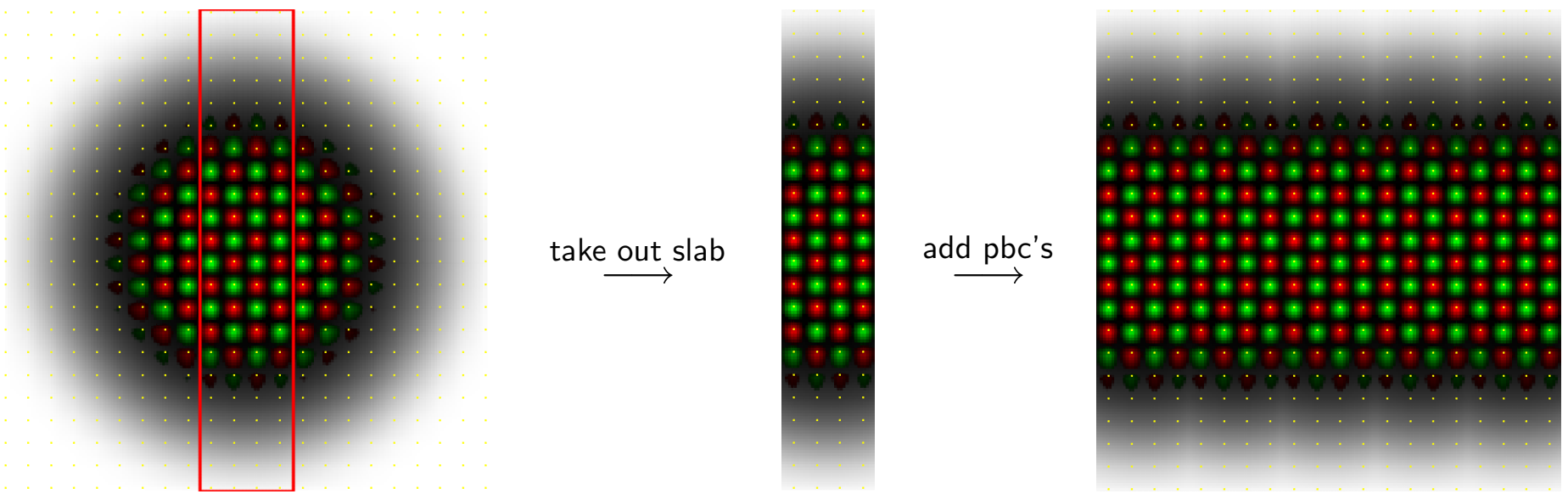
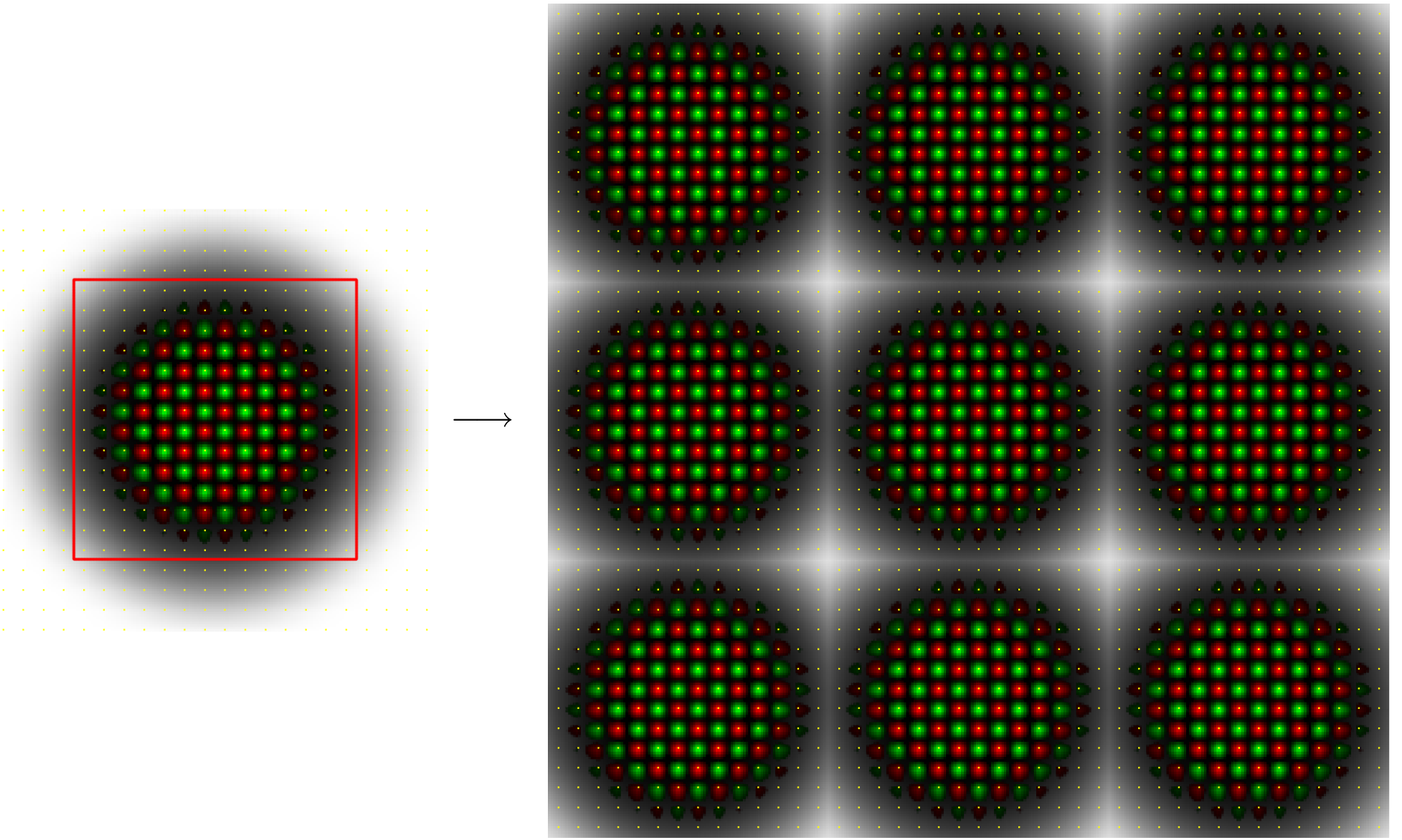


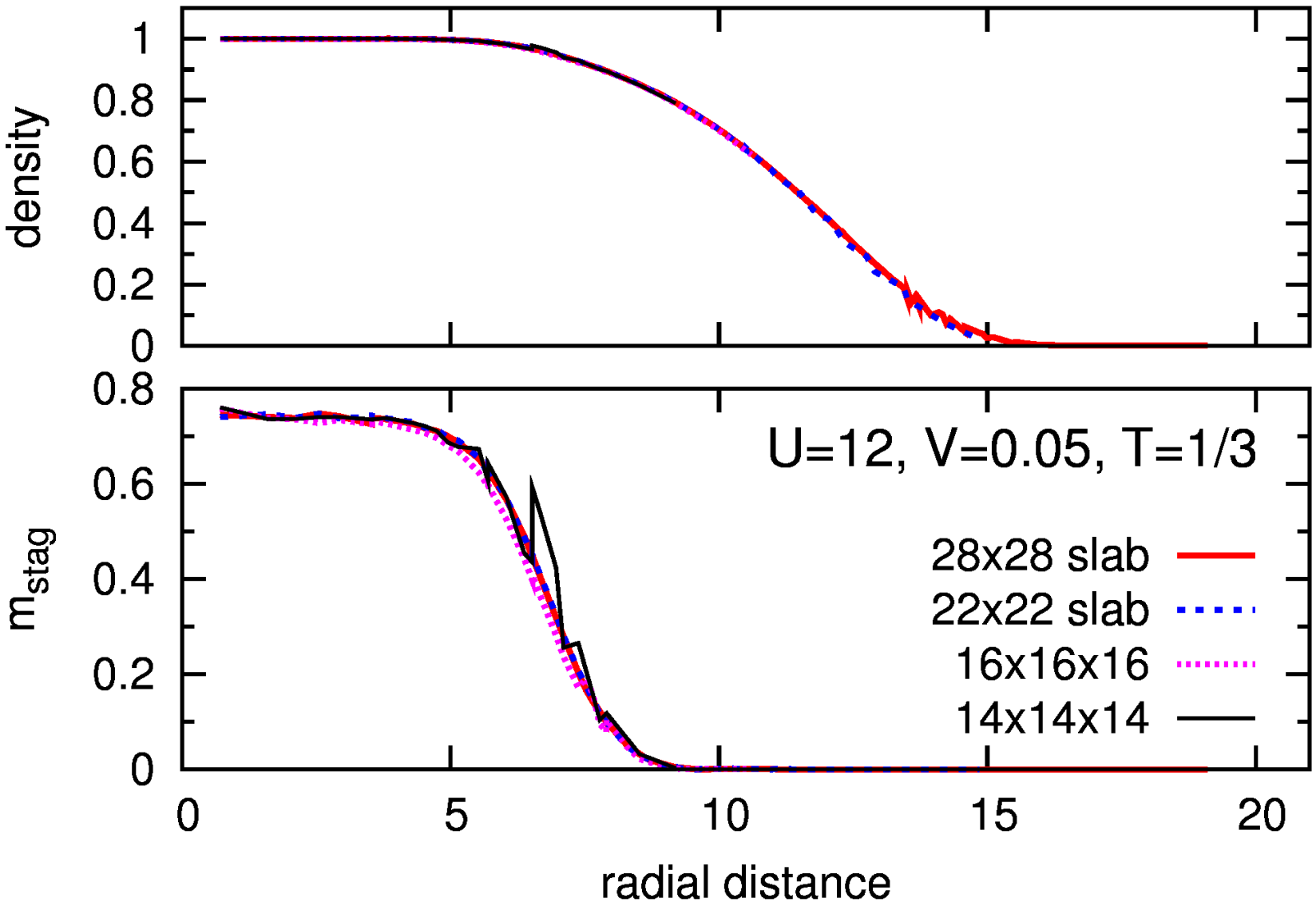
In practice: cylindrical potential (equivalent layers)

Alternative: 3D calculation, but focus on AF core (pbc's in all 3 directions):



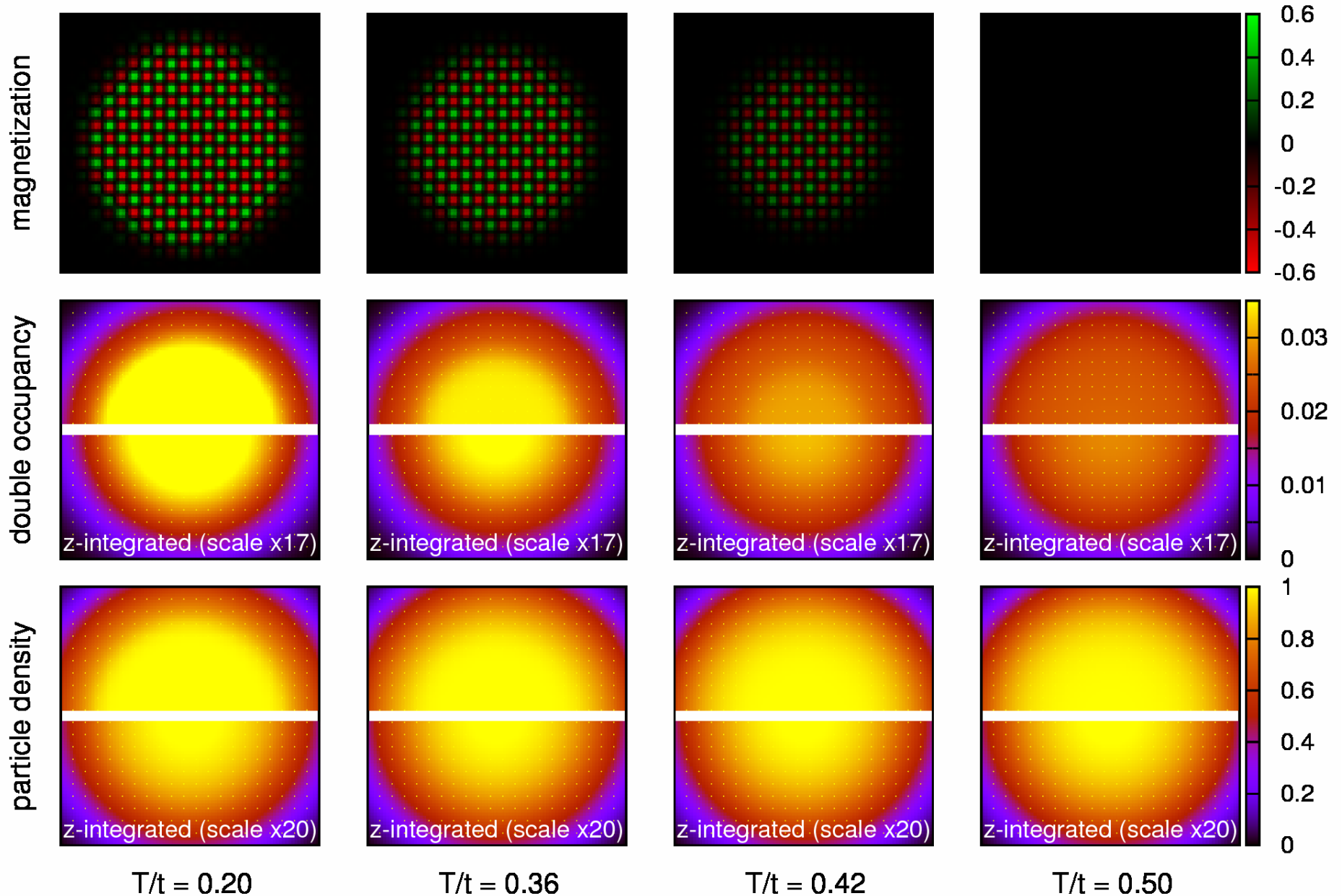
Most efficient: slab calculation focussing on AF core (with pbc)

Test: slab versus minimal core 3D calculation (all with pbc)

