

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

Nils Blümer and Elena Gorelik, Univ. Mainz

Outline

Introduction: SCES, cold atoms on lattices

Approaches for correlated lattice Fermi systems

Paramagnetic Mott transitions in 3-flavor mixtures

AF order at finite T in an optical trap (2D, 3D)

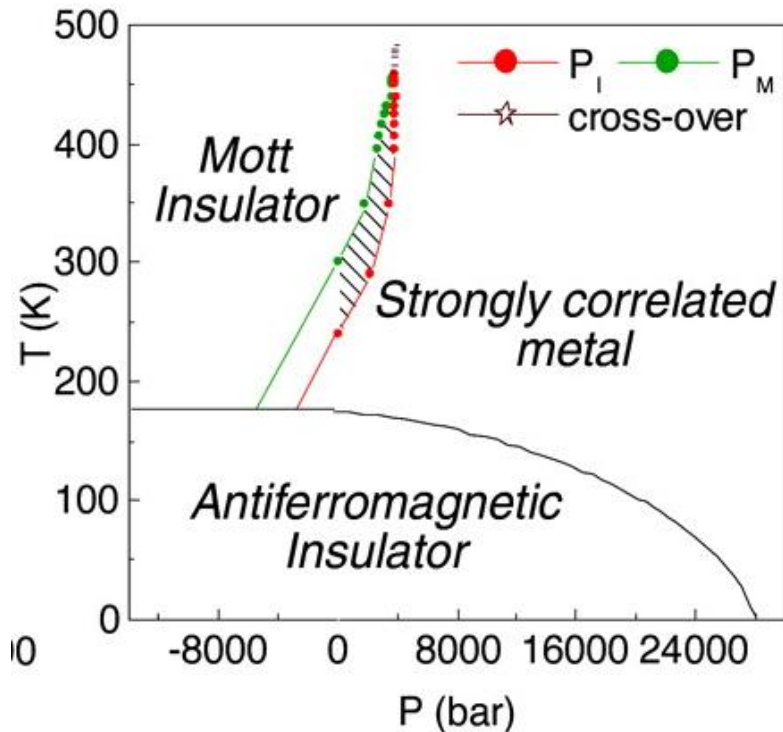
Summary and outlook

Systems with strong electronic/fermionic correlations

Paramagnetic Mott metal-insulator transition

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

Phase diagram

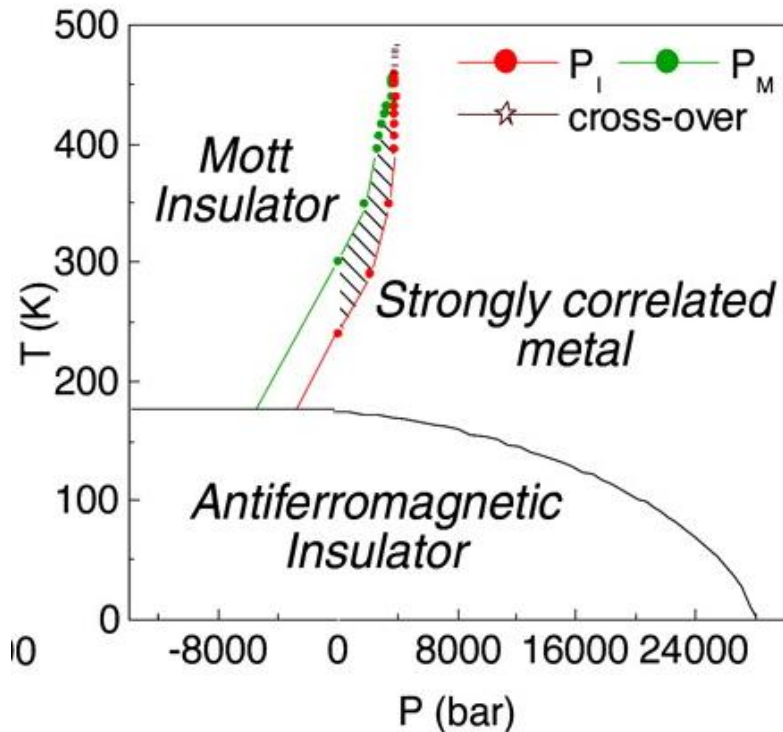


Systems with strong electronic/fermionic correlations

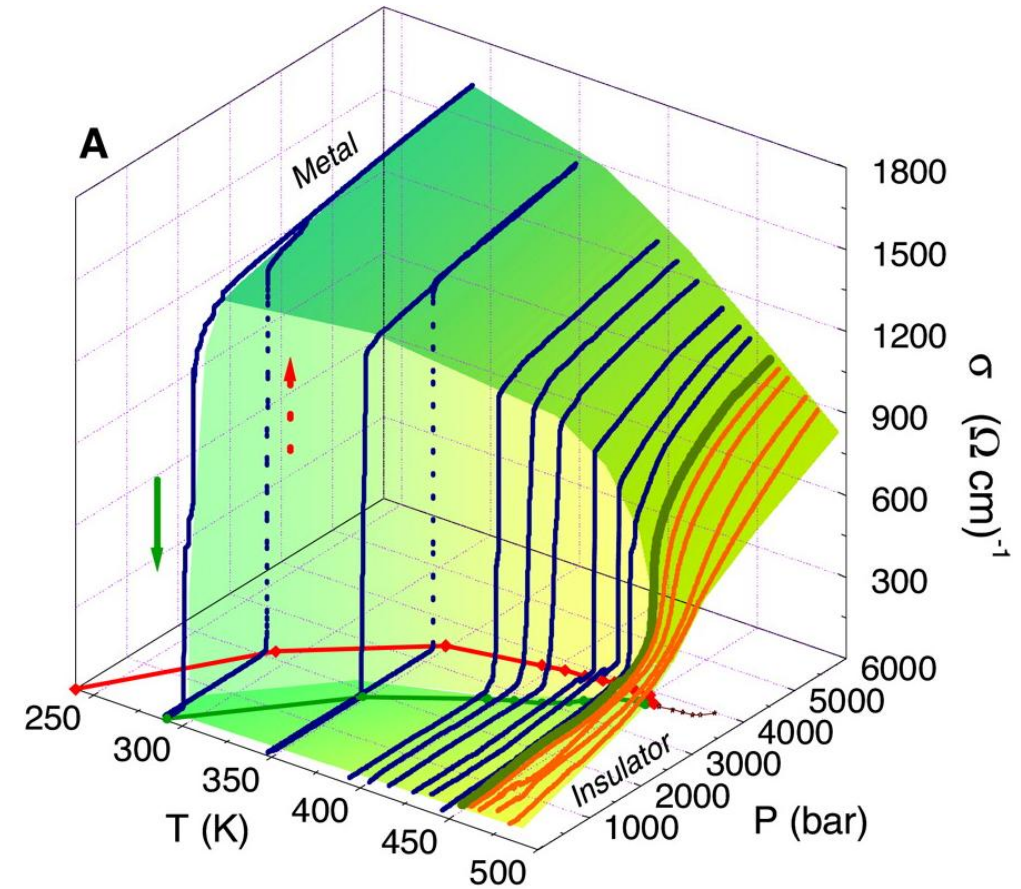
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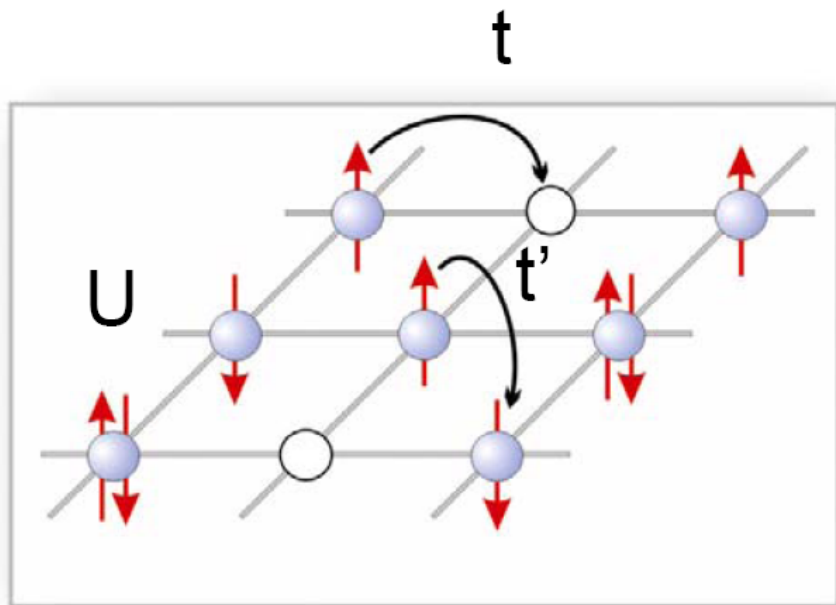
Electrical conductivity



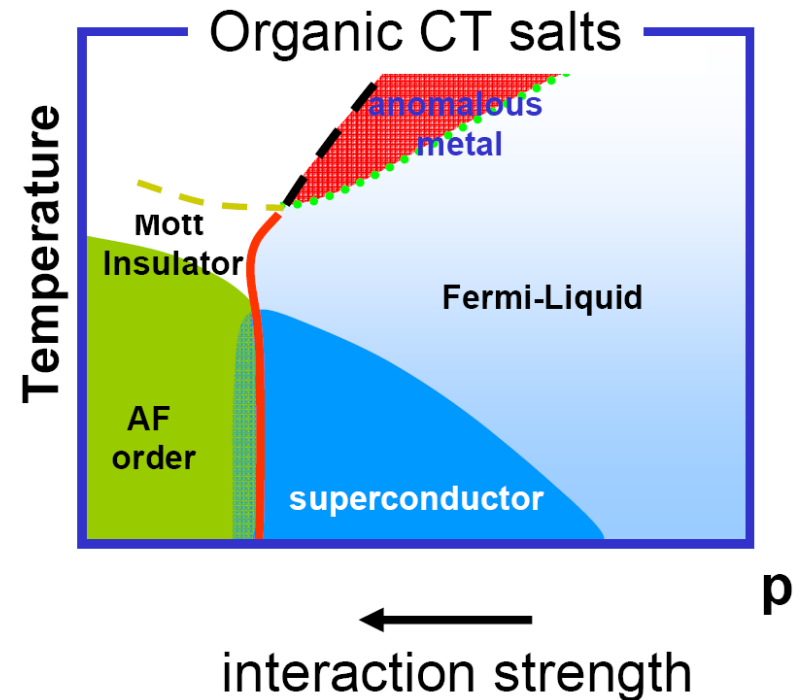
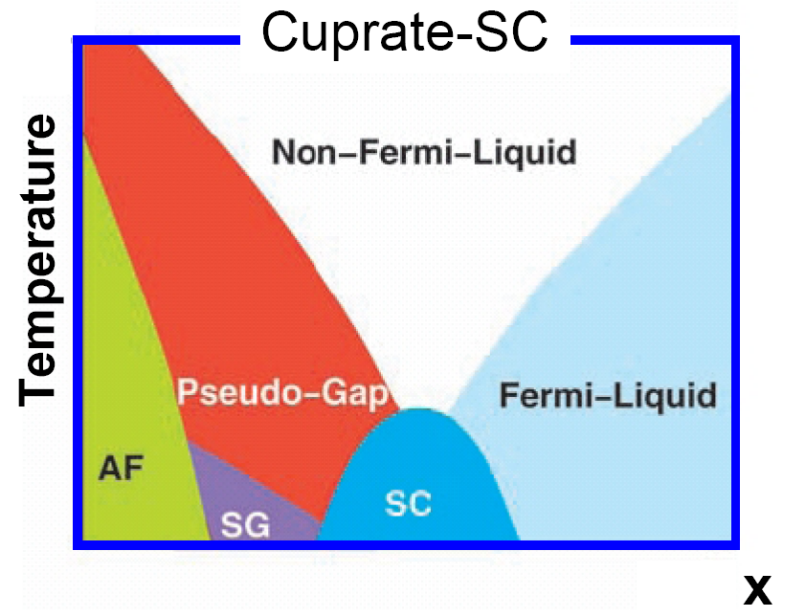
[Limelette et al., Science 302, 89 (2003)]

Complex phases of cuprate and organic superconductors

High- T_c physics contained in 2D Hubbard model?