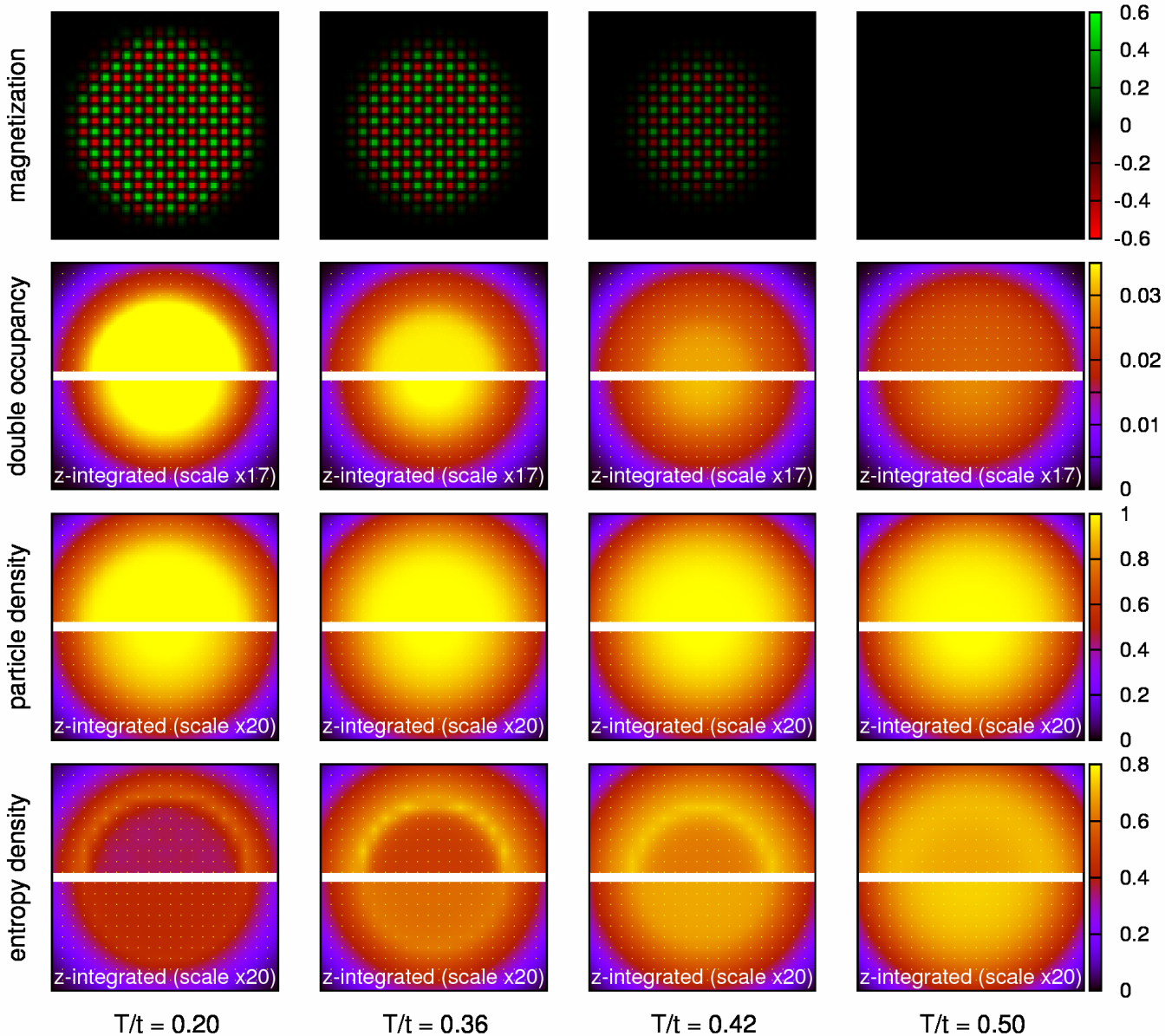


Significant deviations only if core touches boundaries!

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



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



AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

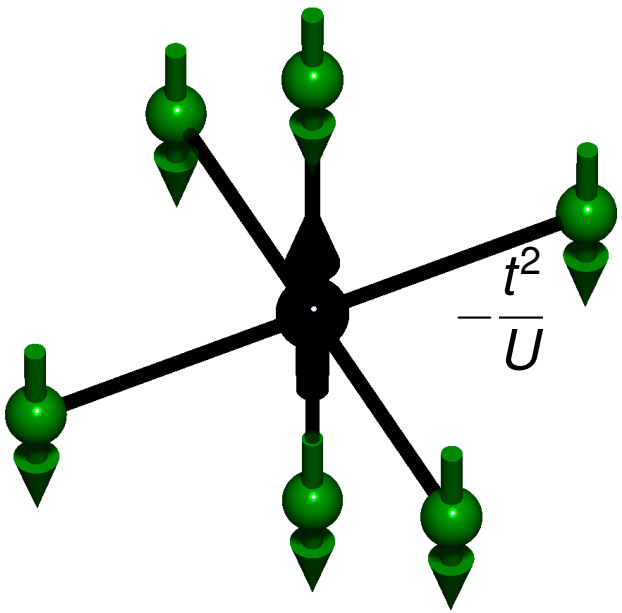
~ 6000 atoms
(naively $\sim 30^3 = 27000$ sites needed)

Entropy

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

Enhanced double occupancy: a signature of AF order

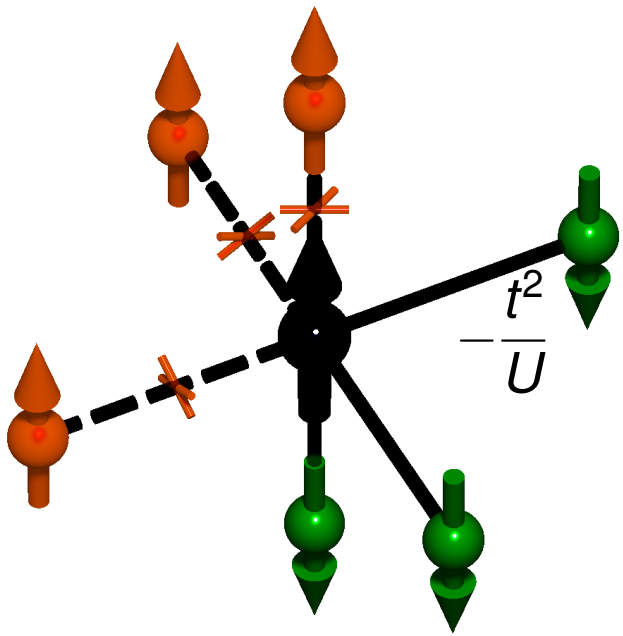
Illustration of mechanism for enhanced double occupancy (at strong coupling):



AF state:

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

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



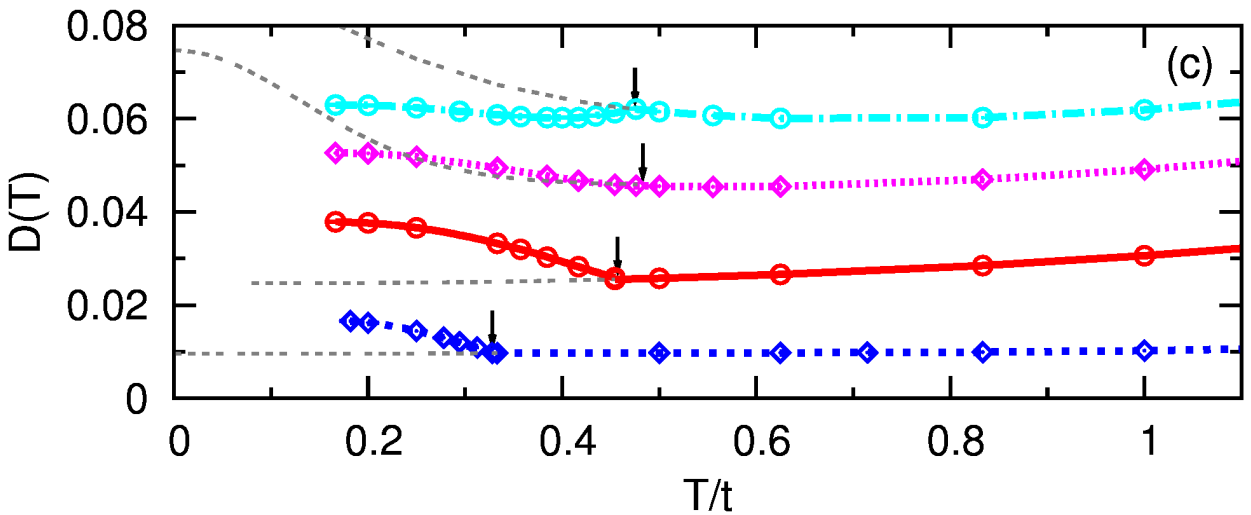
Paramagnetic state:

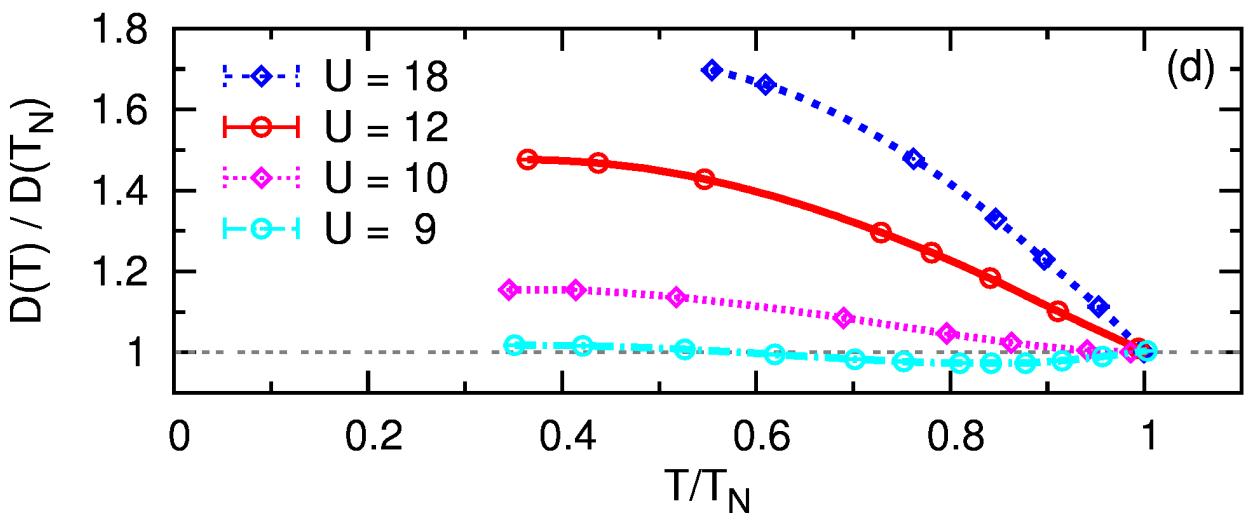
1/2 of the neighboring sites are forbidden for hopping

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

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

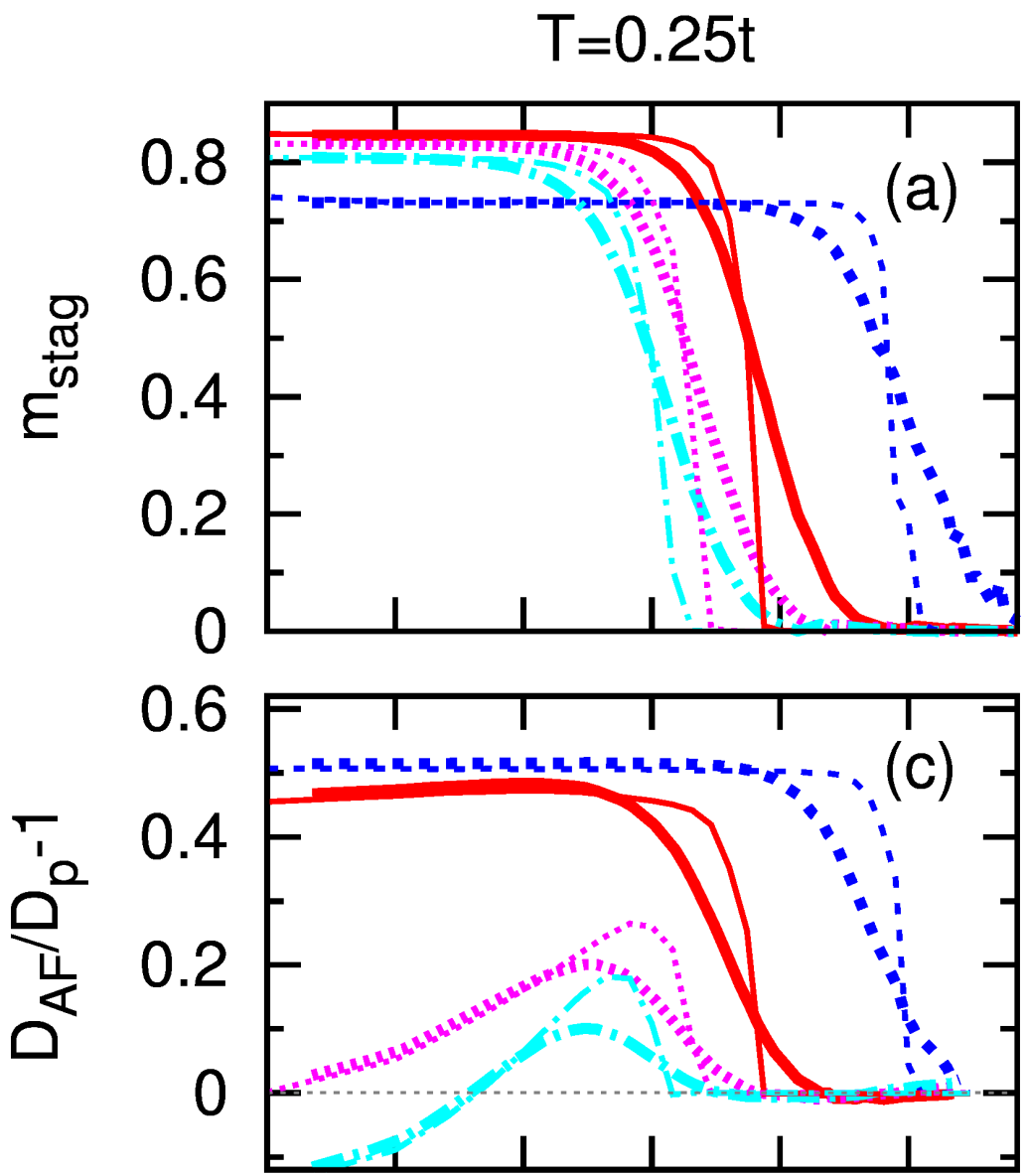
thin lines: metastable paramagnetic phase.

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)]!