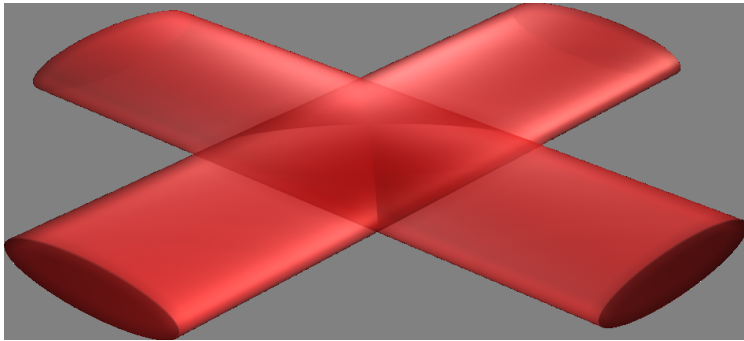
Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?



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)



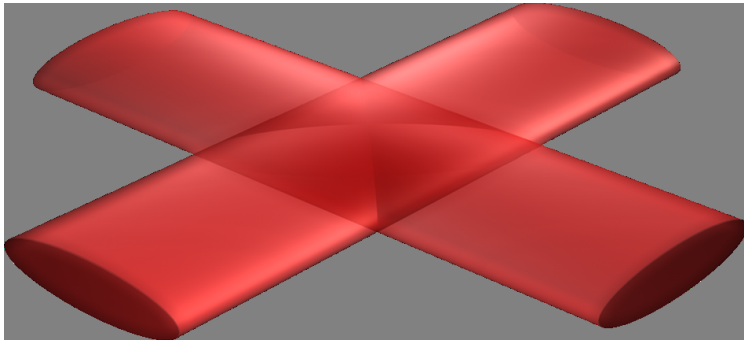
$$V_{\text{dipole}}(\mathbf{r}) = -\mathbf{d} \cdot \mathbf{E}(\mathbf{r}) \propto \alpha(\omega_L) |\mathbf{E}(\mathbf{r})|^2$$

time-averaged
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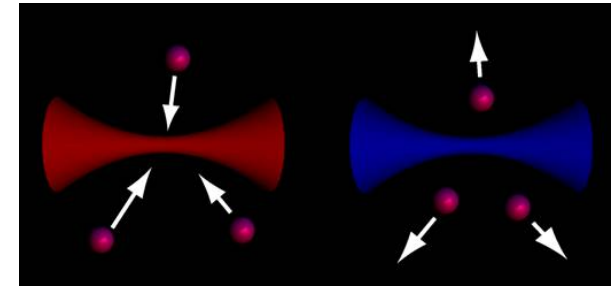
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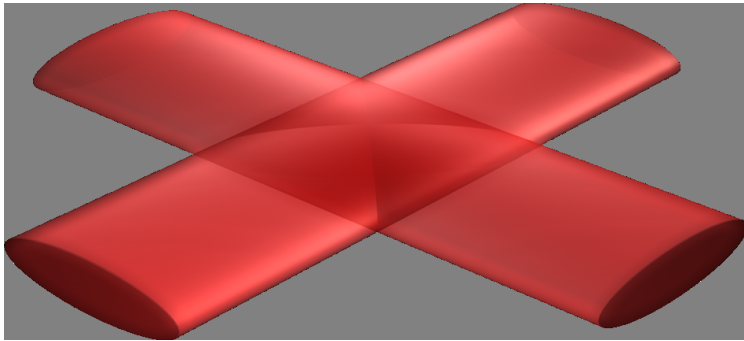
polarizability $\alpha(\omega_L)$
changes sign at ω_0



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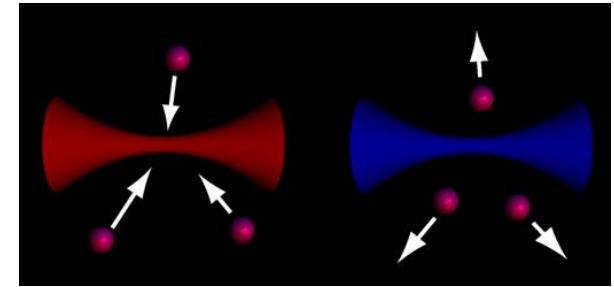
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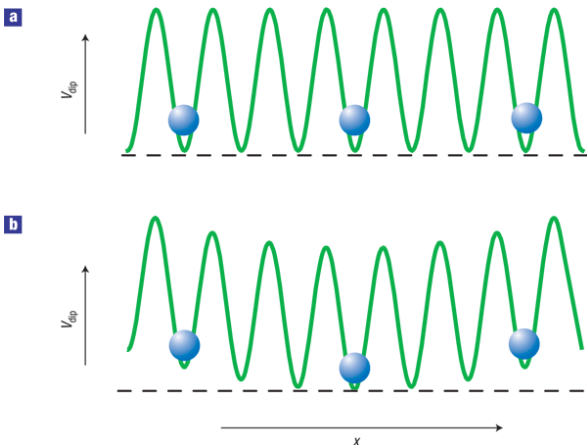
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Standing wave (from coherent counterpropagating beams) \rightsquigarrow modulated potential

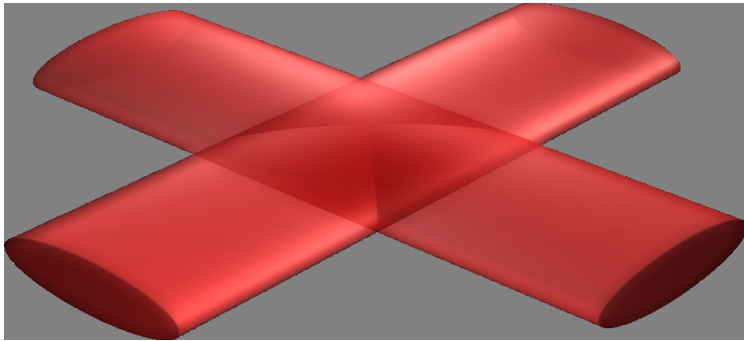


Beam profile: (anti) trapping

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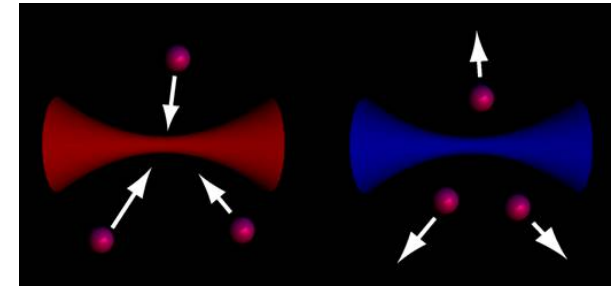
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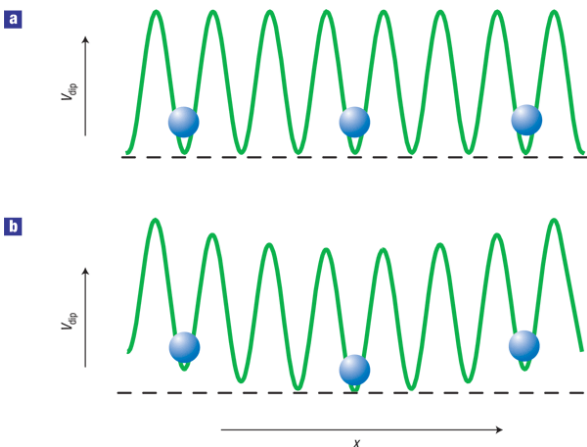
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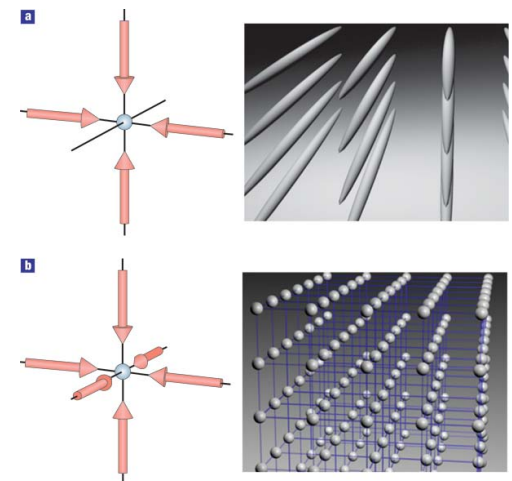
Beam profile: (anti) trapping

1 pair of lasers \rightsquigarrow pancakes

2 pairs of lasers \rightsquigarrow tubes

3 pairs of lasers \rightsquigarrow 3D lattice

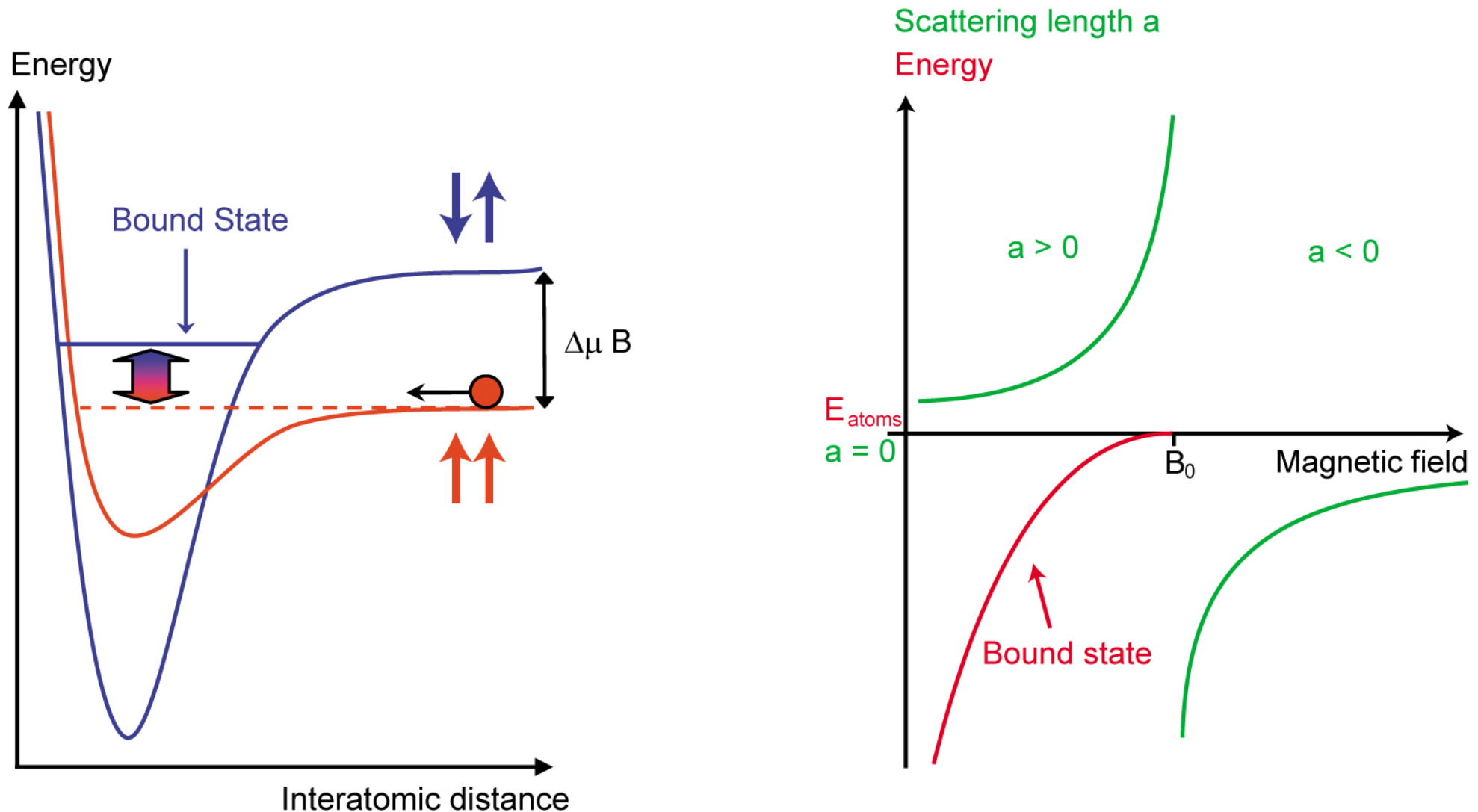
hopping t tunable by laser



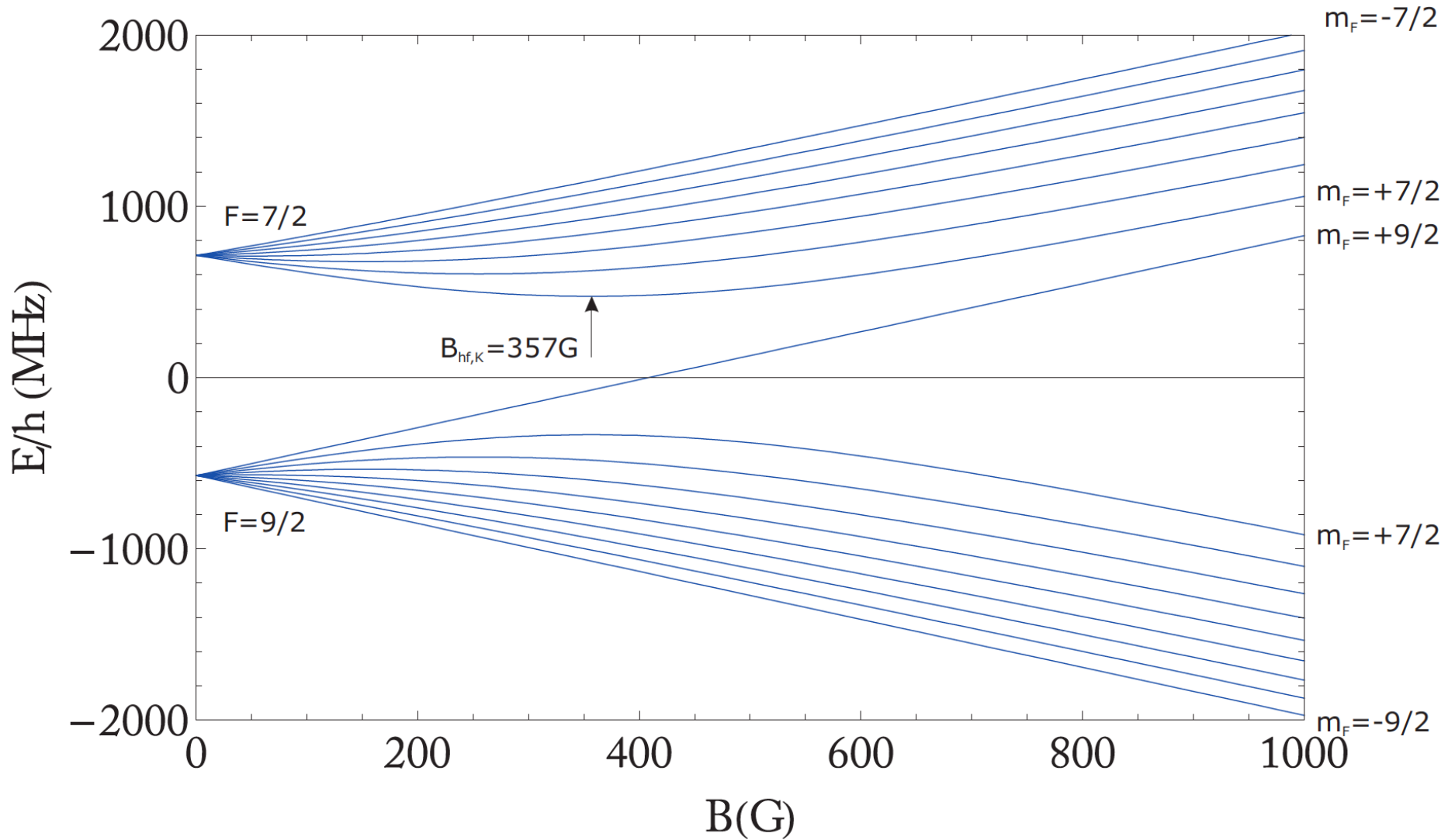
Interactions can be tuned via Feshbach resonances

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

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



Large multiplets: reservoir of “flavors”

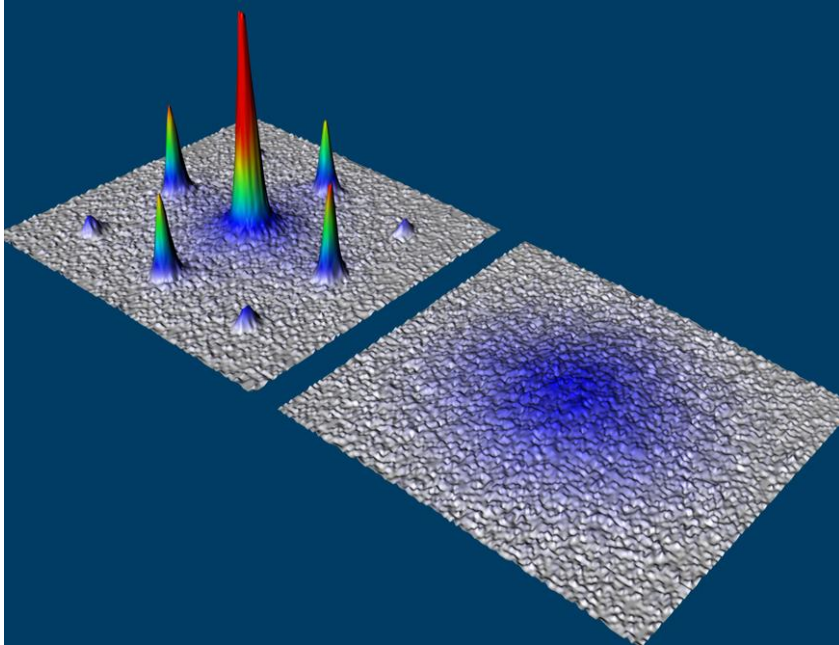


Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

[Tiecke, unpublished]

Correlated ultracold quantum gases on optical lattices: bosons

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

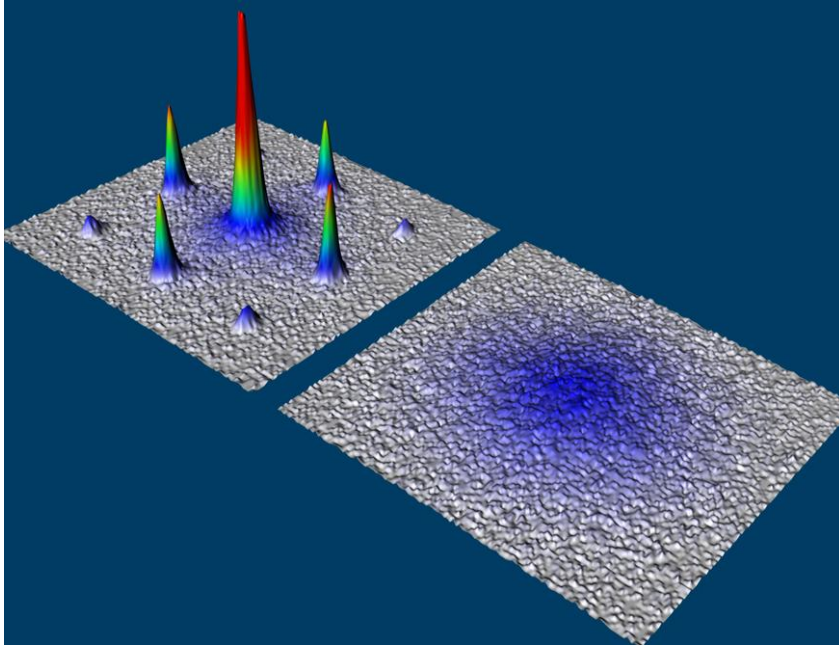


Time-of-flight image – momentum distribution

ultracold bosons on optical lattice
(Bloch group, 2002)

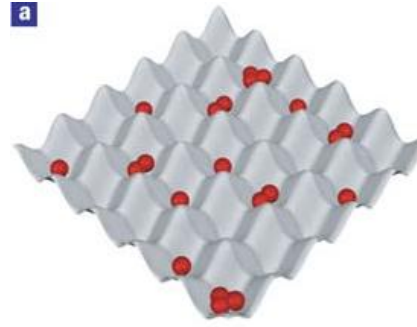
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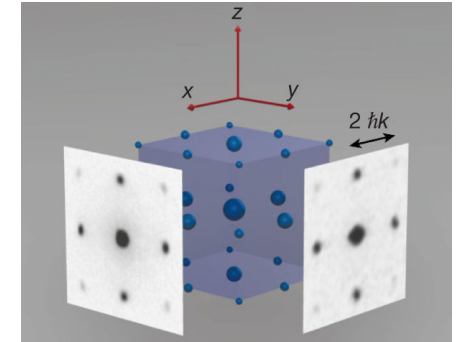
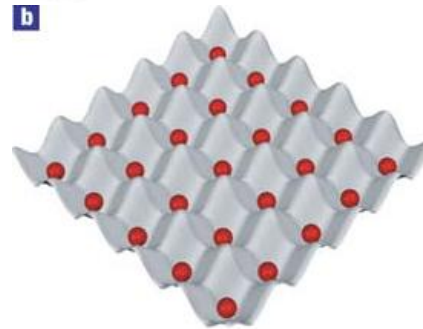


Time-of-flight image – momentum distribution

a



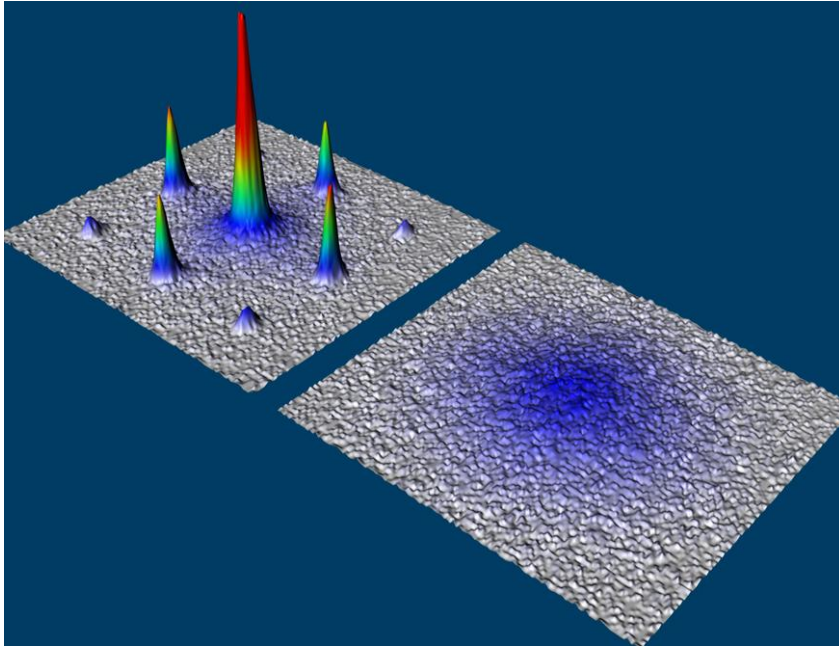
b



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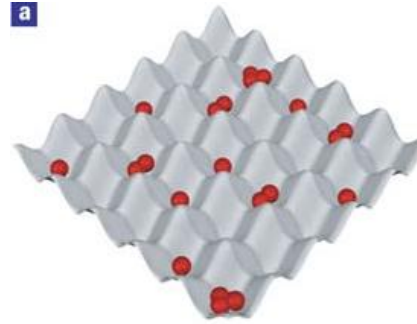
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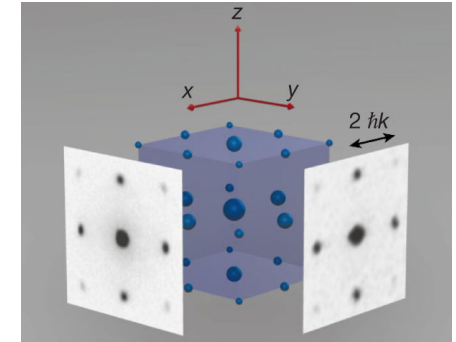
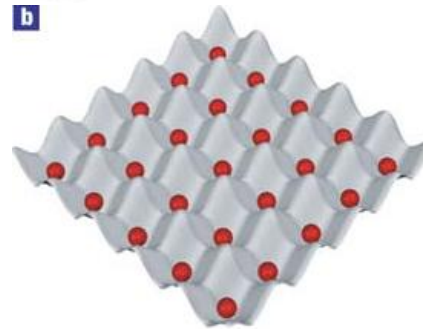