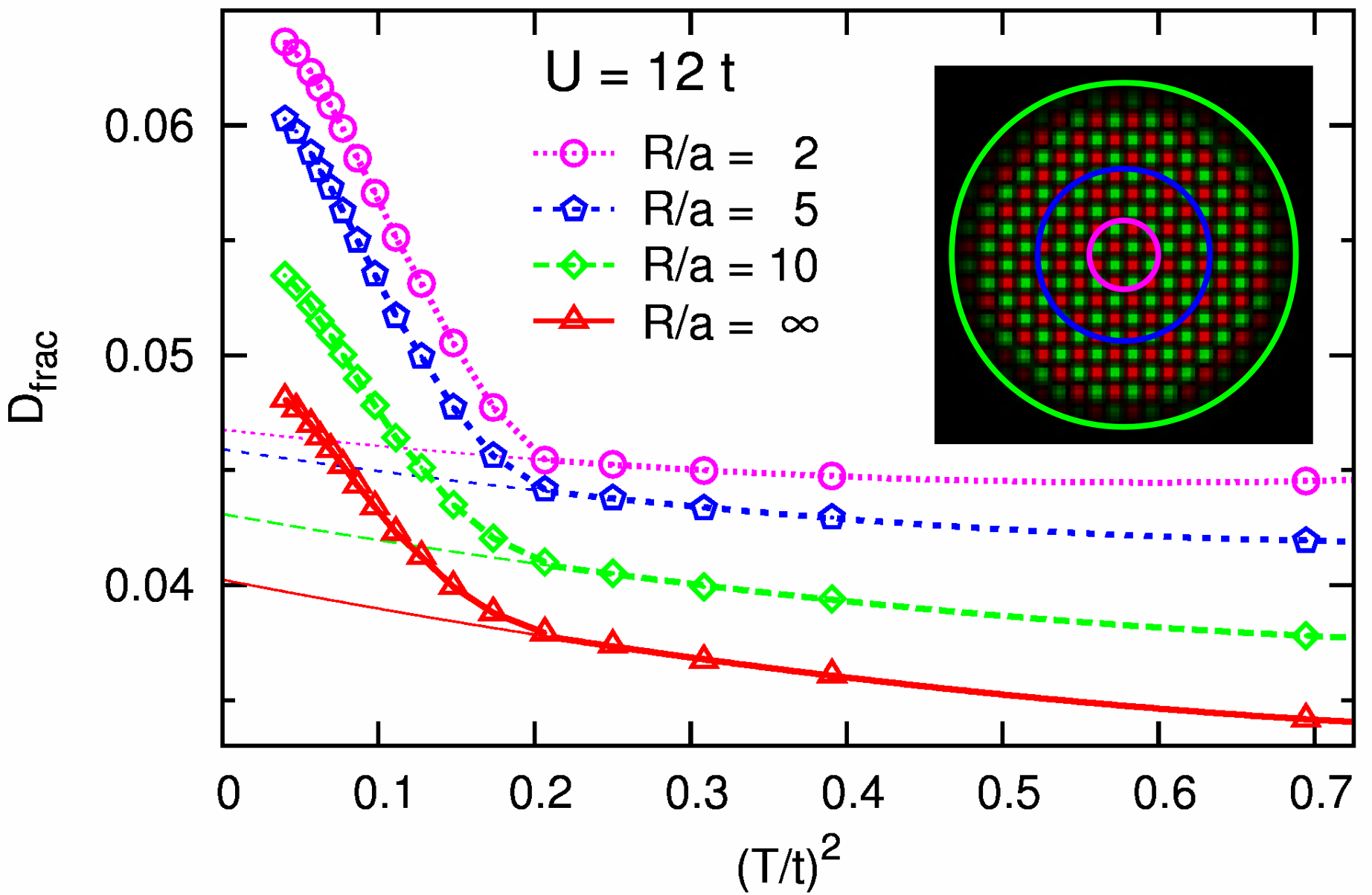
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



Strong proximity effects beyond LDA (thin lines)

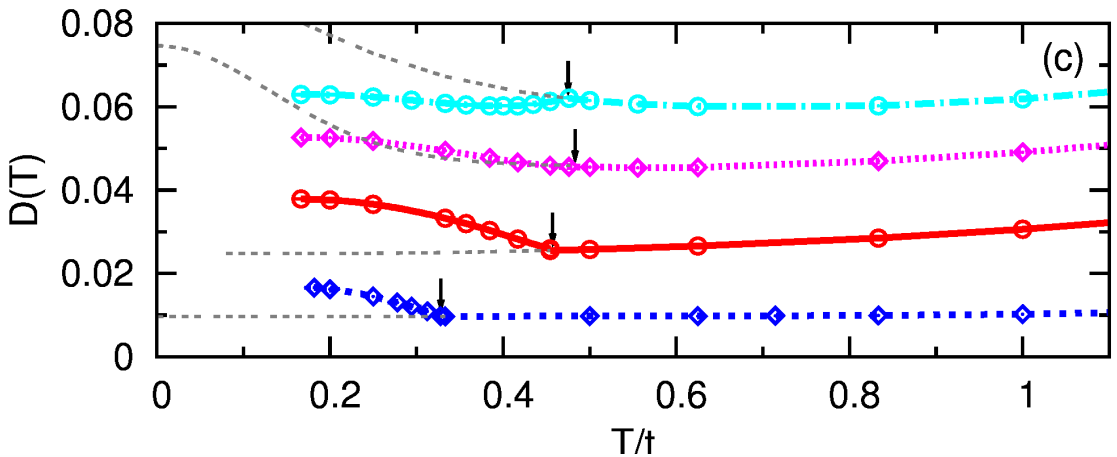
significant enhancement of D only at strong coupling

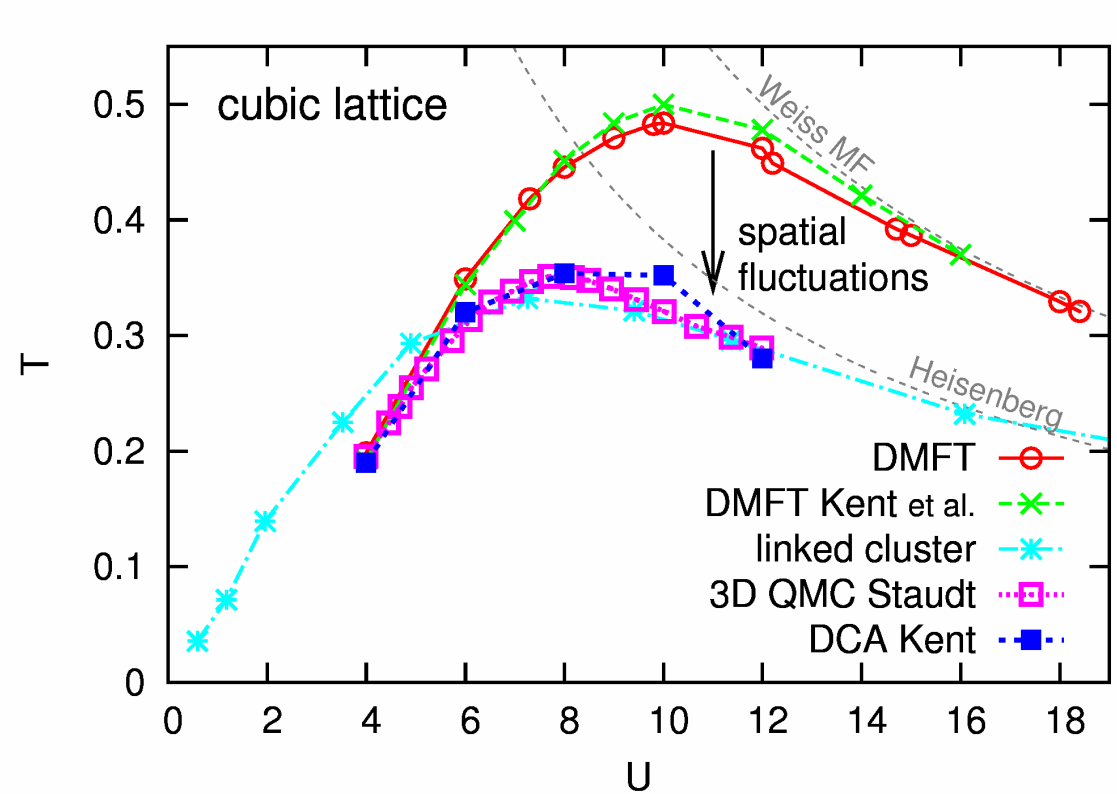
Néel transition visible in integrated quantities? Yes!



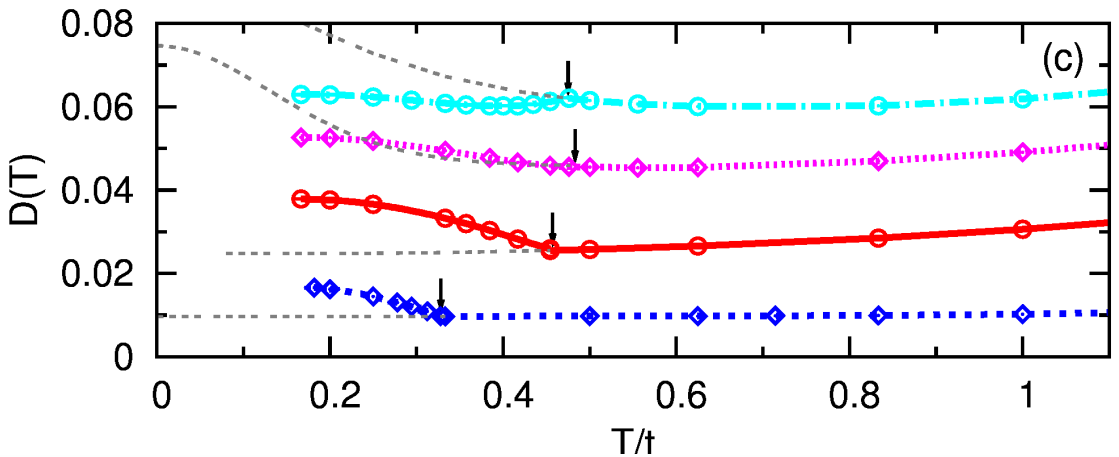
Effects of nonlocal correlations?

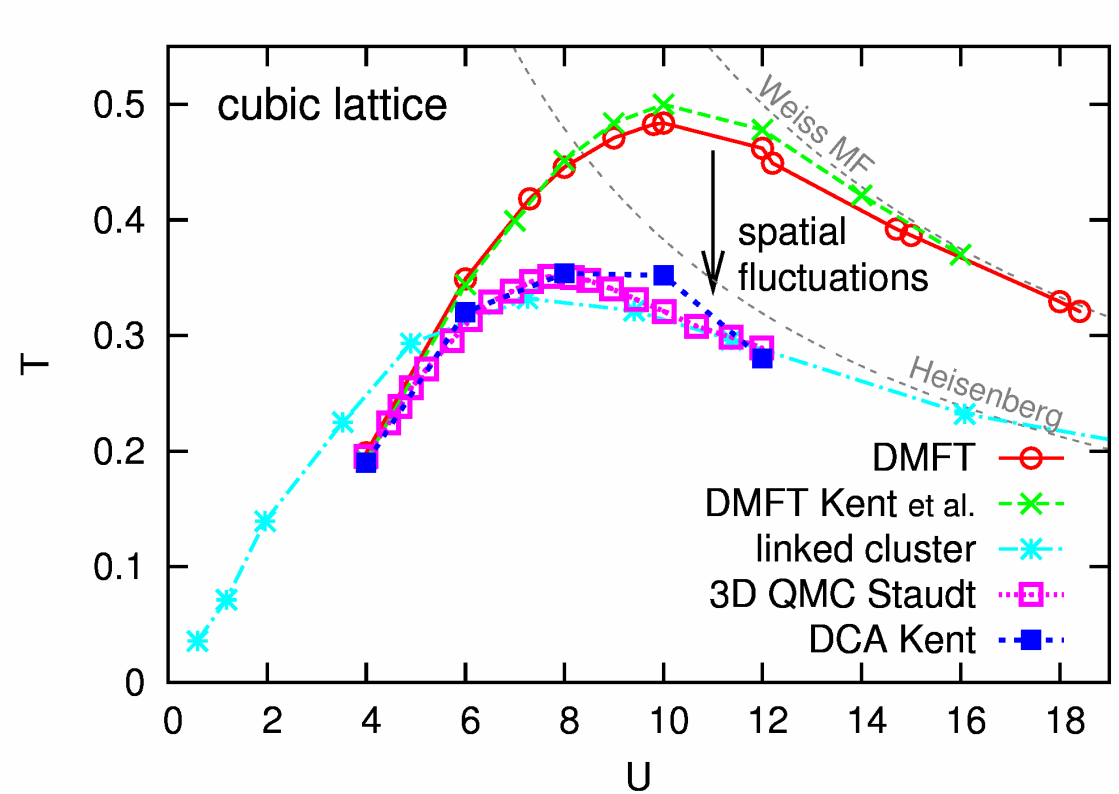
Modification of DMFT predictions by spatial fluctuations in 3d: how?





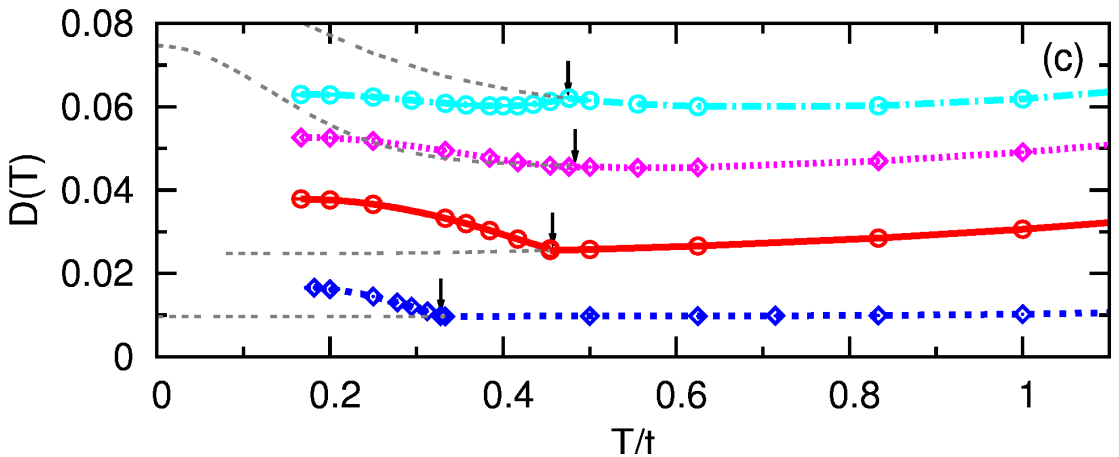
Modification of DMFT predictions by spatial fluctuations in 3d: how?