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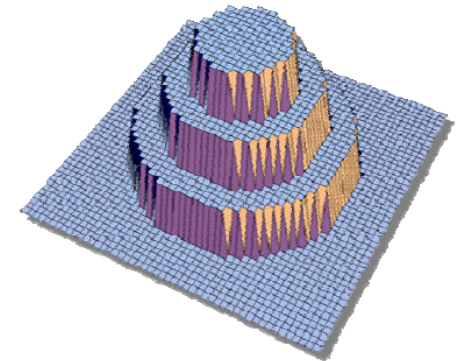


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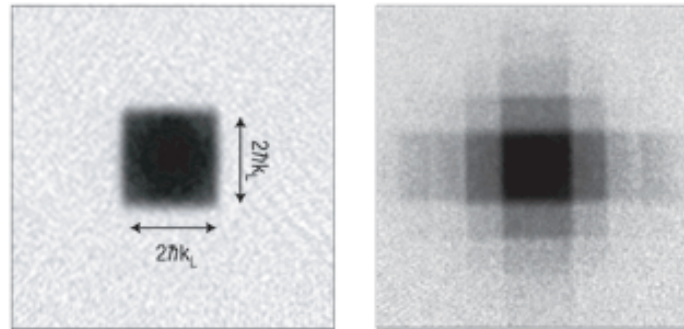
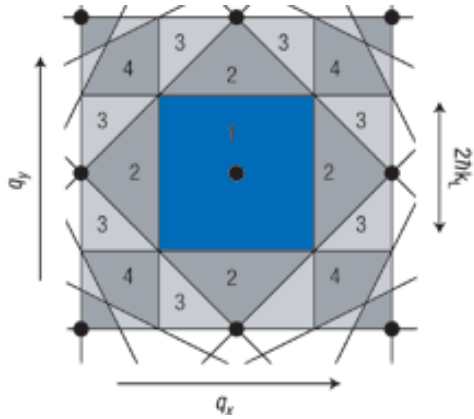


ultracold bosons on optical lattice
(Bloch group, 2002)

superfluidity destroyed by density constraint at large U ;
trapping potential \rightsquigarrow wedding cake structure



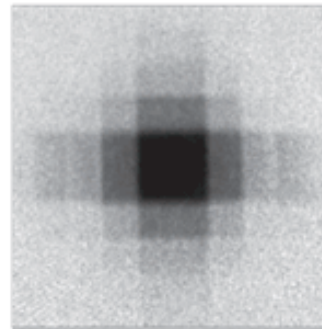
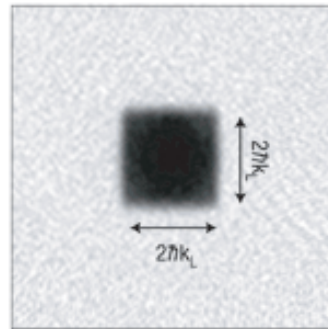
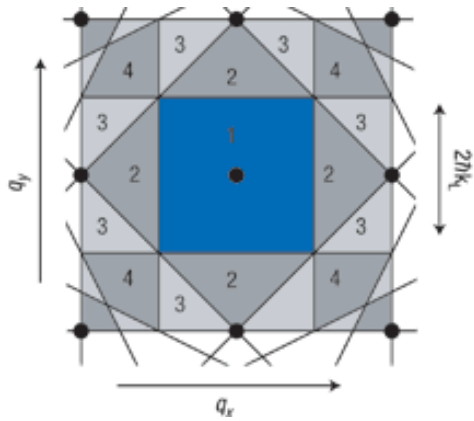
Correlated ultracold quantum gases on optical lattices: fermions



1 species: band insulator for filled 1st Brillouin zone:

[Köhl et al, PRL (2005)]

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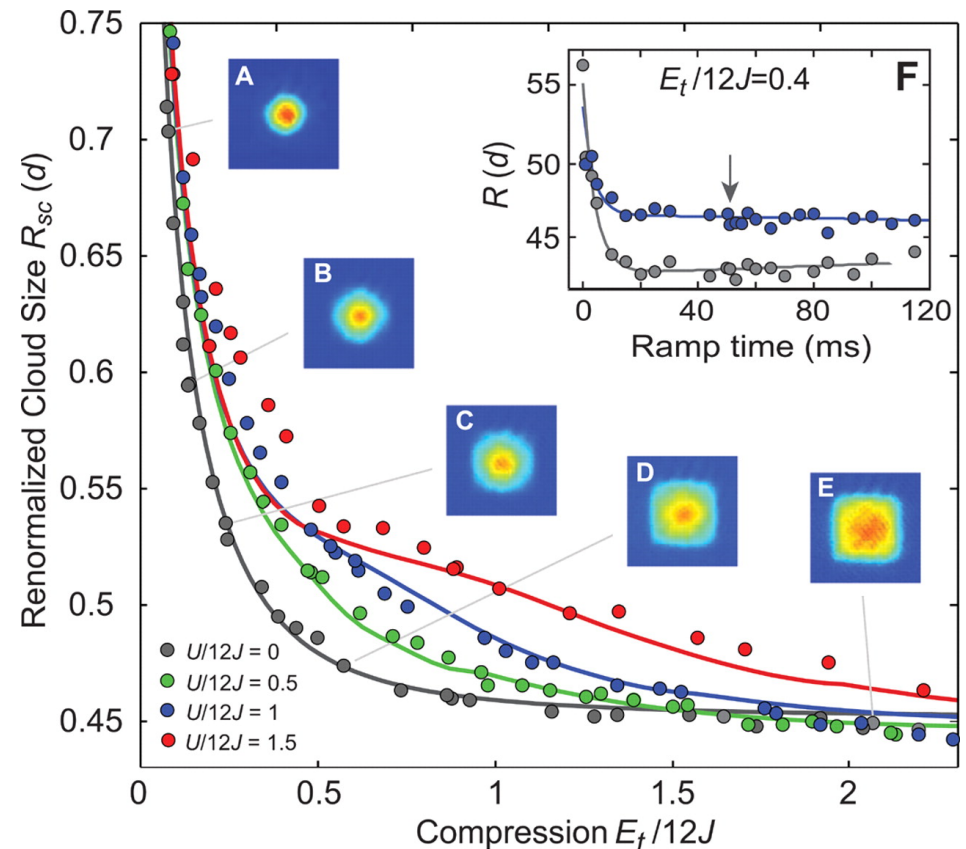
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Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

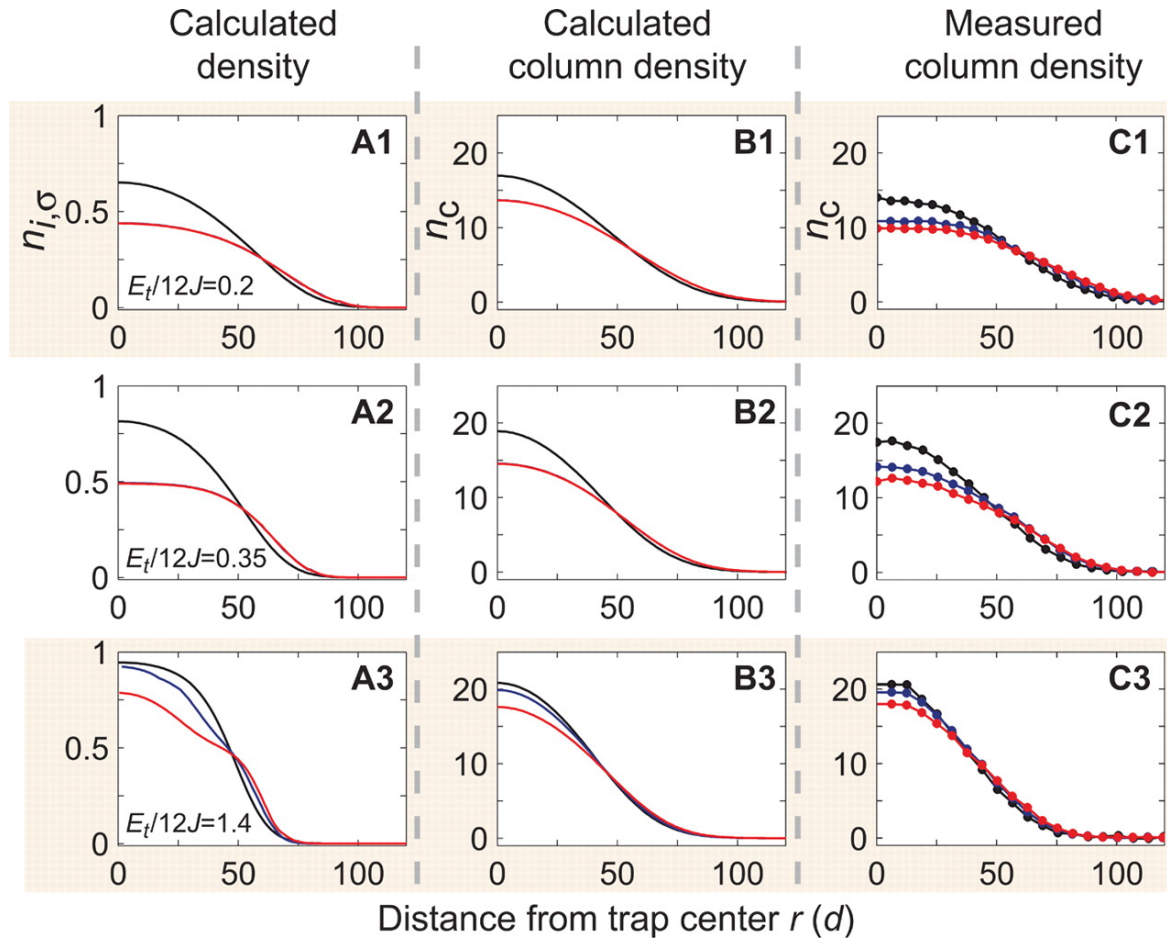
Detection method: measure cloud diameter vs. trap strength

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

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

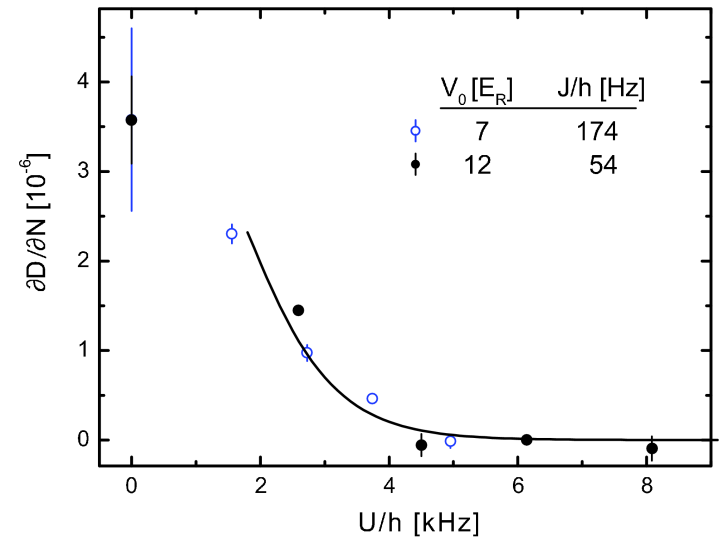
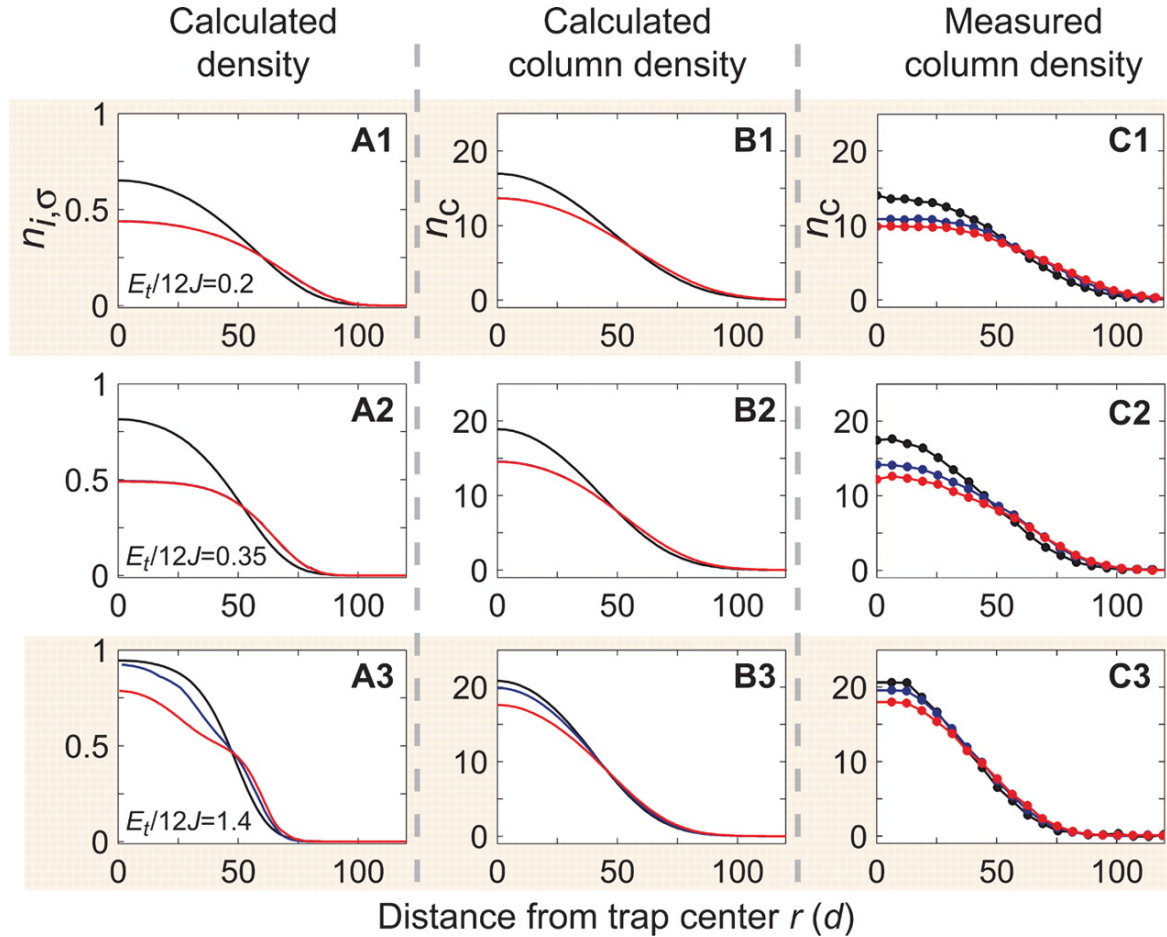


Further MIT observables: **column density**, fraction of atoms with **double occupations**



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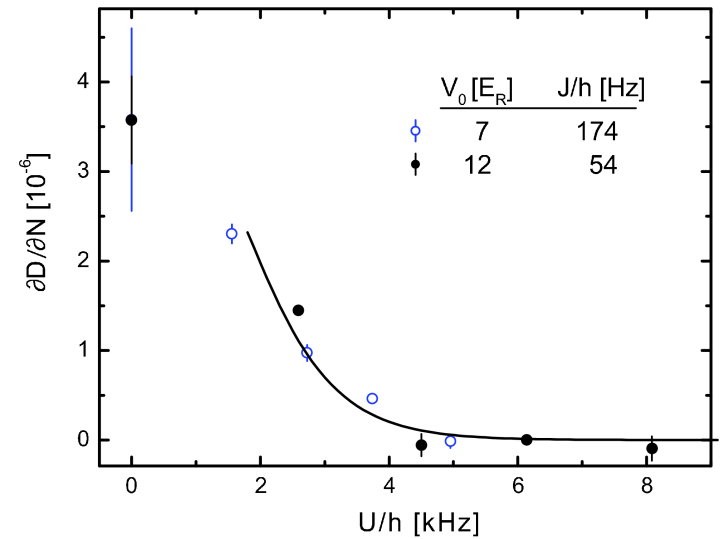
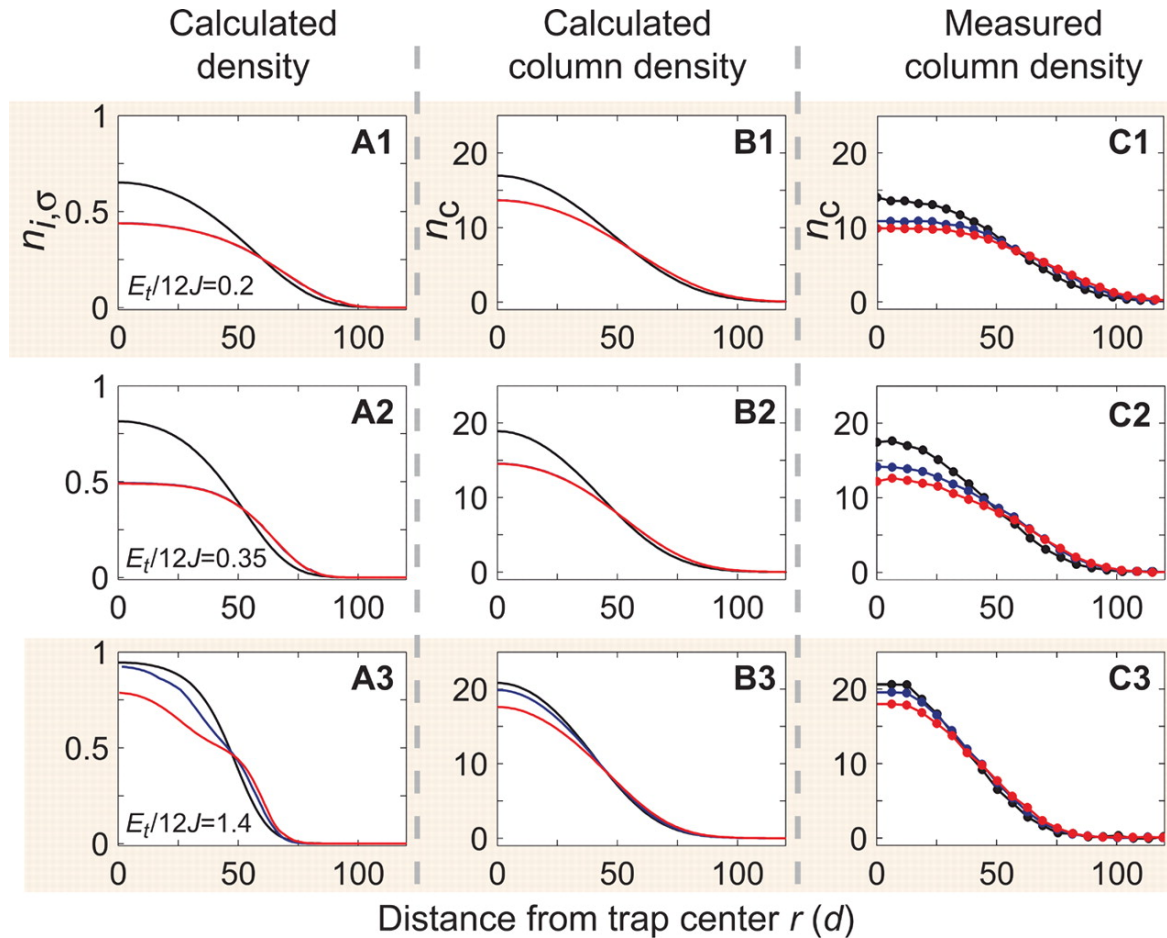
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Many other phenomena seen: **superconductivity**, **vortices**, **BEC-BCS crossover**, ...

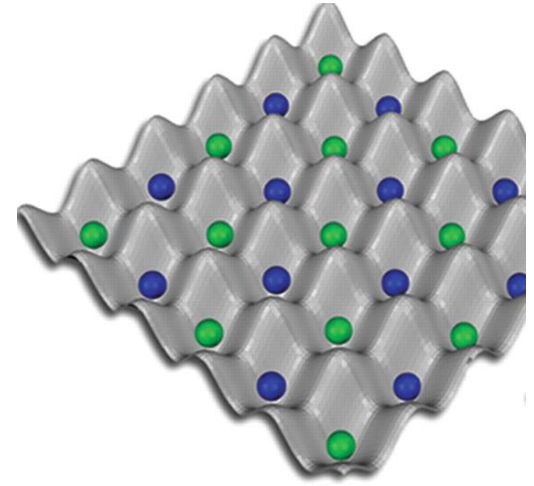
Next grand challenges:

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!

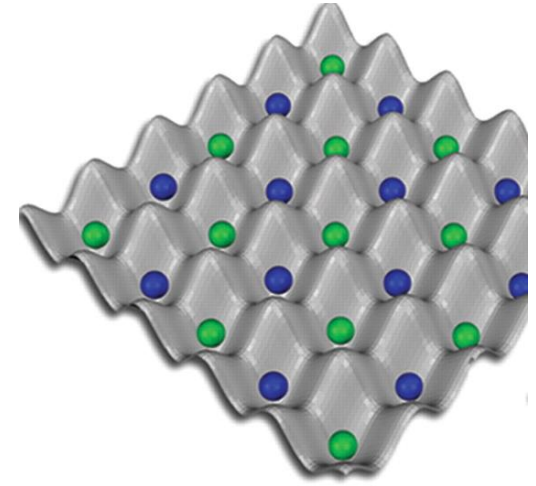


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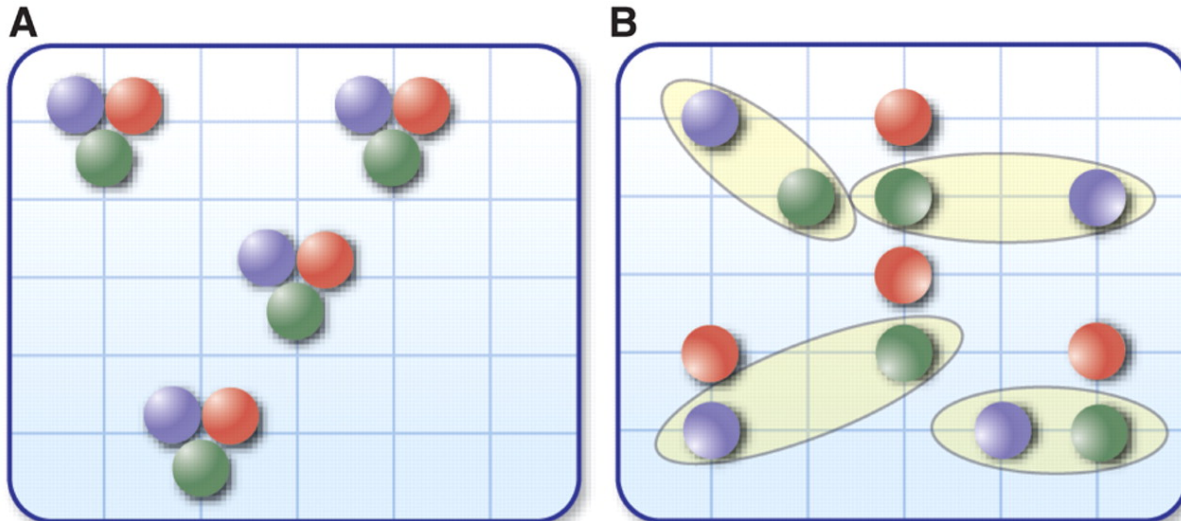
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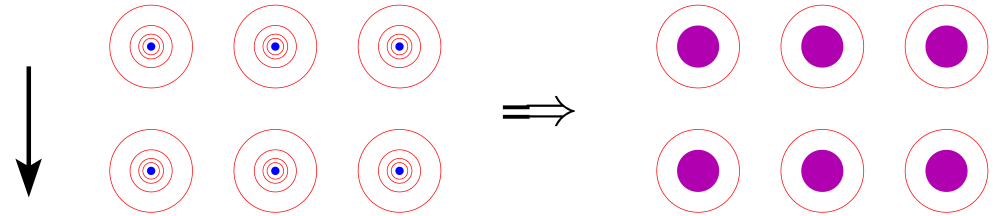
Multiflavor phenomena, e.g. trions versus color superconductivity