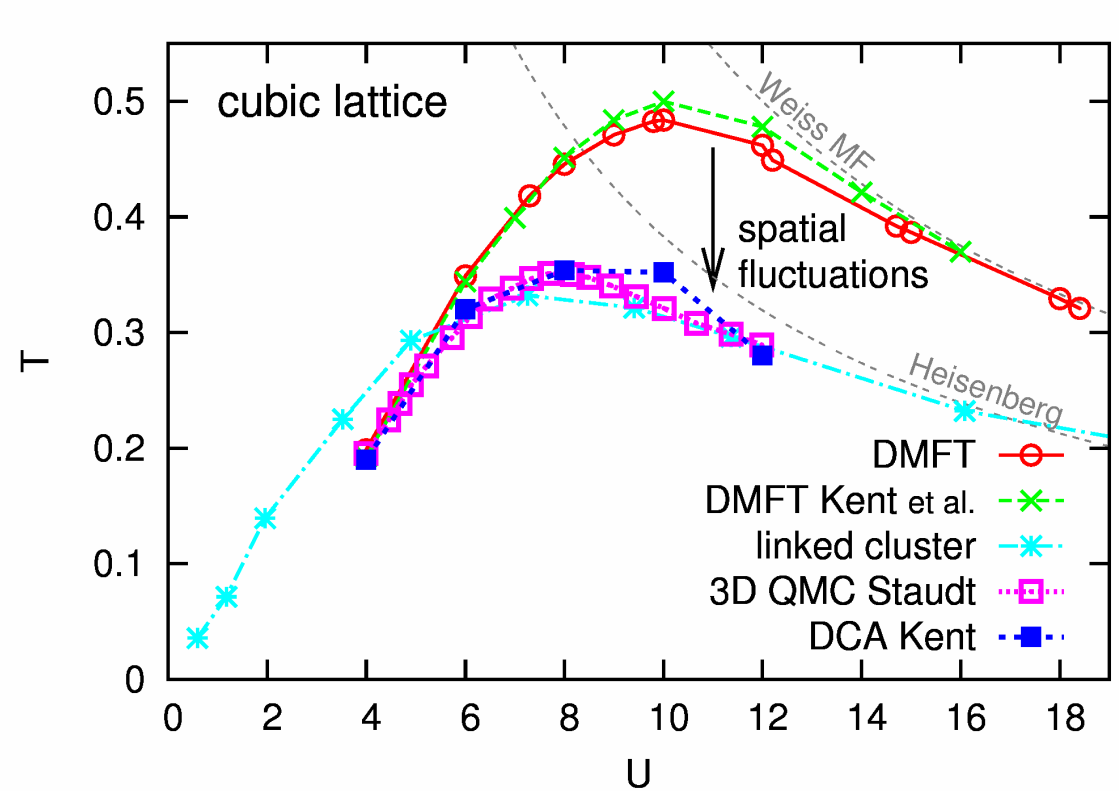




Unavoidable change: kinks cannot remain at $T = T_N^{DMFT} > T_N$!

Modification of DMFT predictions by spatial fluctuations in 3d: how?





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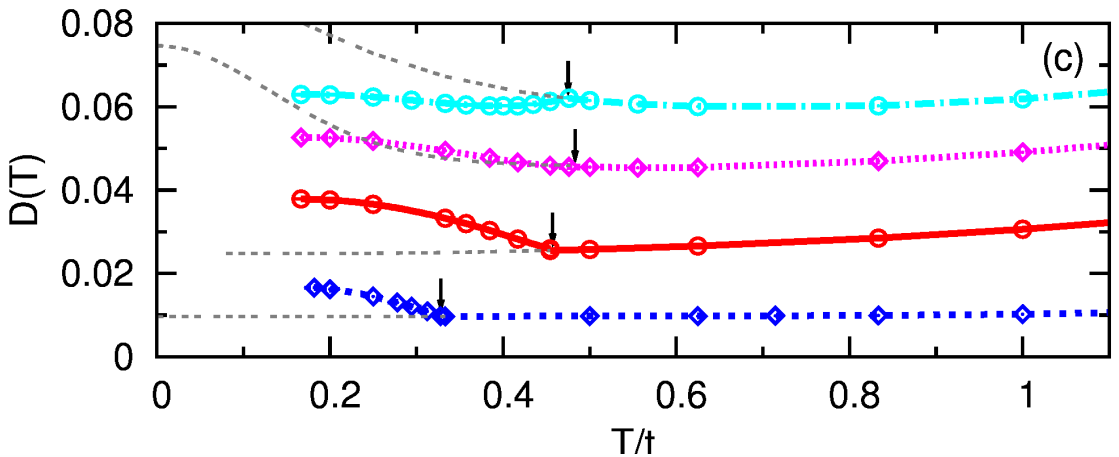
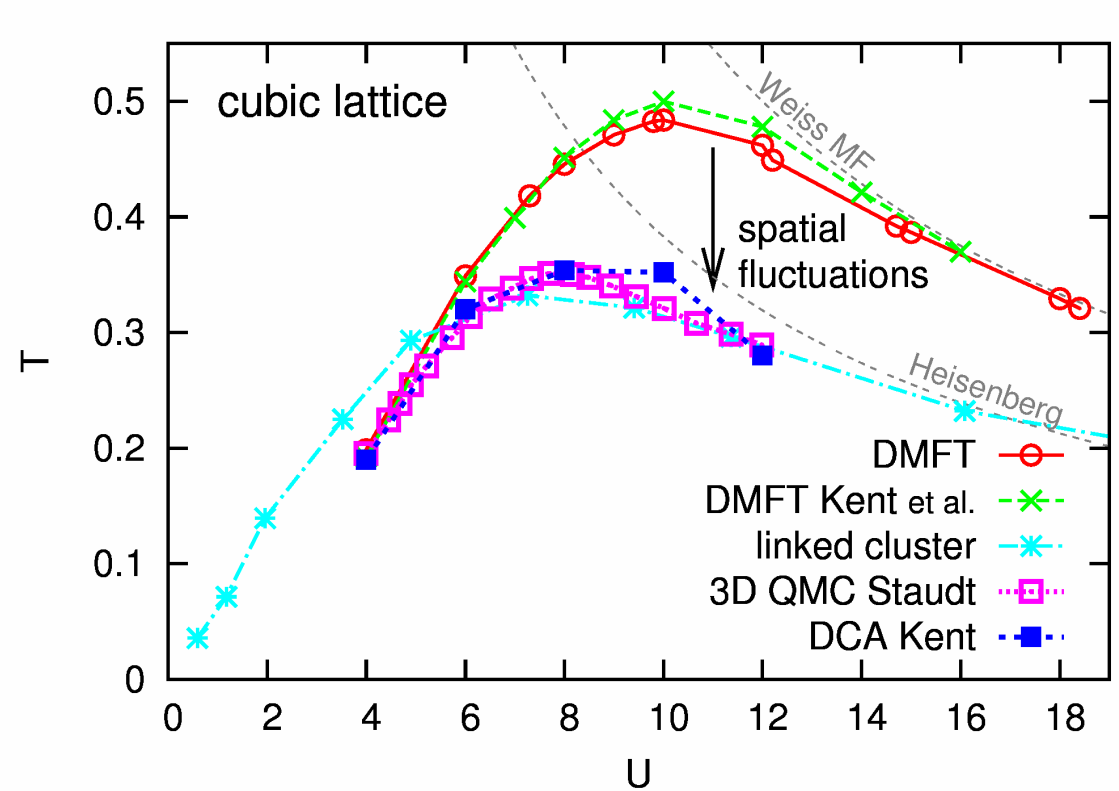
Constraints:

- DMFT results for D(T) agree with high-T expansion at $T >> T_N$

[Jördens et al., PRL (2010)]

Modification of DMFT predictions by spatial fluctuations in 3d: how?





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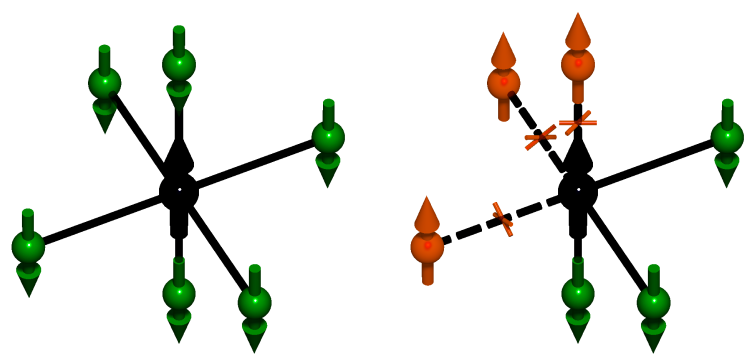
- argument for $D_{AF}/D_{para} \overset{U\to\infty}{\longrightarrow} 2$ is independent of dimension



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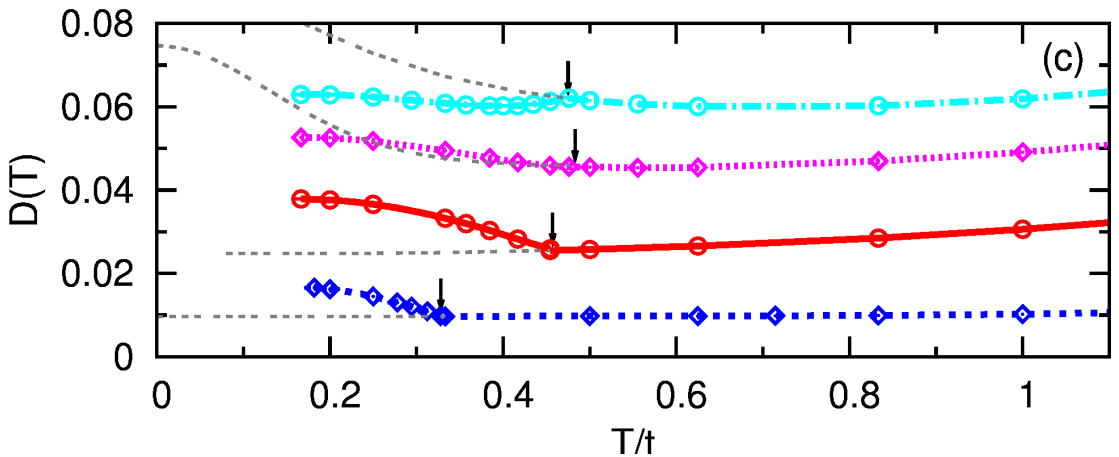

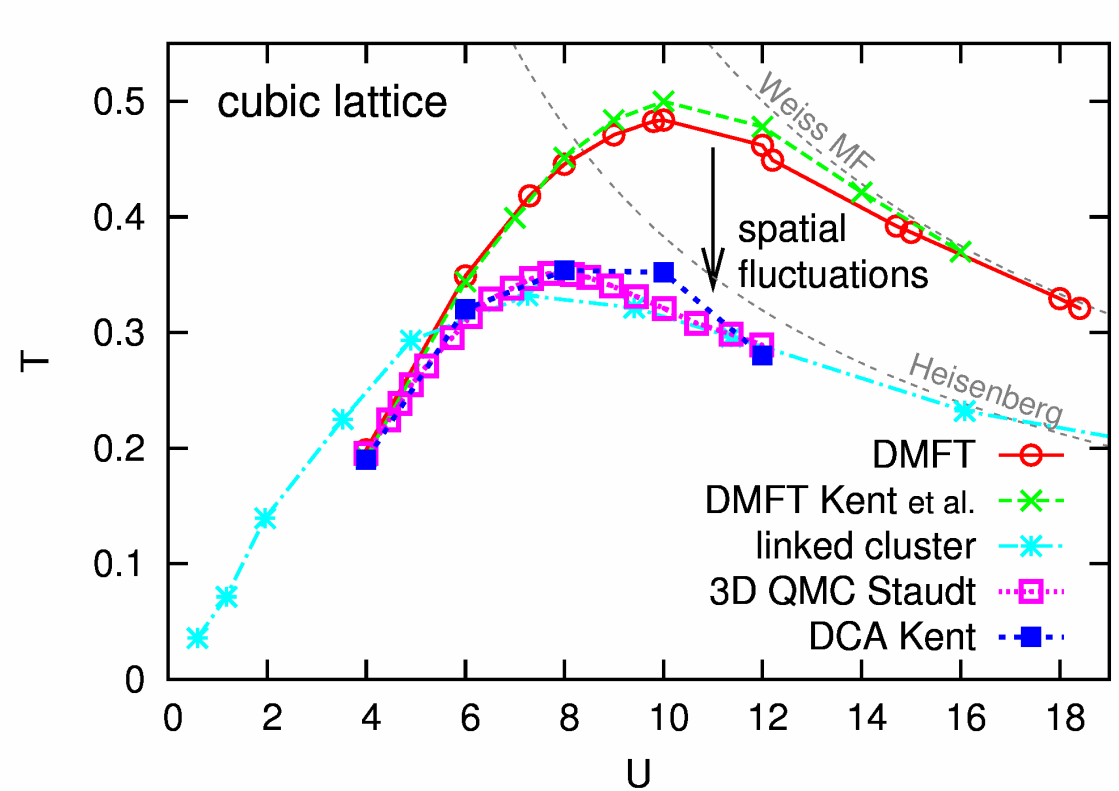

Unavoidable change: kinks cannot remain at $T = T_N^{DMFT} > T_N$!

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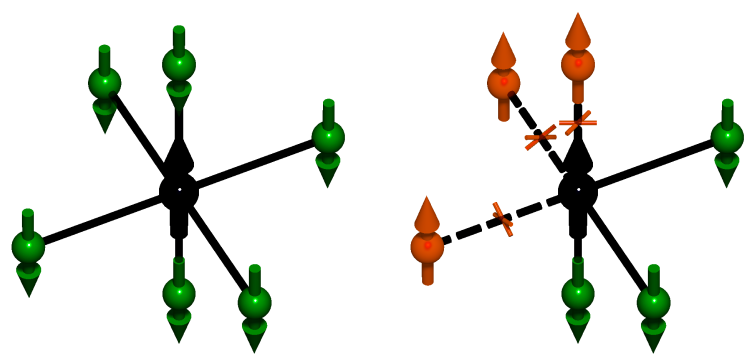
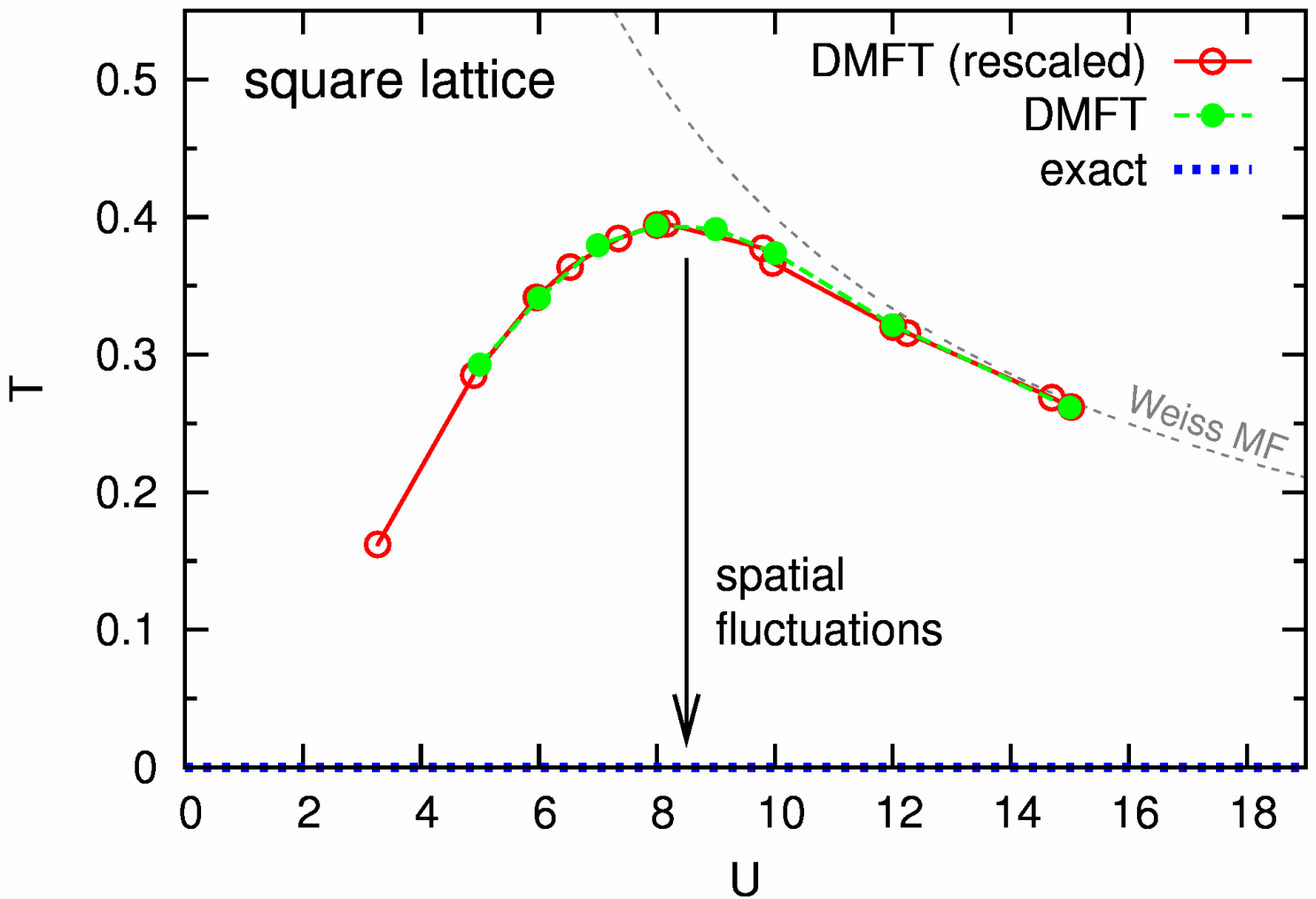


and independ. of long-range order

Situation "worse" in 2d: no antiferromagnetism at finite T!