Approaches for correlated lattice Fermi systems

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

reduction to valence electrons

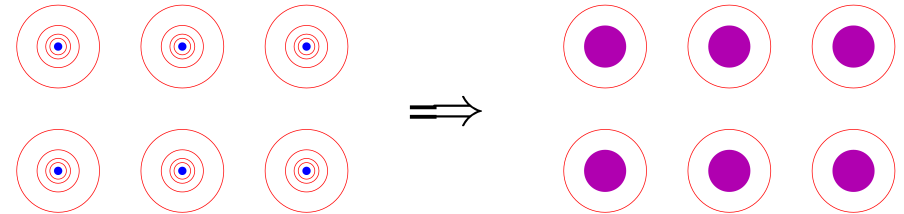


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occupation number formalism

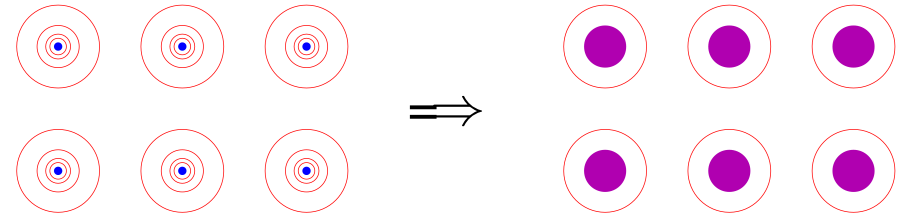
Wannier orbitals

$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu} \hat{c}_{i\nu\sigma}^{\dagger} \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'} \hat{c}_{i\nu\sigma}^{\dagger} \hat{c}_{j\nu'\sigma'}^{\dagger} \hat{c}_{n\mu'\sigma'} \hat{c}_{m\mu\sigma}$$

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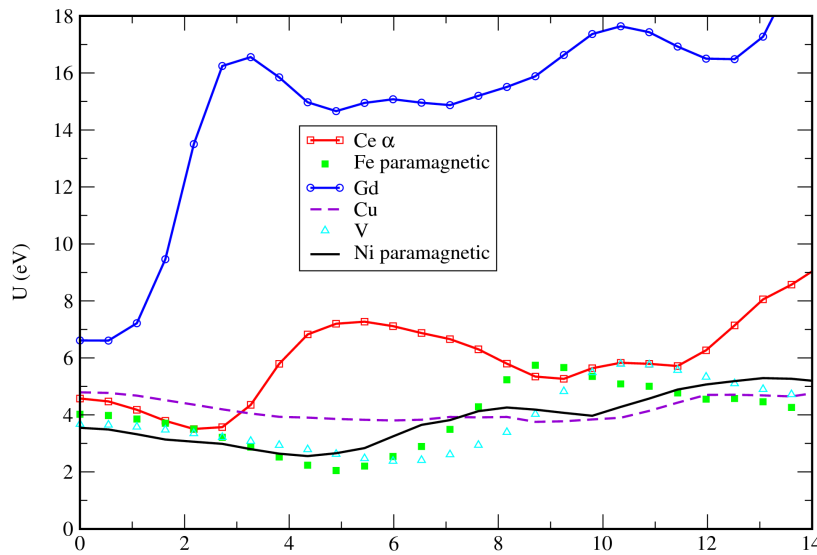
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Hubbard model

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

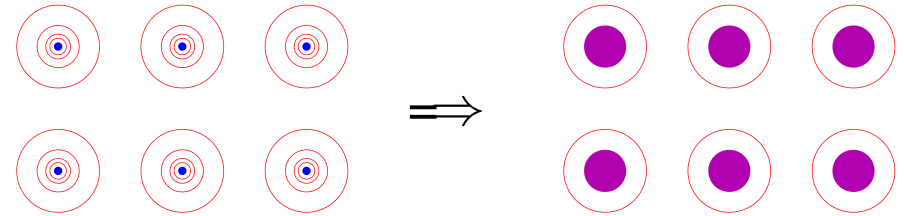
related lattice Fermi systems



[Aryasetiawan et al, PRB 2006]

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

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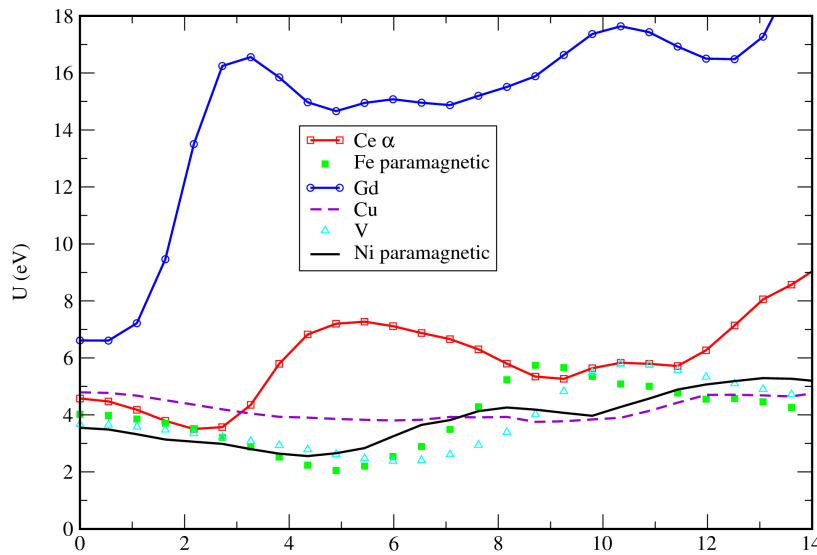
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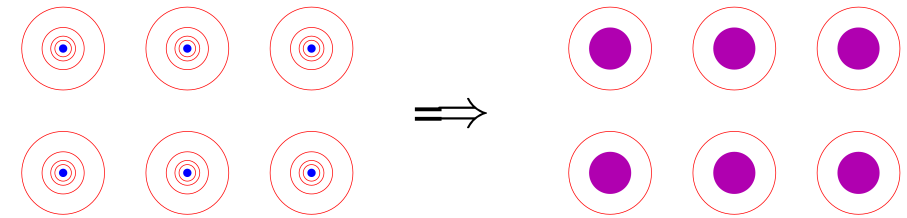
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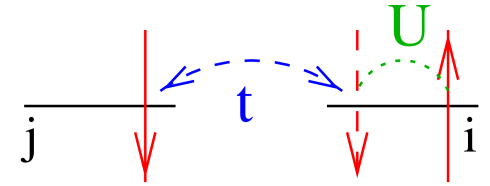
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Note: no core states in quantum gas case!

Approaches for Hubbard-type models

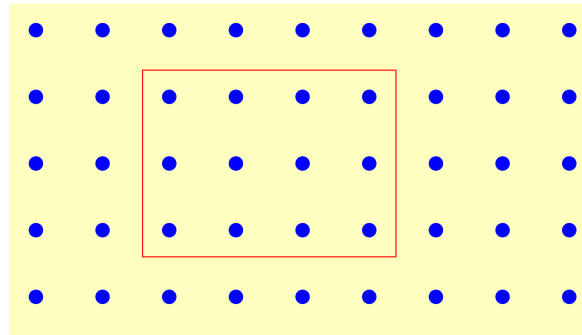
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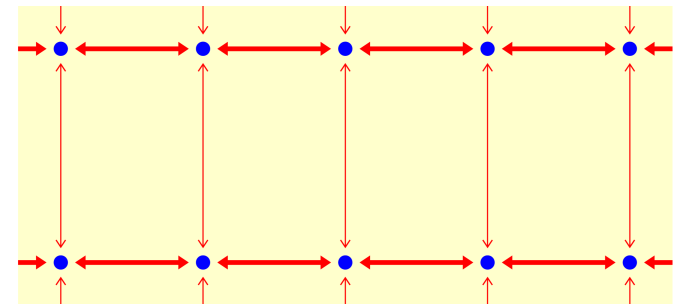
Perturbation theory

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

finite clusters: ED, QMC

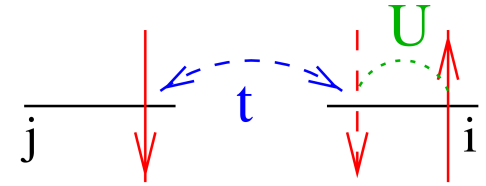


$d \rightarrow 1$: Bethe ansatz, DMRG



Approaches for Hubbard-type models

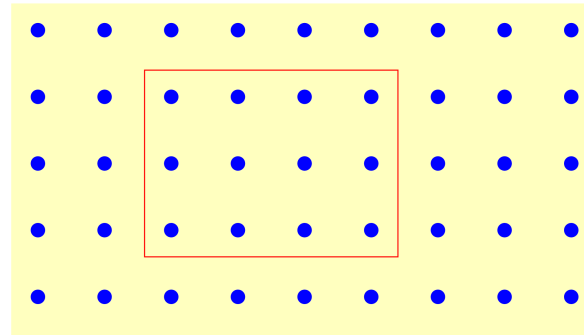
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



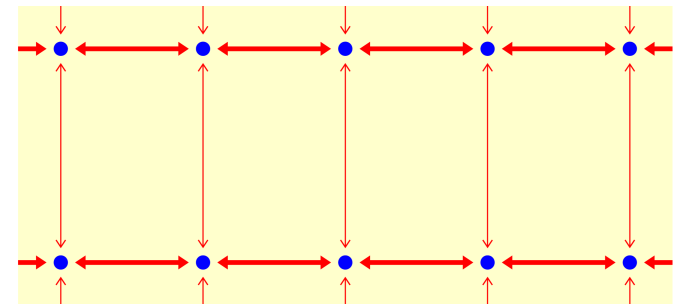
Perturbation theory

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

finite clusters: ED, QMC



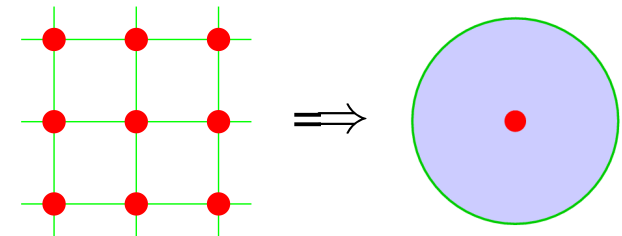
$d \rightarrow 1$: Bethe ansatz, DMRG



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

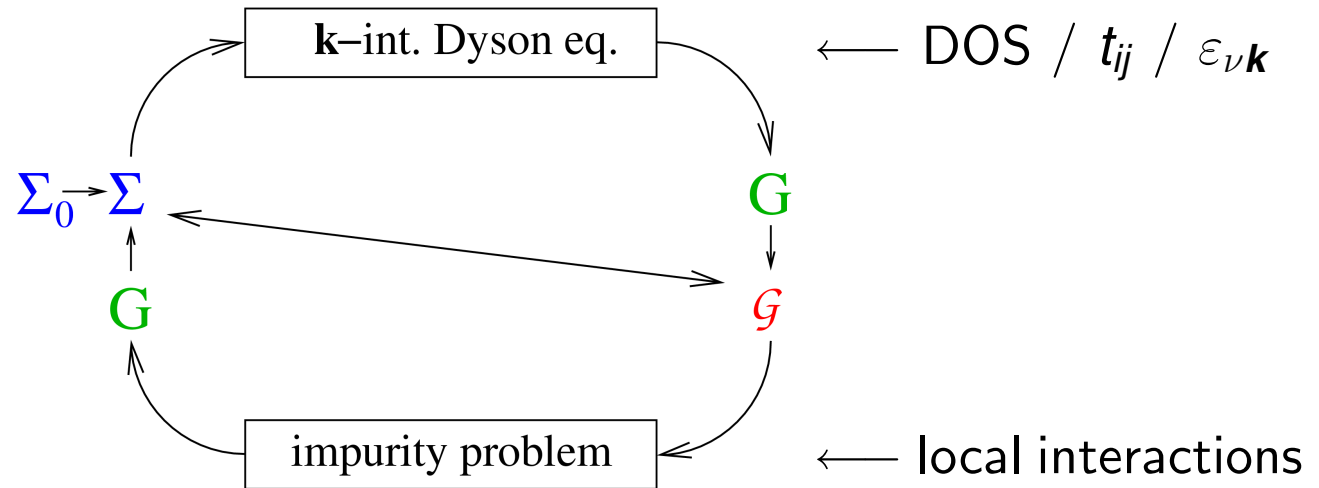
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

- + non-perturbative \rightsquigarrow valid at MIT
- + dynamical on-site correlations preserved
- + in thermodynamic limit
- +/- exact for coordination $Z \rightarrow \infty$