Will any enhancement of D at low T remain? At which temperature scale?

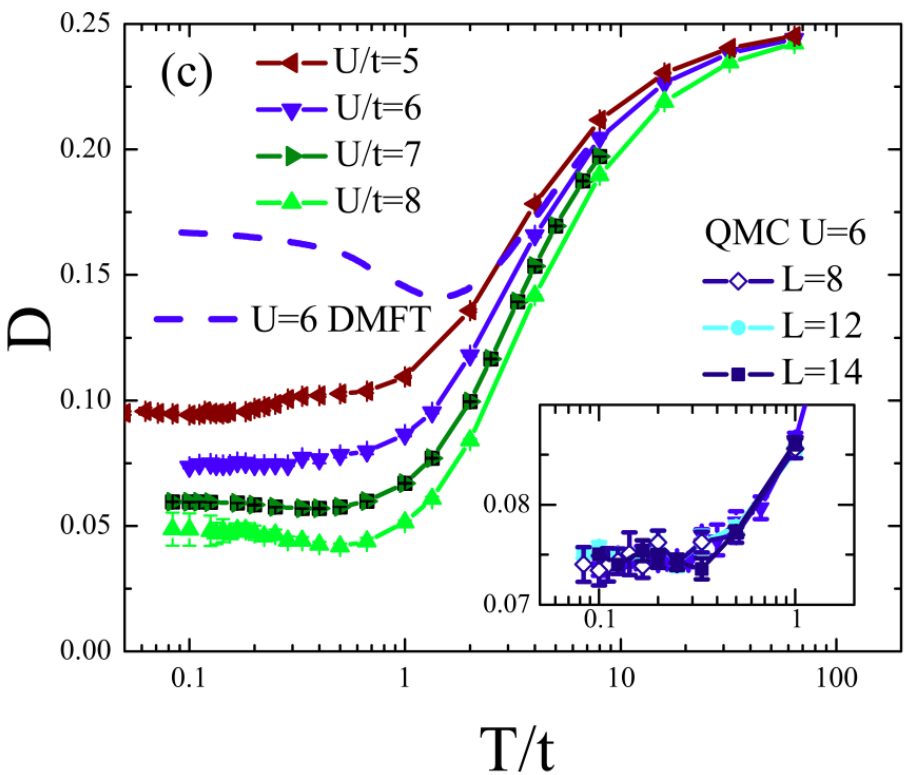
How large are the DMFT errors in $D(T)$ for $T \gtrsim T_{\mathrm{N}}^{\mathrm{DMFT}}$?

Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity

Thereza Paiva,[1] Richard Scalettar,[2] Mohit Randeria,[3] and Nandini Trivedi[3]

[1]*Instituto de Fisica, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[2]*Department of Physics, University of California, Davis, California 95616, USA*
[3]*Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA*

(Received 18 June 2009; published 11 February 2010)



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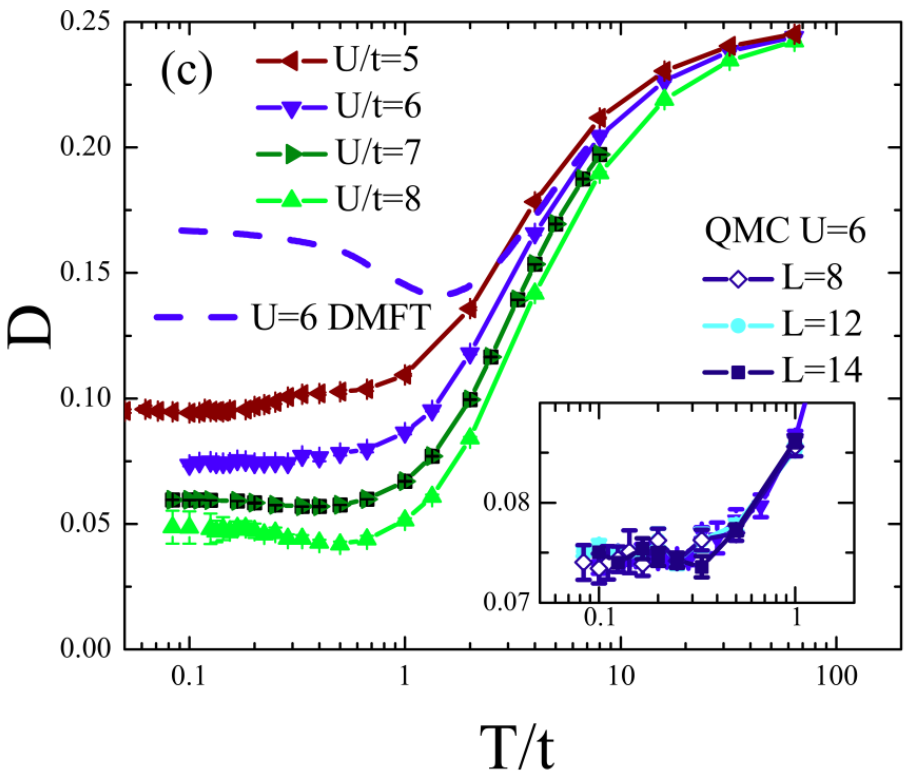

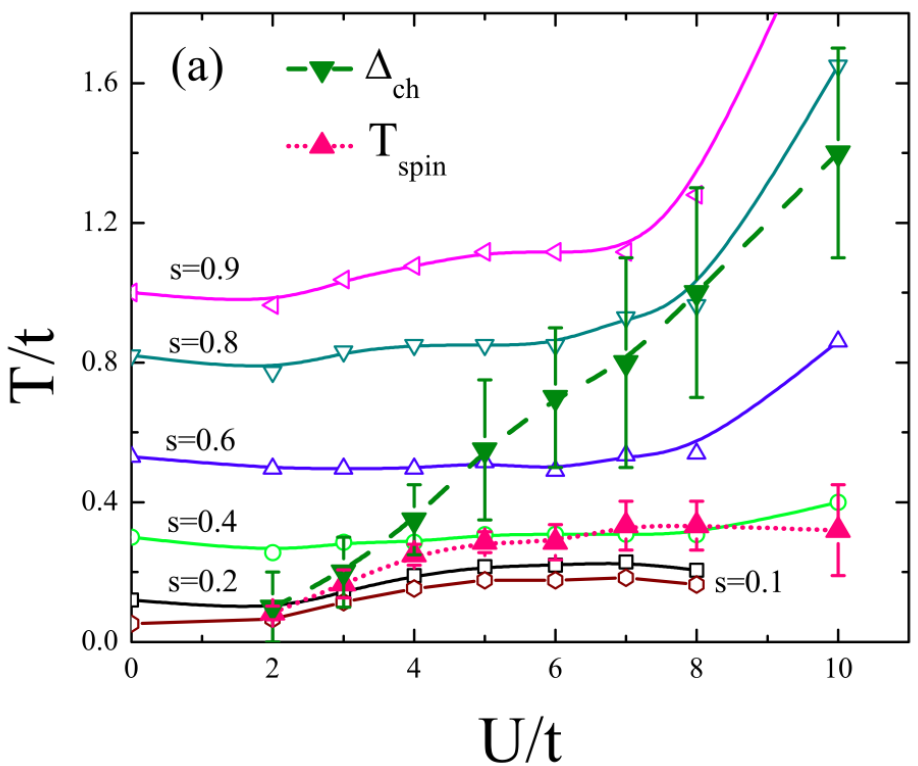

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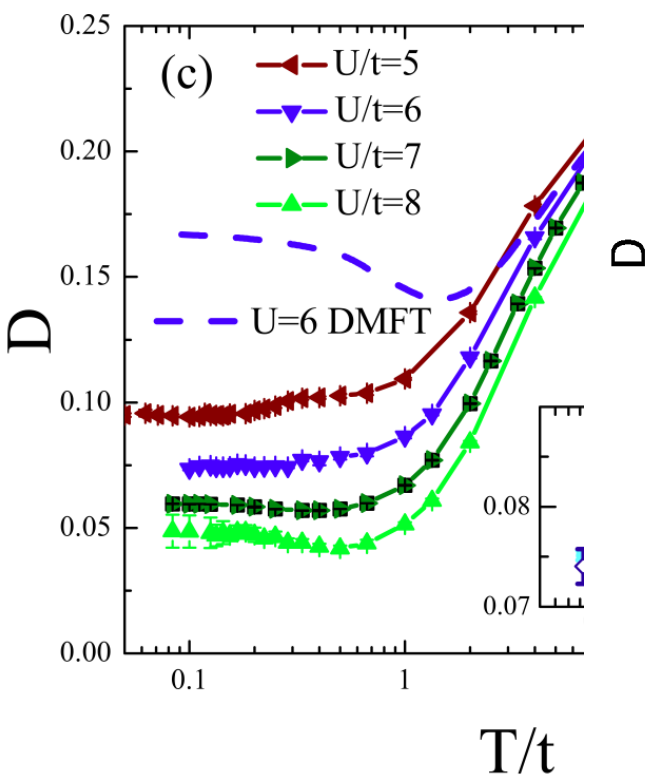
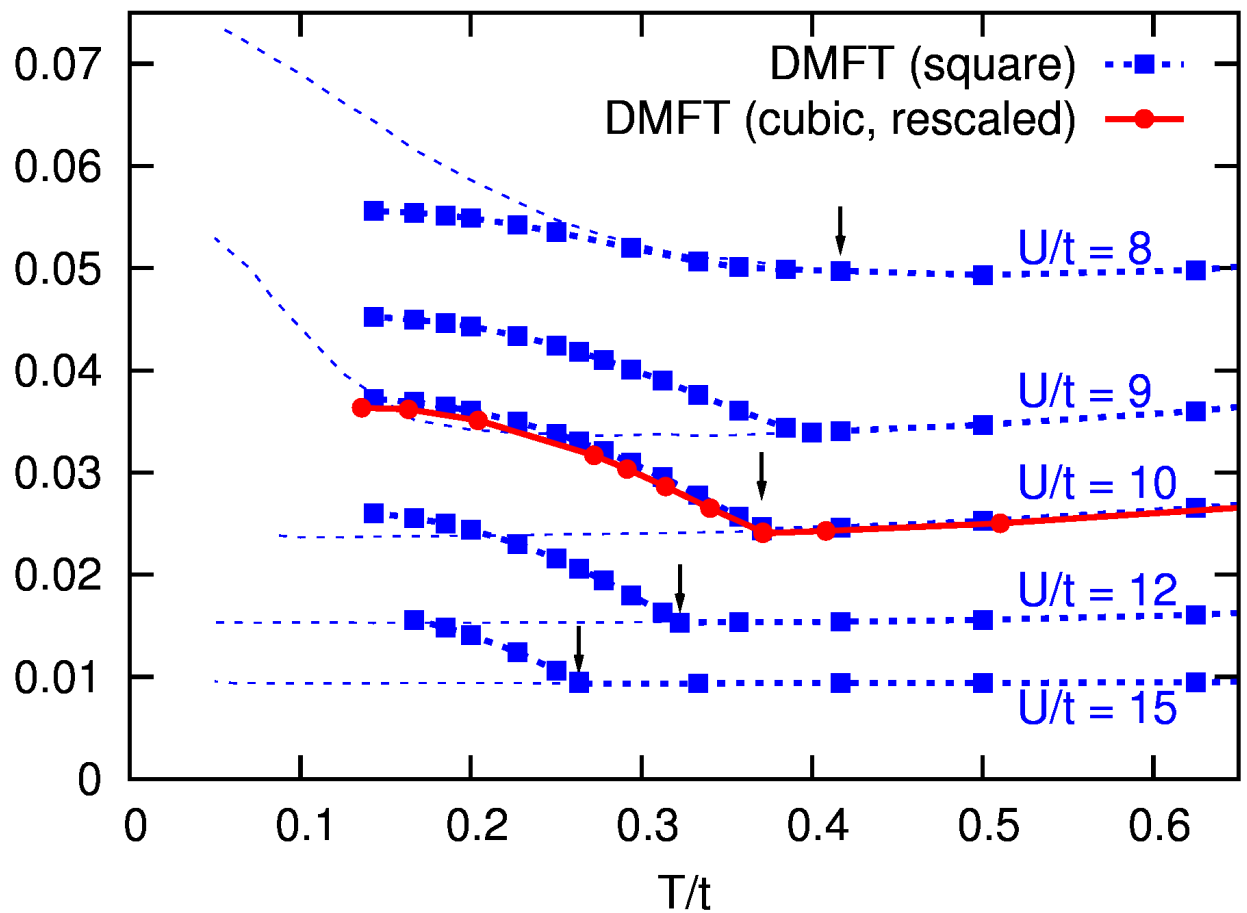
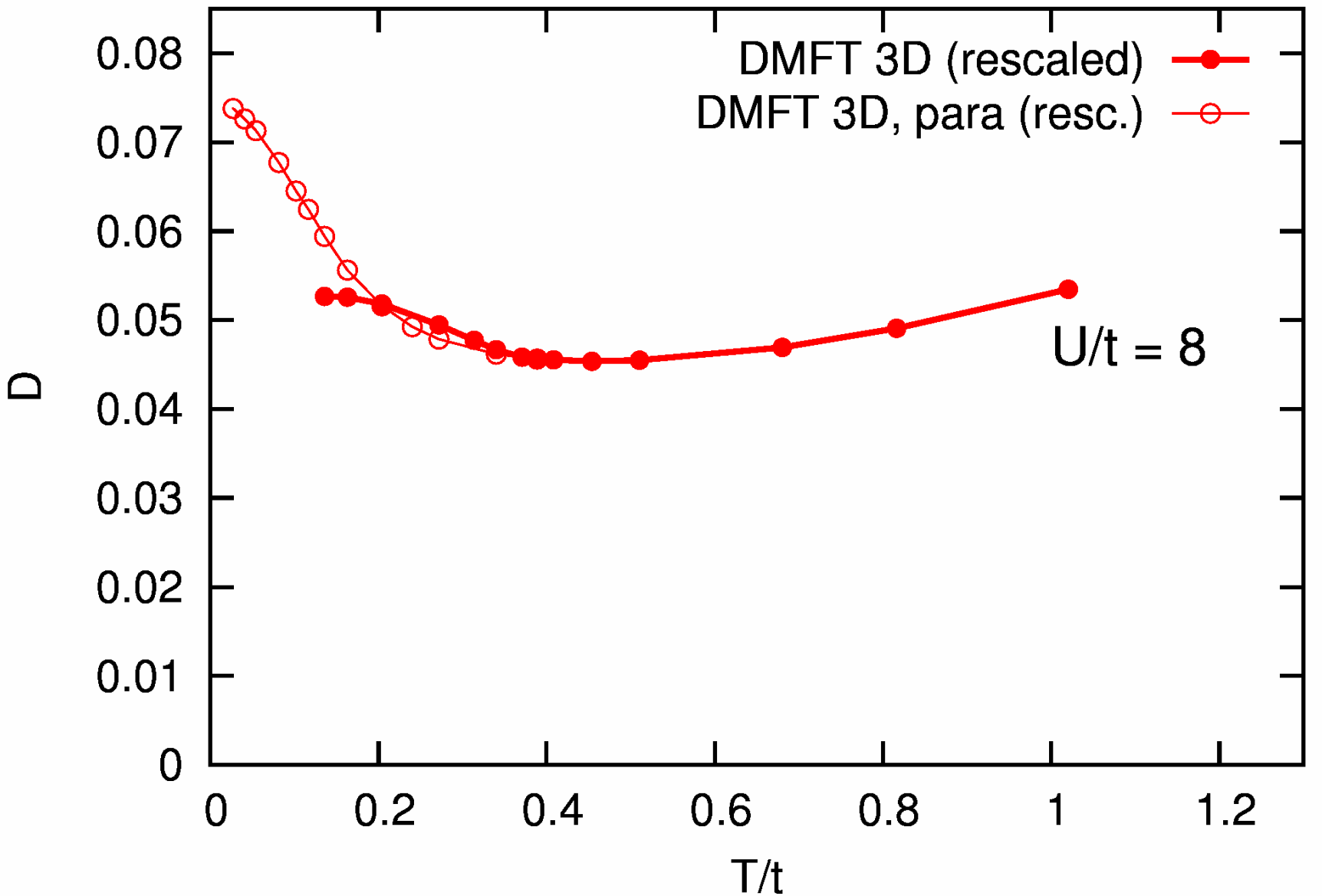




Comparison DMFT – direct QMC for the 2d square lattice



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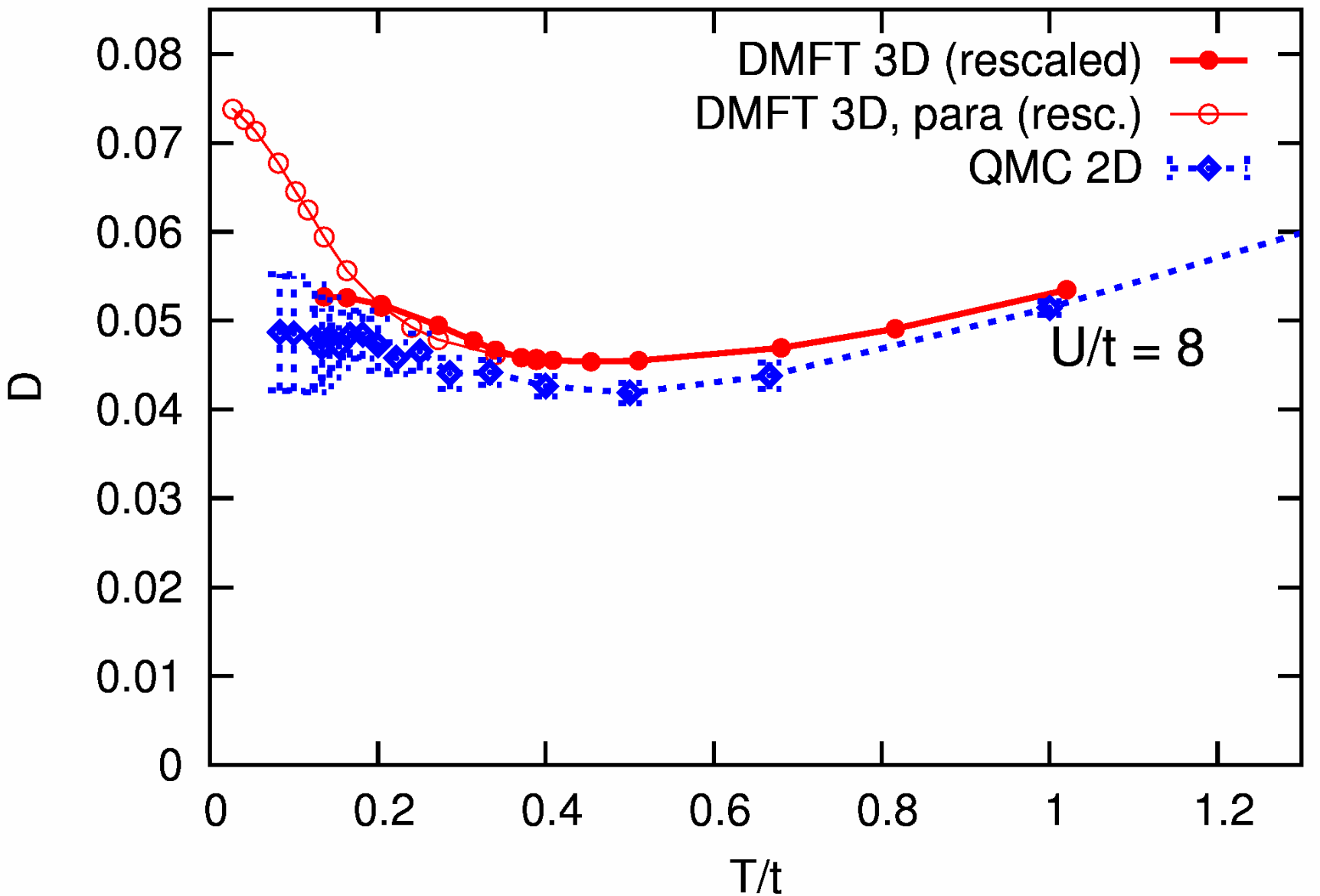

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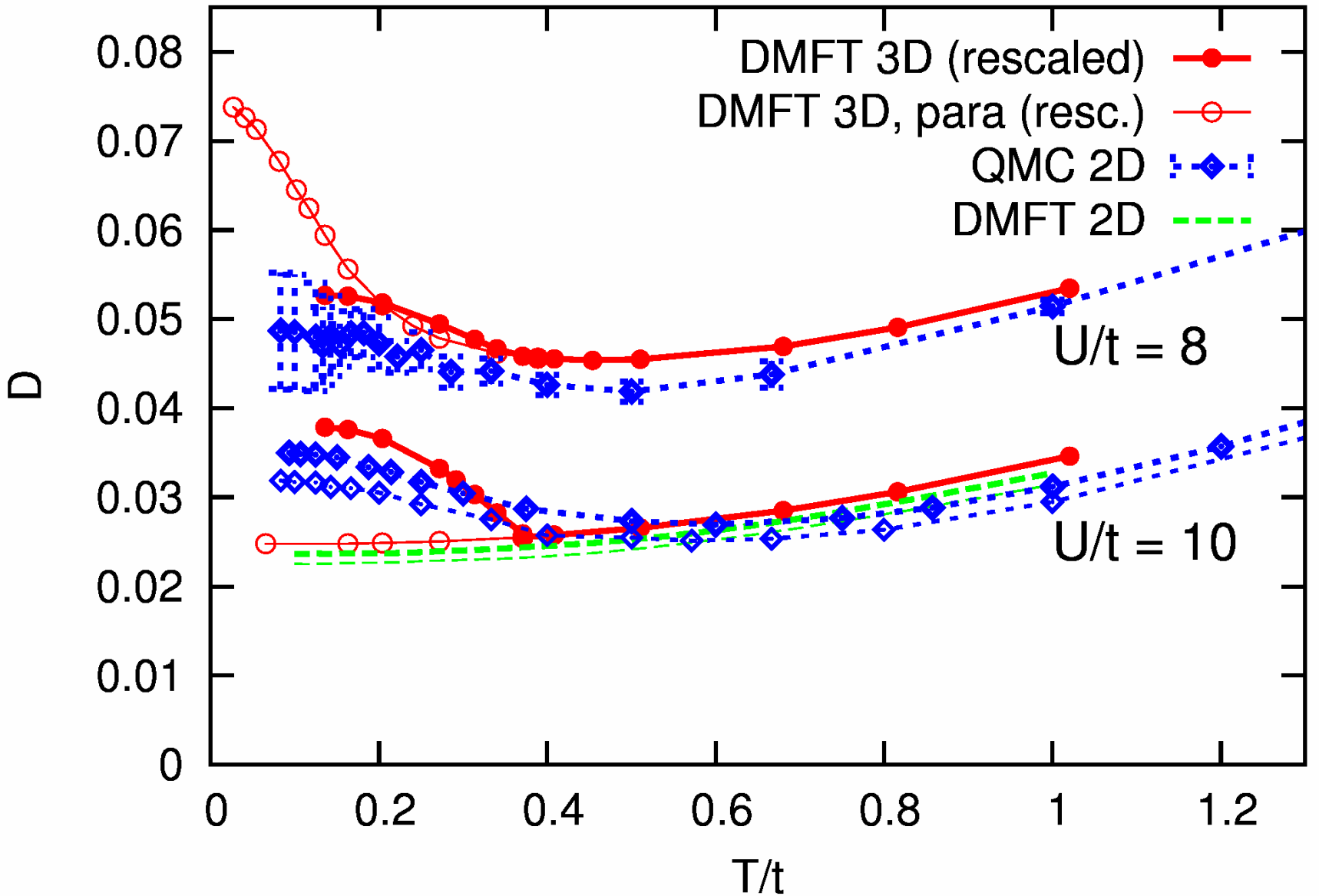
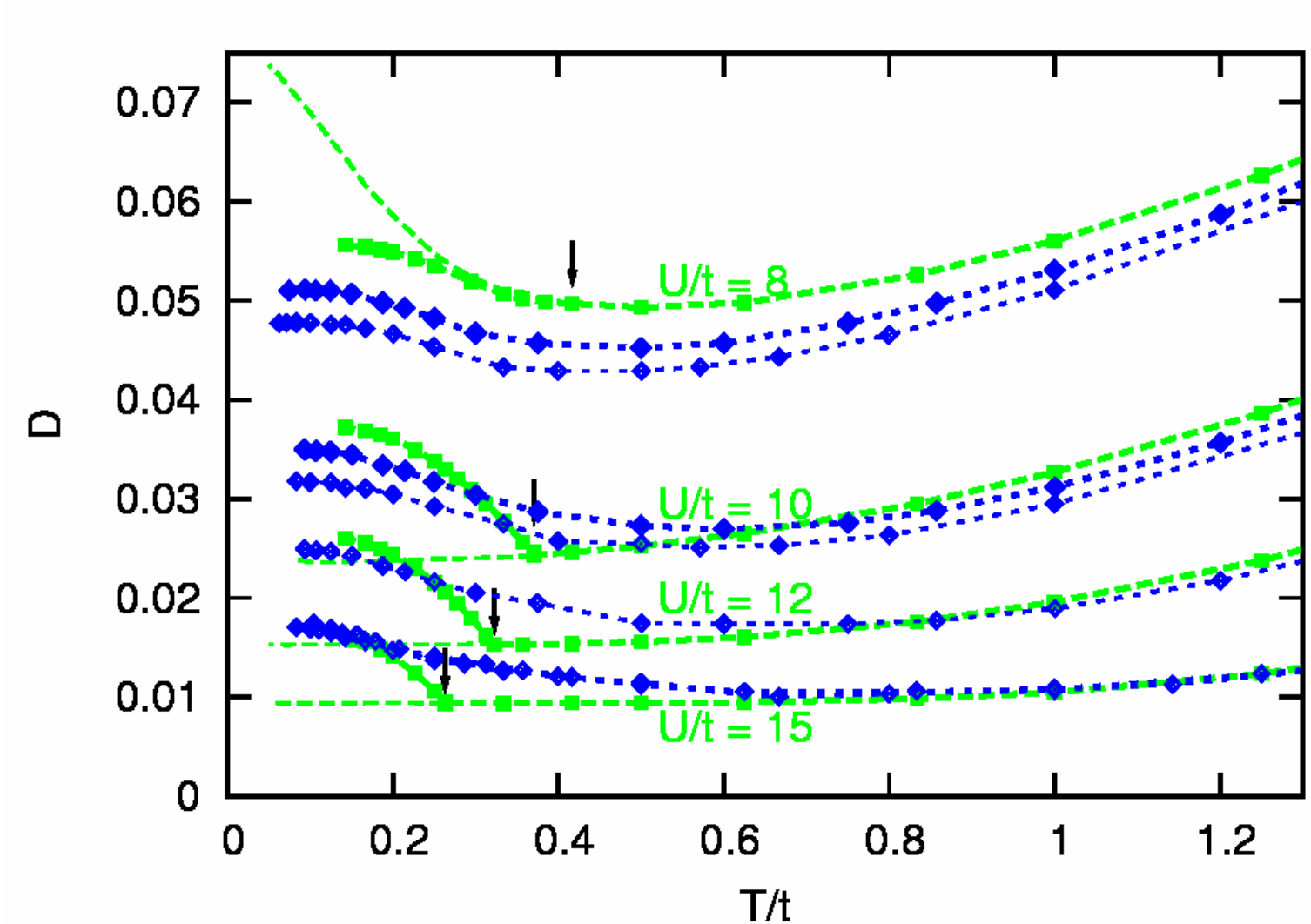
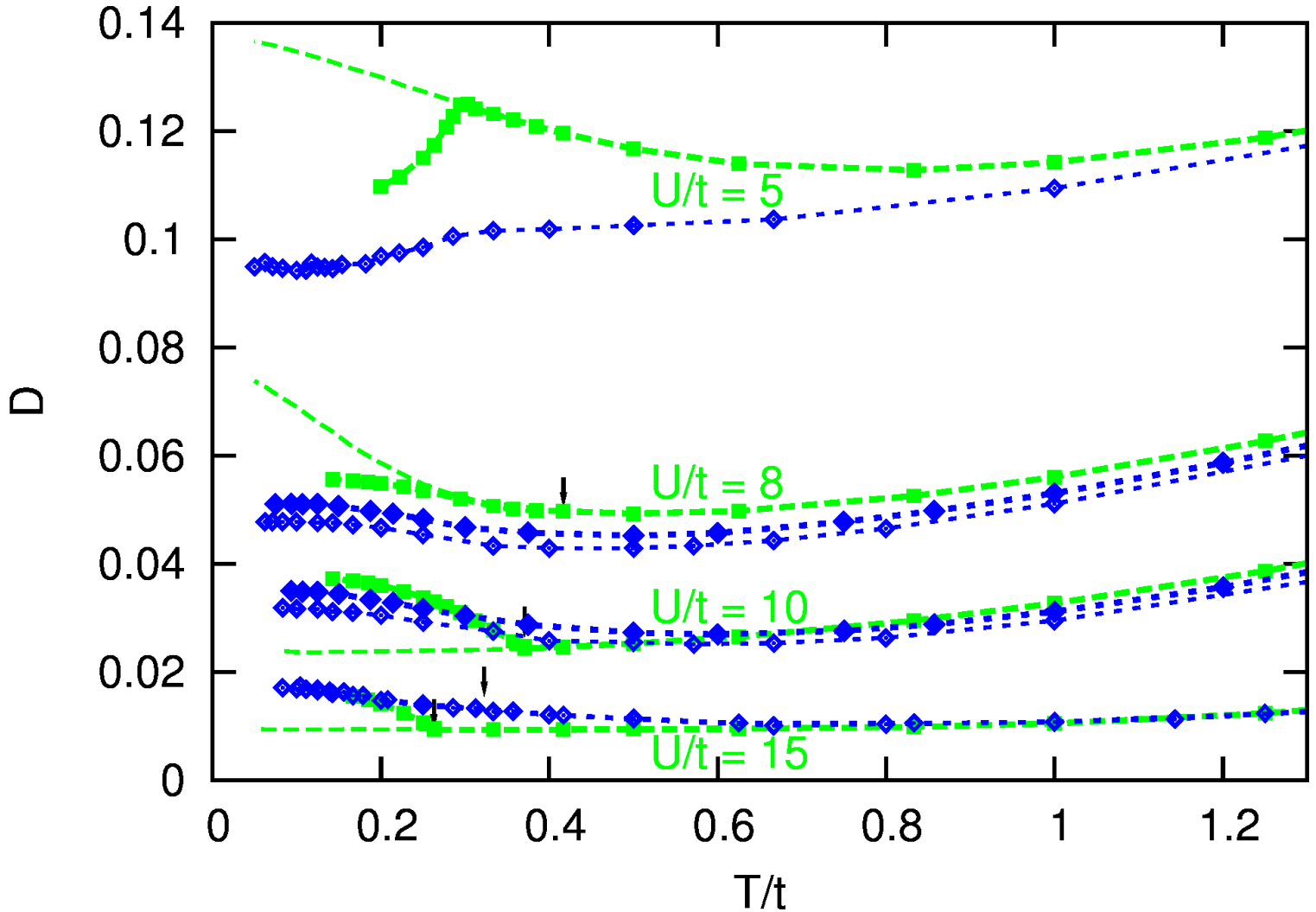