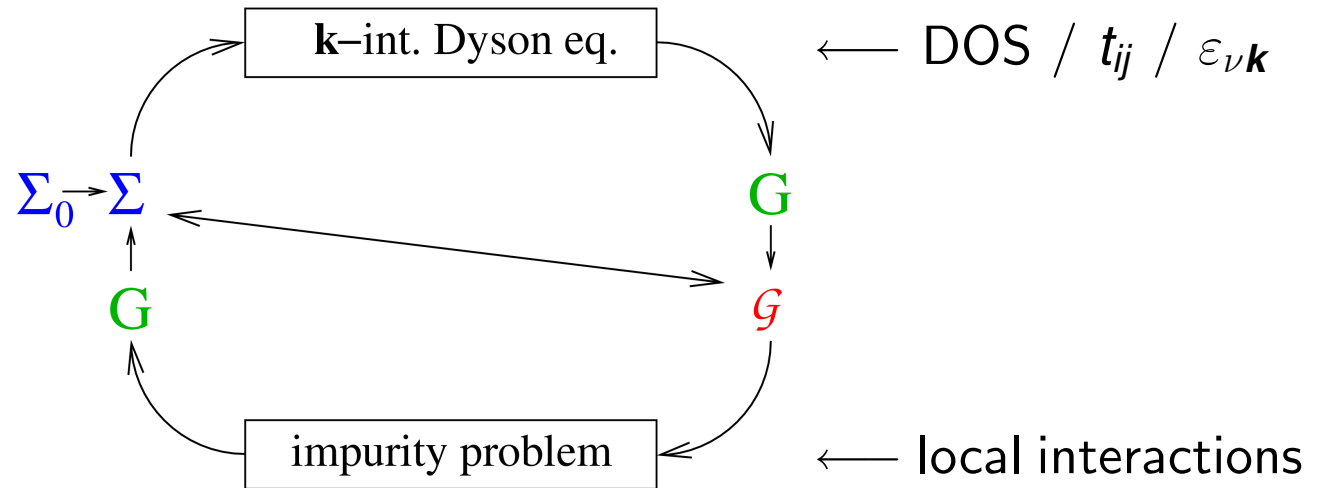
Iterative solution of DMFT equations

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



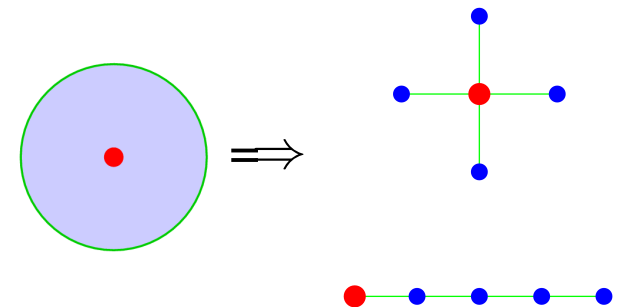
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Impurity solver:

- 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^*):

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

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(i) Imaginary-time discretization $\beta = \Lambda \Delta\tau$

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

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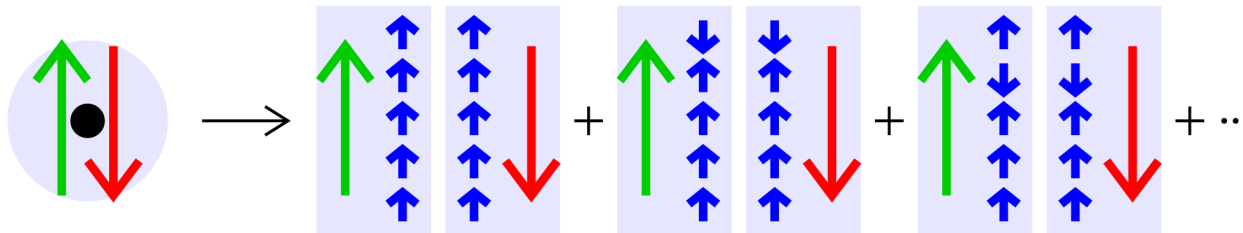
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Wick theorem:

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

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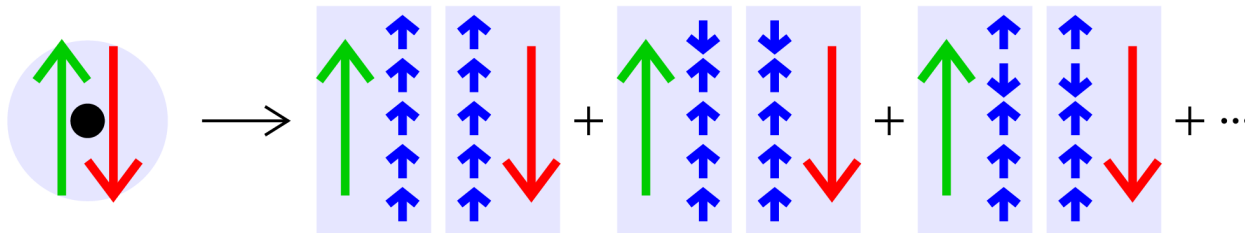
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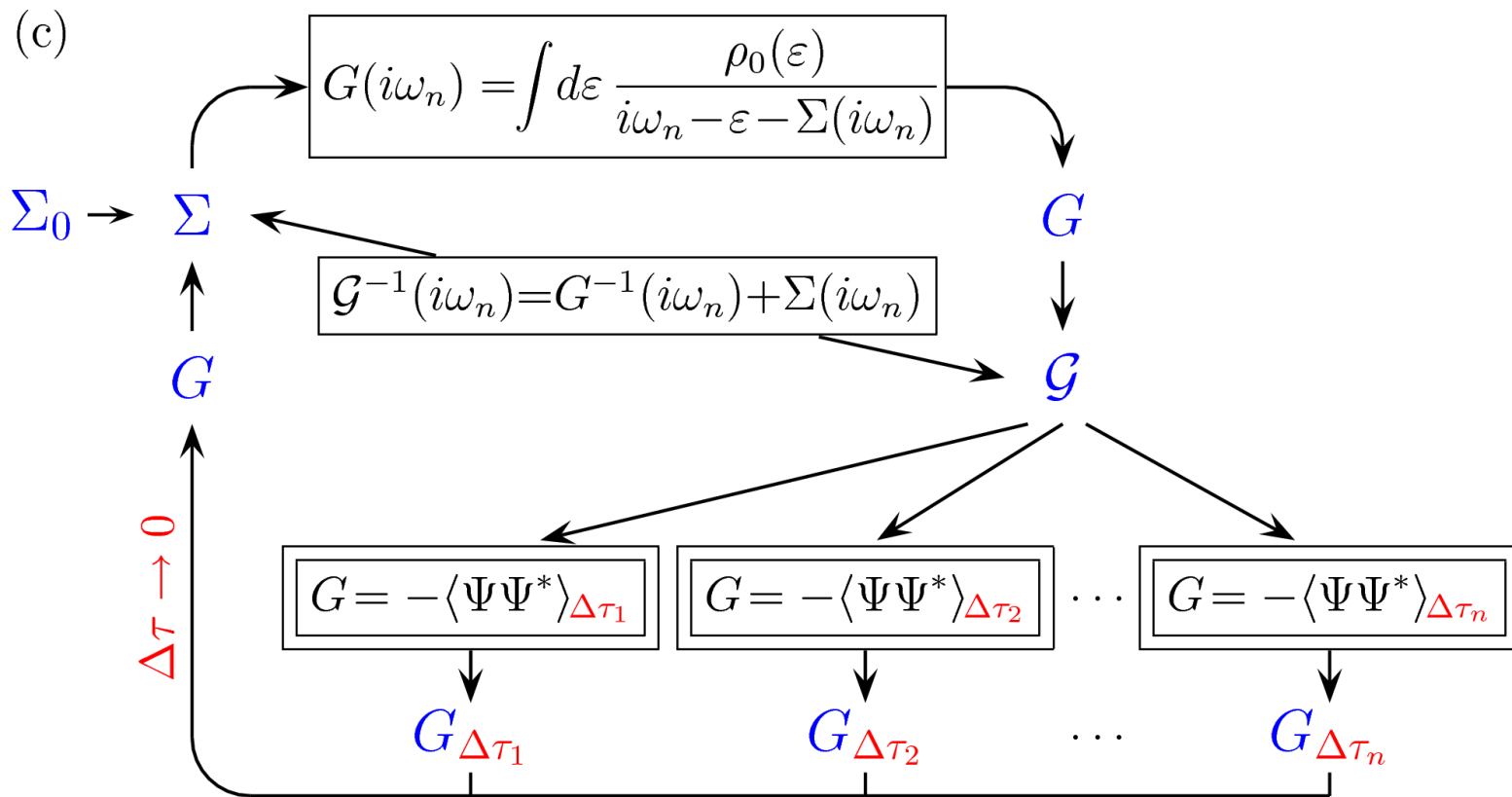
(iv) MC importance sampling over auxiliary Ising field $\{s\}$: 2^{Λ} configurations

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

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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

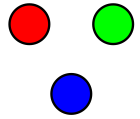
(b) *a posteriori* extrapolation of selected observables



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

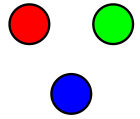
\rightsquigarrow quasi CT-QMC algorithm [NB, arXiv:0801.1222, PRA(2009)]

Paramagnetic Mott transitions in 3-flavor mixtures



3 flavors: simplest case beyond electronic systems
1st approximation: all flavors equivalent, bulk calc.

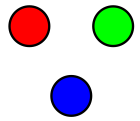
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 - Color superconductivity
 - Trionic phase
 - ...

Paramagnetic Mott transitions in 3-flavor mixtures

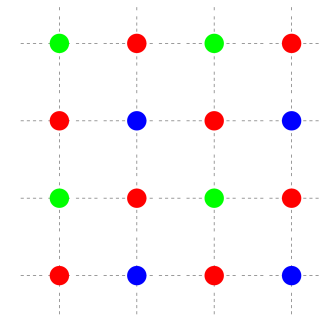
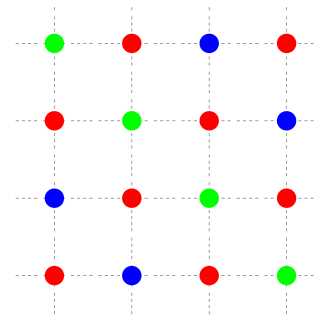
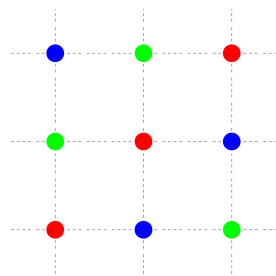
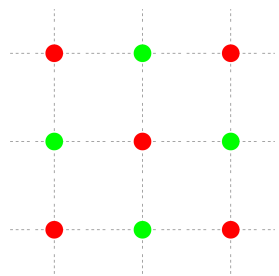


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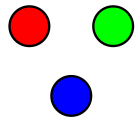
- Ordered phases: $U > 0$, $n = 1$



2 spins/flavors

3 spins/flavors

Paramagnetic Mott transitions in 3-flavor mixtures

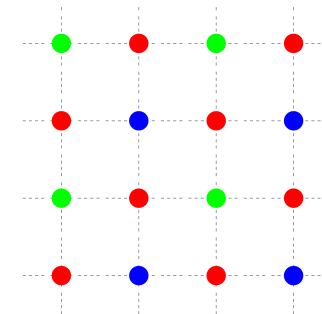
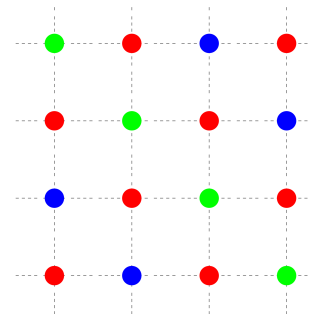
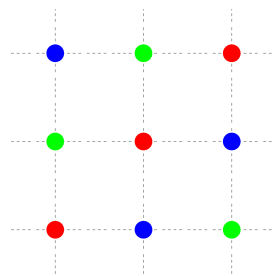
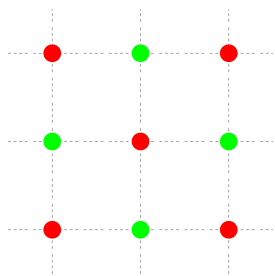