green: DMFT, blue: BSS-QMC (thicker lines: smaller $\Delta\tau$)

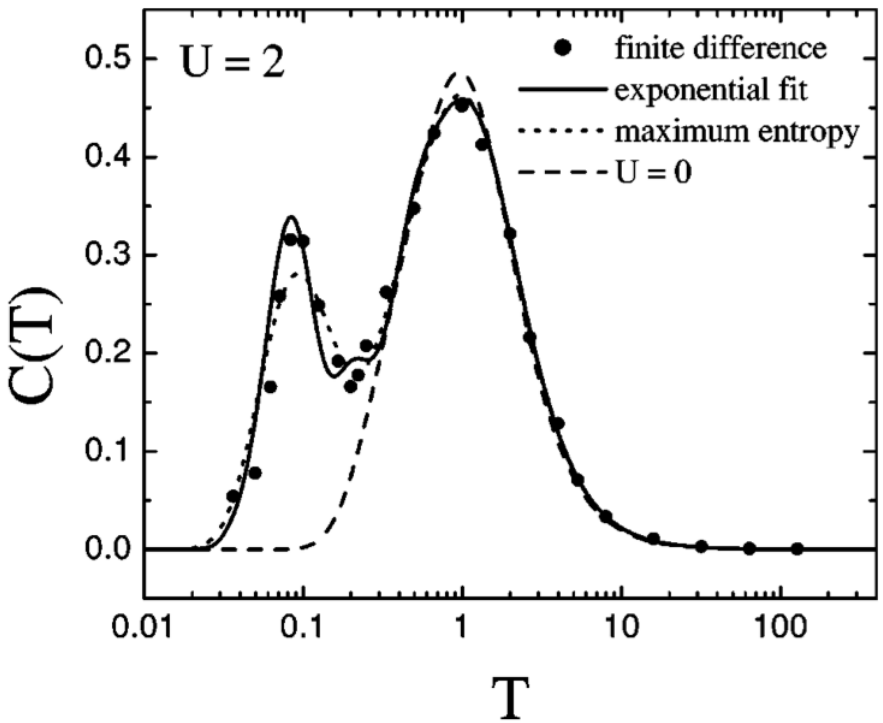
excellent agreement at $U = 8$; rounding off at $T \gtrsim T_N^{\mathrm{DMFT}}$ for larger U

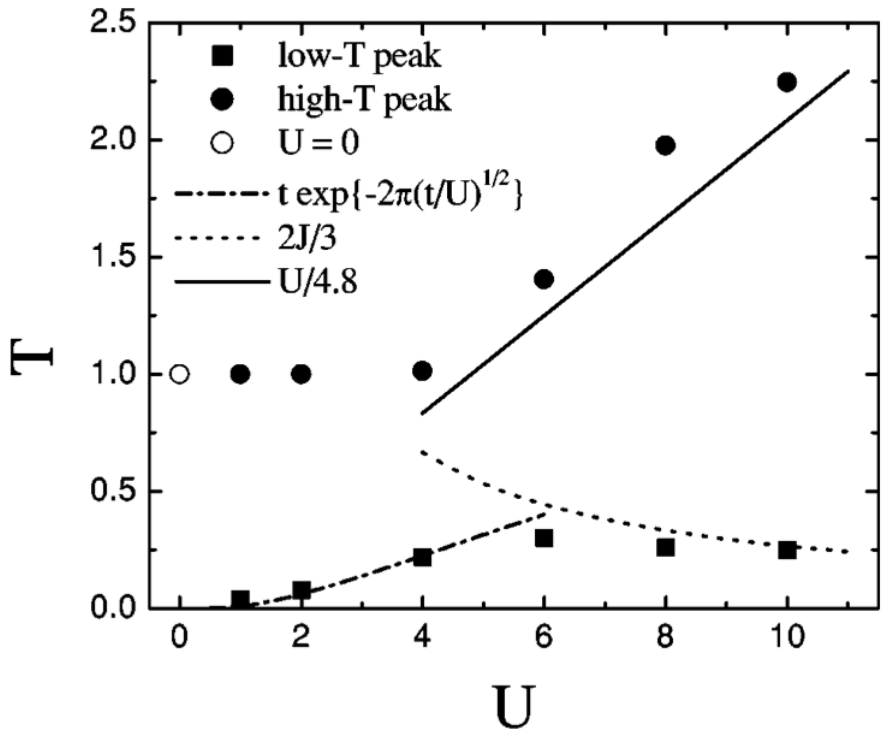
Even the low-T suppression of D at small U corresponds with direct QMC:



How is this possible? How much better is the agreement in 3 dimensions?

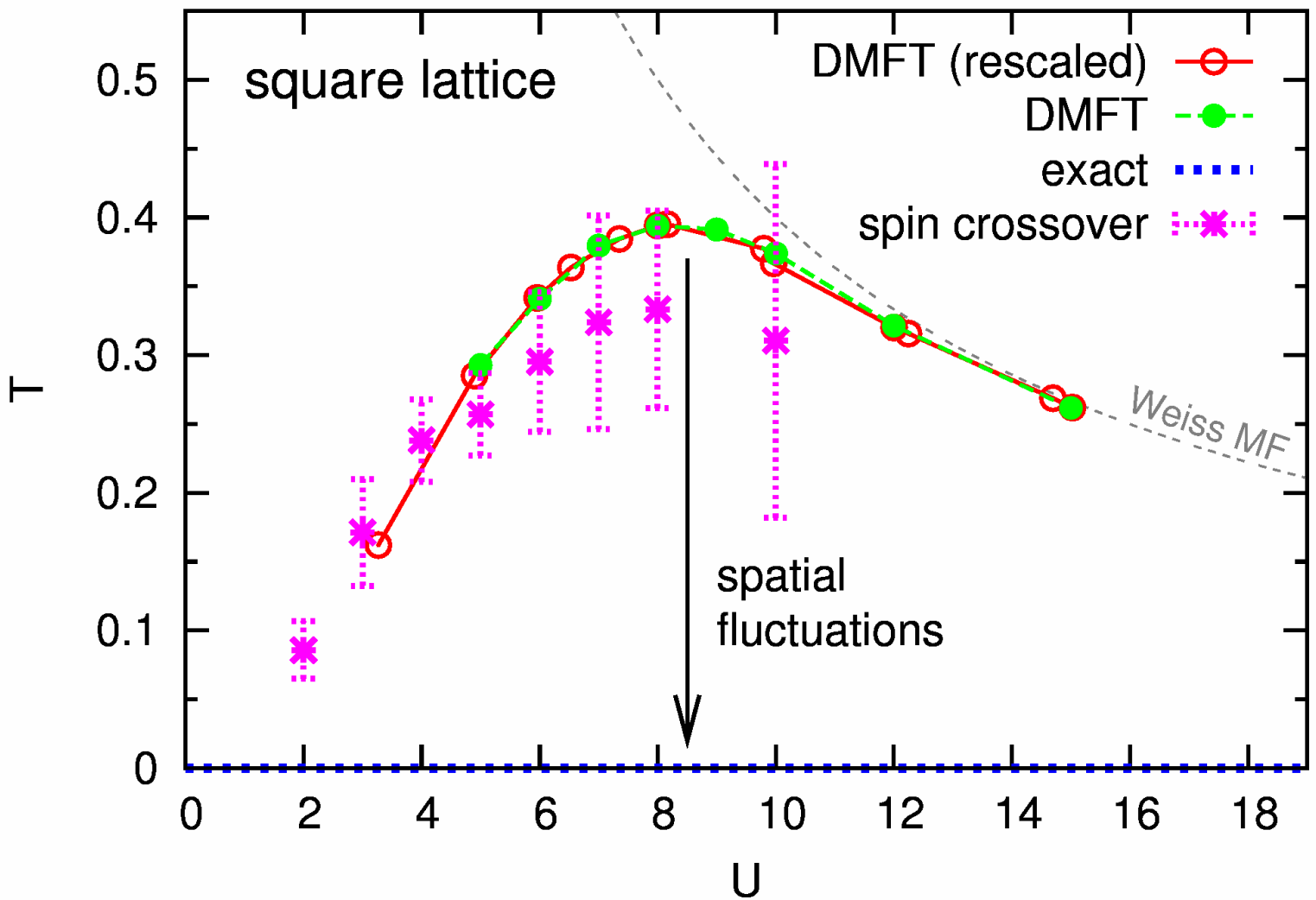
Spin crossover scale in 2 dimensions – definition?





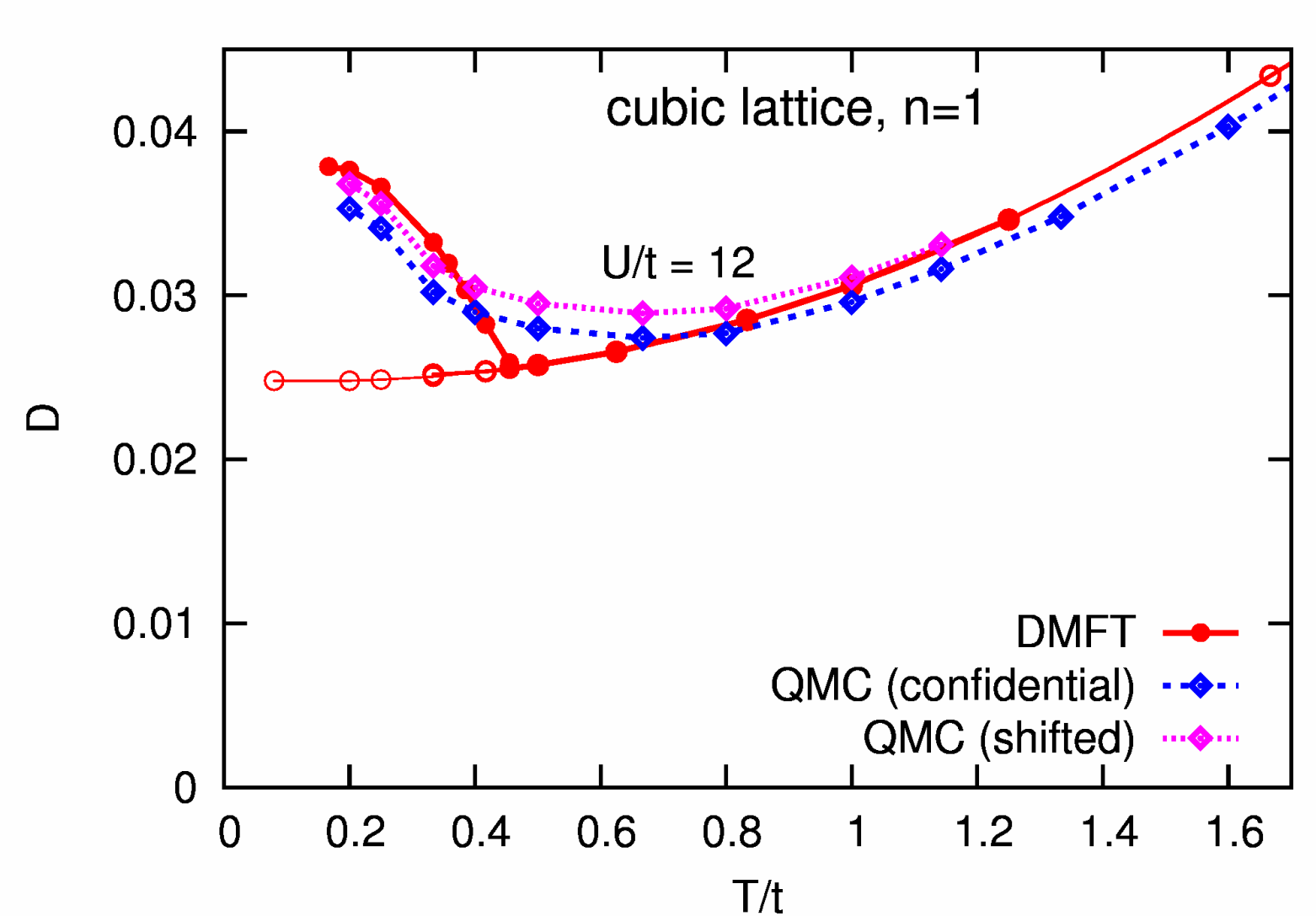
[Paiva, Scalettar, Huscroft, McMahan, PRB (2001)]

Comparison for square lattice: spin crossover temperature vs. T_N^{DMFT}



Nearly perfect agreement!!!

Comparison in 3 dimensions



Summary

Multigrid HF-QMC method: numerically exact (quasi CT) + efficient

Mott transition for 3 degenerate flavors in (U, T, μ) space

Novel semi-compressible phase, spectra, small lattice effects

[E. V. Gorelik, N. Blümer, Phys. Rev. A **80**, 051602(R) (2009)]

Real-space DMFT study of antiferromagnetism

Efficient and flexible RDMFT-QMC code

AF order at finite T signaled by enhanced D

Proximity effects important – LDA deficient

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

DMFT surprisingly accurate in low dimensions

Outlook

3D calculations for realistic trap parameters and system sizes

Inequivalent spins/flavors: OSMT-like physics, ordered phases

Multigrid HF-QMC for RDMFT; impact of higher Bloch bands

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3D calculations for realistic trap parameters and system sizes

Inequivalent spins/flavors: OSMT-like physics, ordered phases

Multigrid HF-QMC for RDMFT; impact of higher Bloch bands

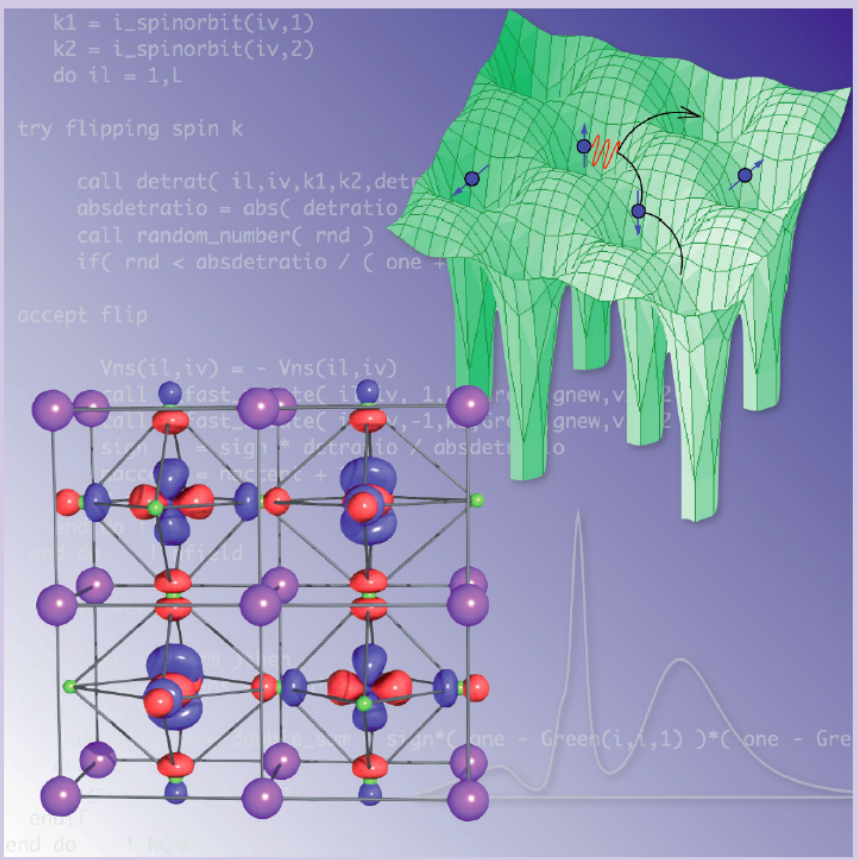
Spin-off: solids with large unit cells (distortions, surfaces, impurities, . . .)

Thanks to: E. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek,
U. Schneider, I. Bloch, H. Moritz, L. Tarruell,
R. Scalettar, T. Paiva, and DFG (TR49)

General method development: new initiative DFG-FG 1346

Positive evaluation on 2010/04/15+16, senate decision on 2010/06/30.

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



Dieter Vollhardt, University of Augsburg (Spokesperson)
Alexander Lichtenstein, University of Hamburg (Co-Spokesperson)

General method development: new initiative DFG-FG 1346

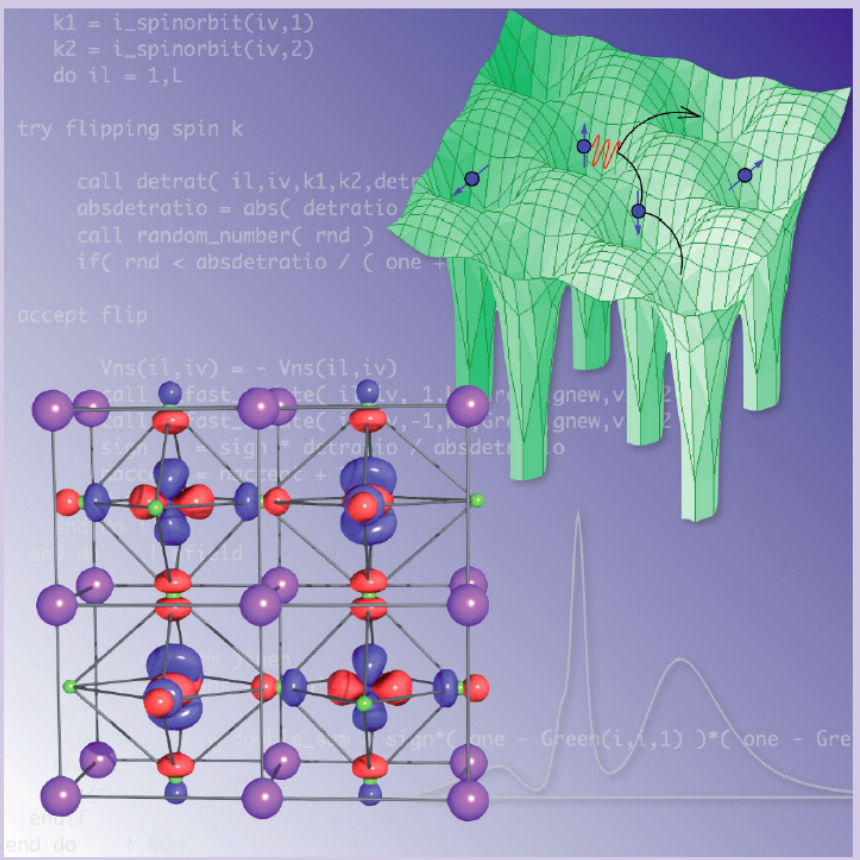
Positive evaluation on 2010/04/15+16, senate decision on 2010/06/30.

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

P7: GW+DMFT (Held,Toschi,Kresse)

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



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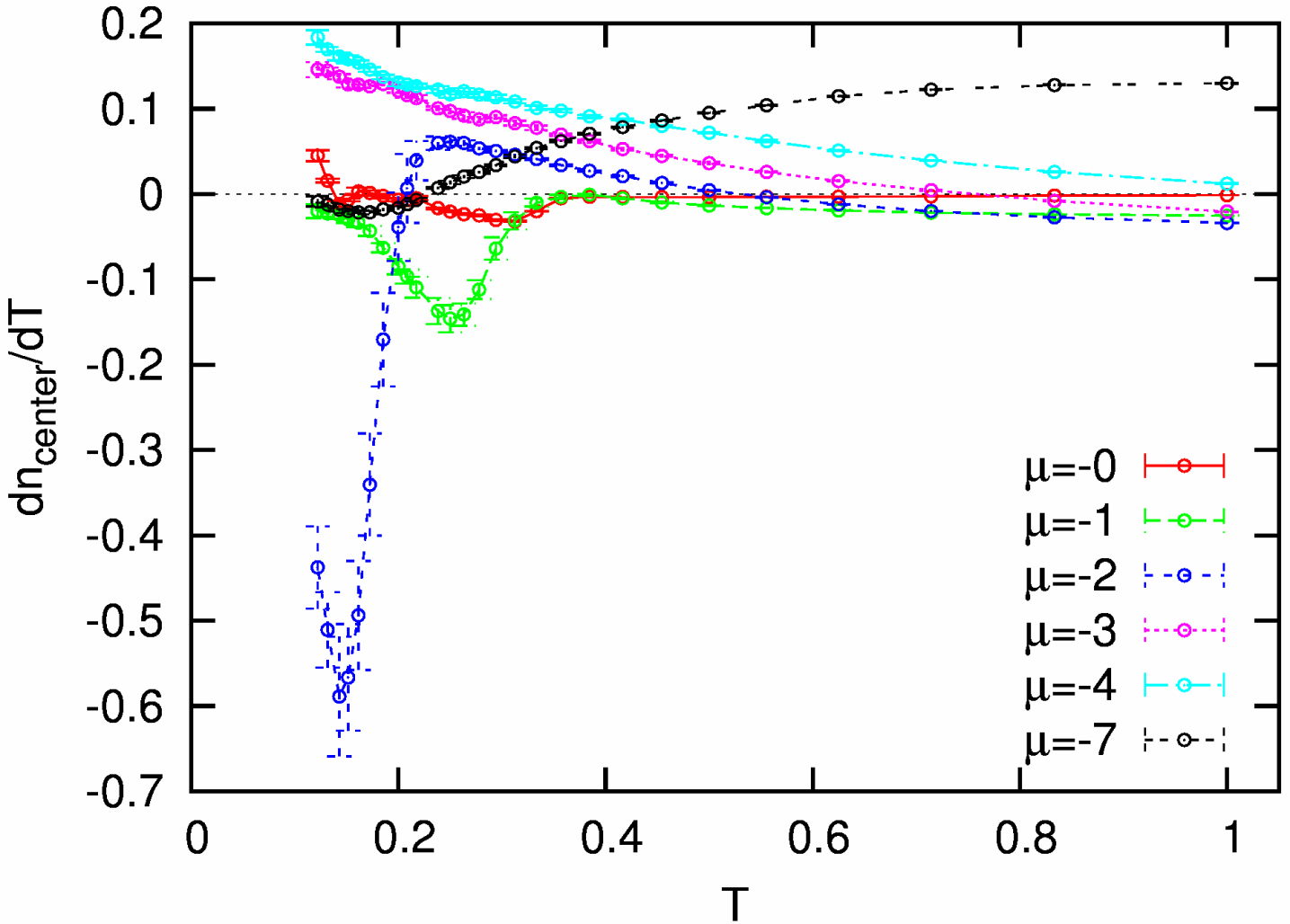
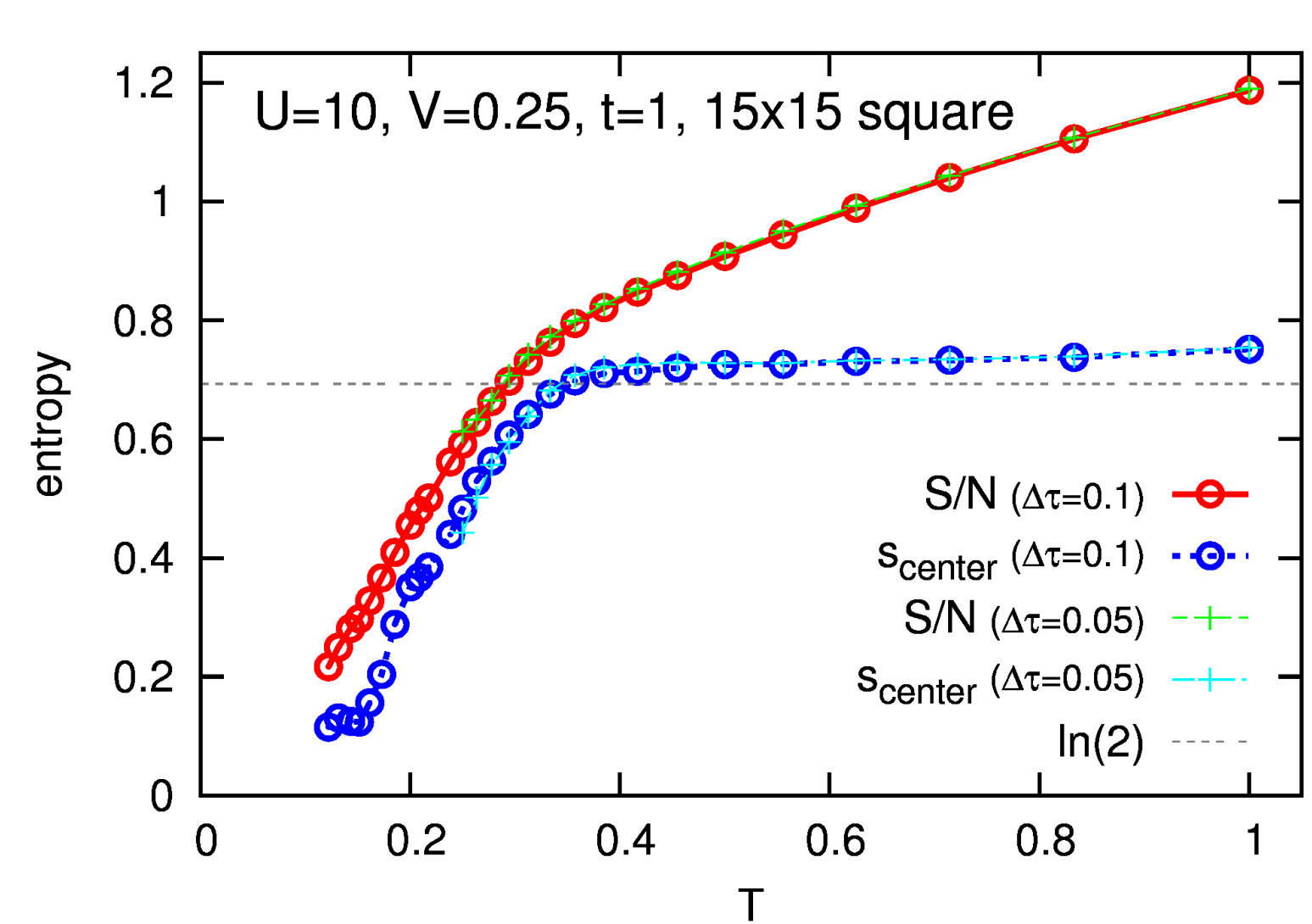
Entropy: no direct computation, but from relations such as $dS/d\mu = dN/dT$



Example: derivative of central density (at $U/t = 10$, $V/t = 0.25$) for square lattice

Strong negative peak at Neel temperature ($\rightsquigarrow$ need fine integration grid)



very small discretization dependence

Important: central entropy can be much smaller than average entropy!