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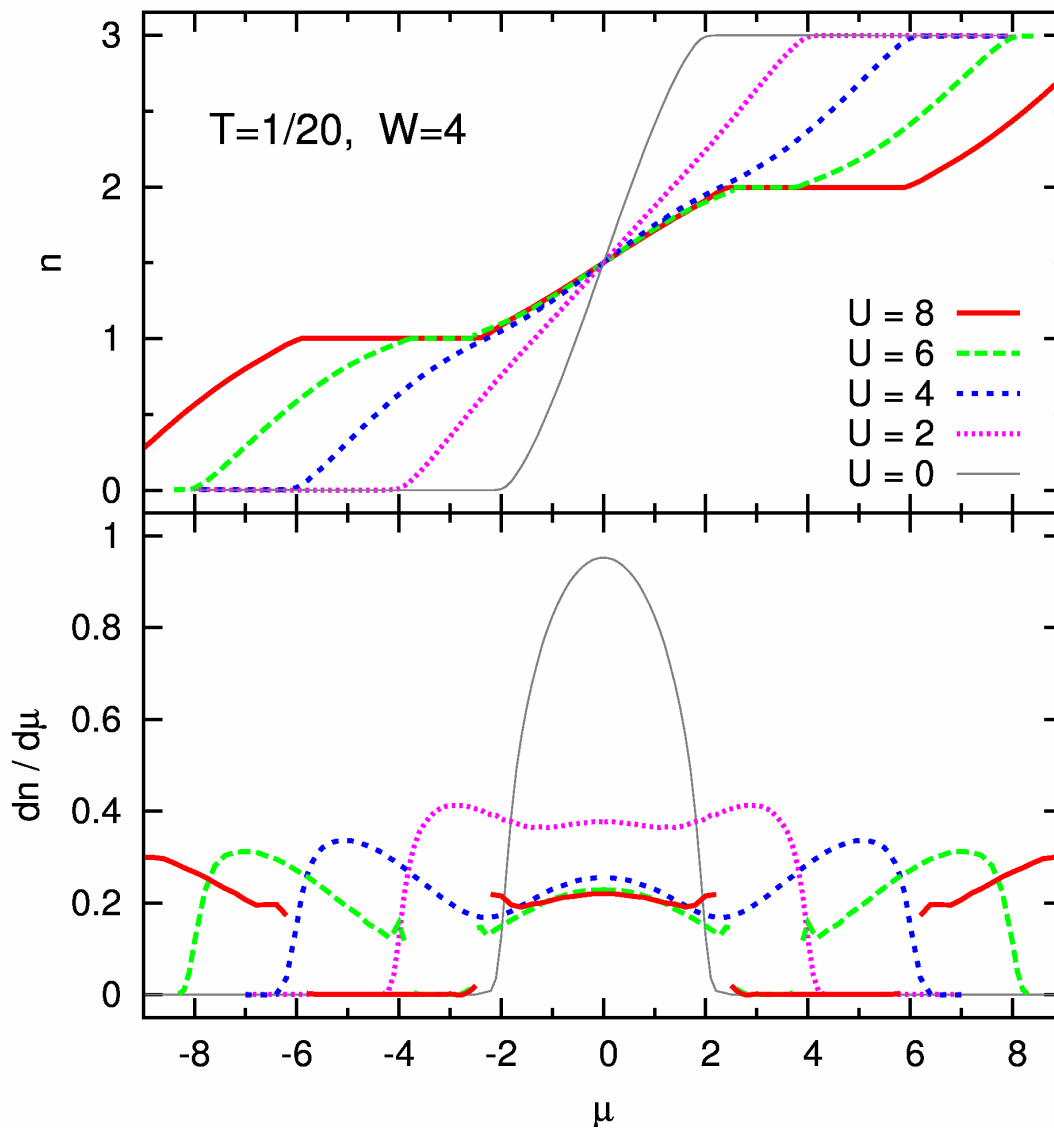
Most “electron-like”: $U > 0$, paramagnetic phase

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

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

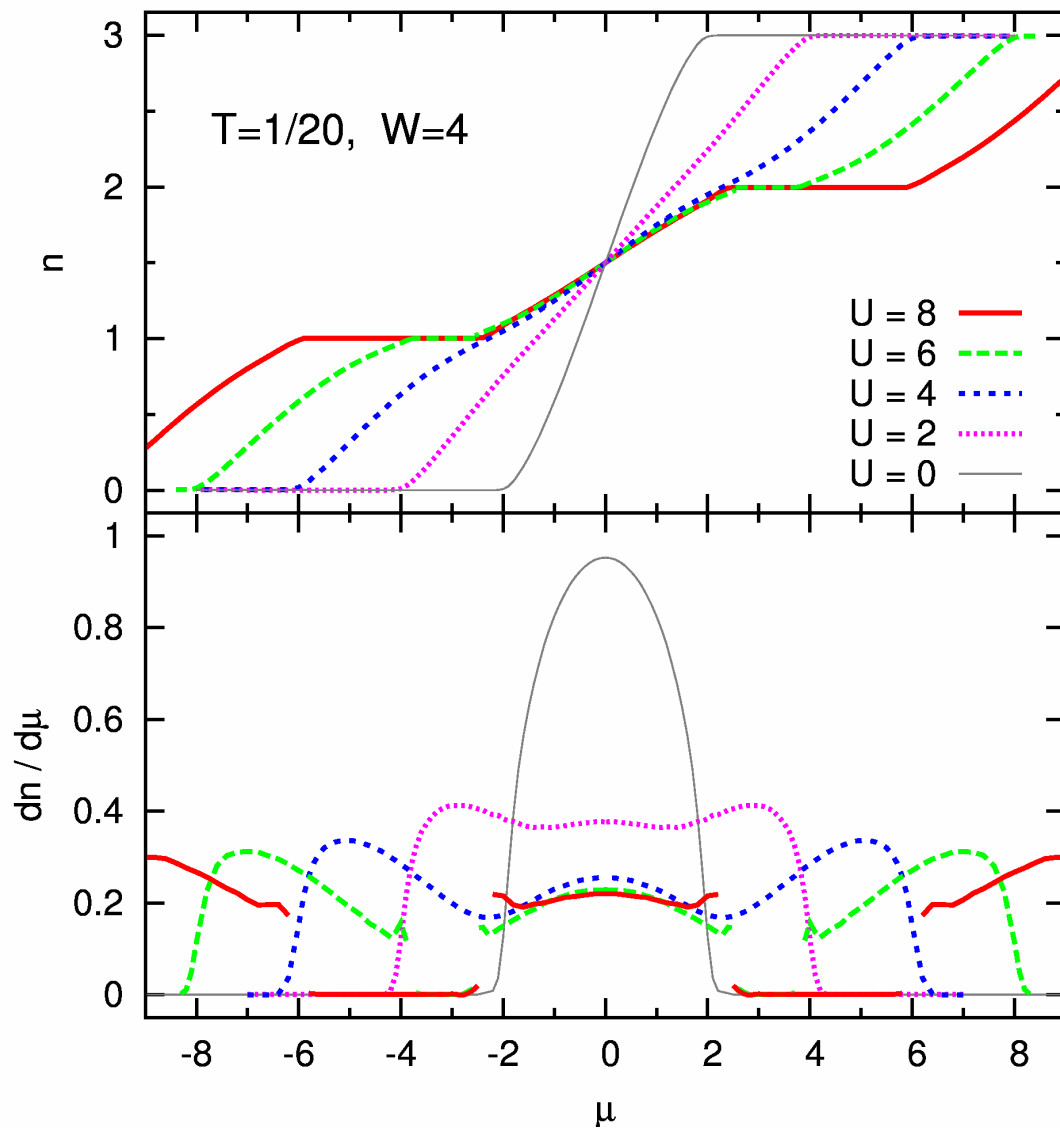
Plateaus at integer filling ($U \gtrsim 5.5$)

\rightsquigarrow incompressible Mott phases



[E. Gorelik, N. Blümer, PRA(2009)]

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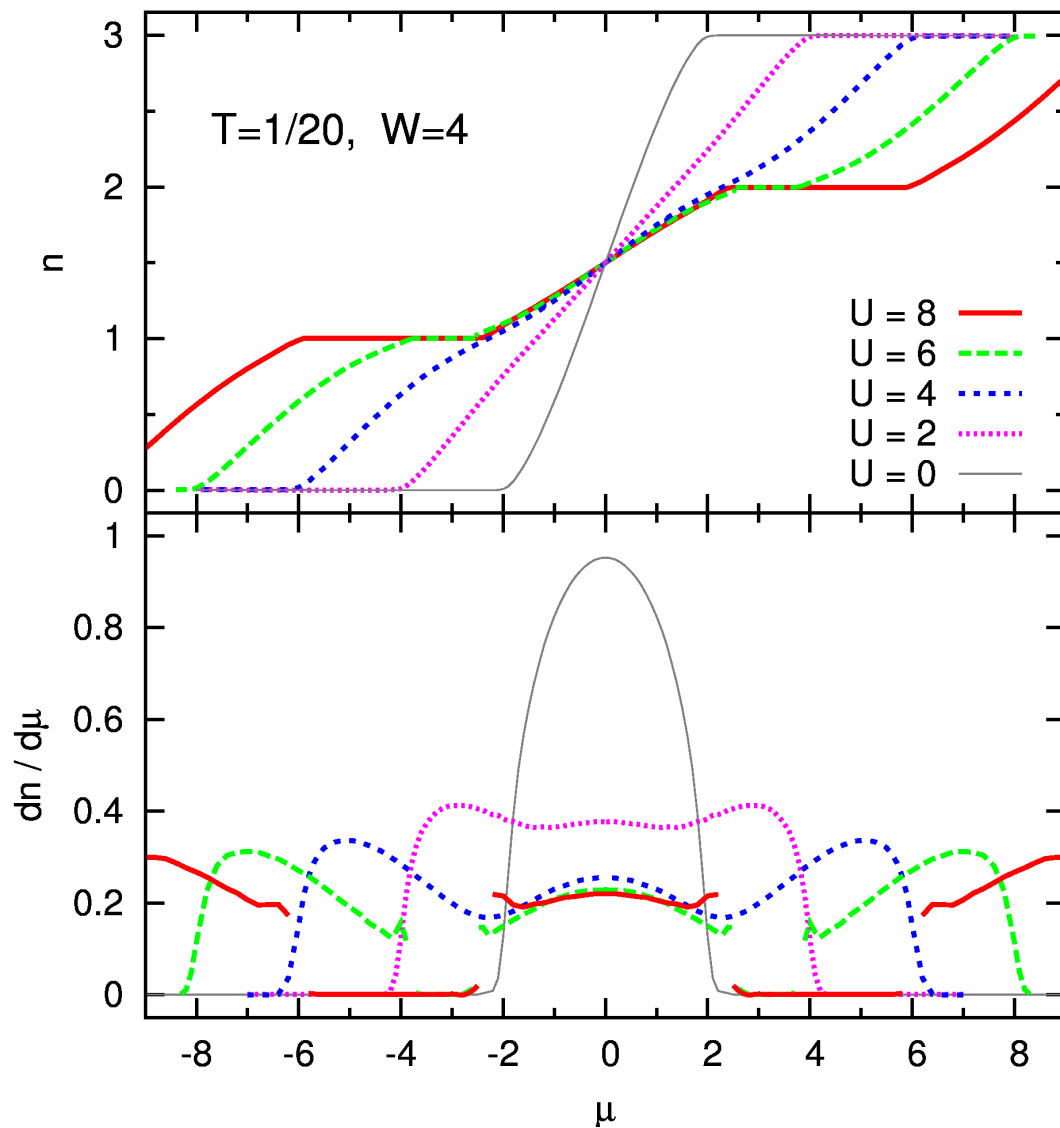
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$1 < n < 2$: semi-compressible phase

κ independent of μ, U, T

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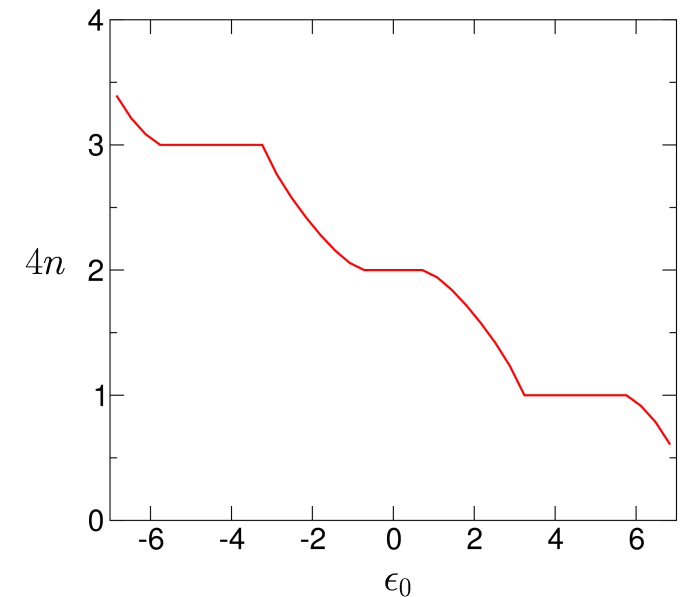
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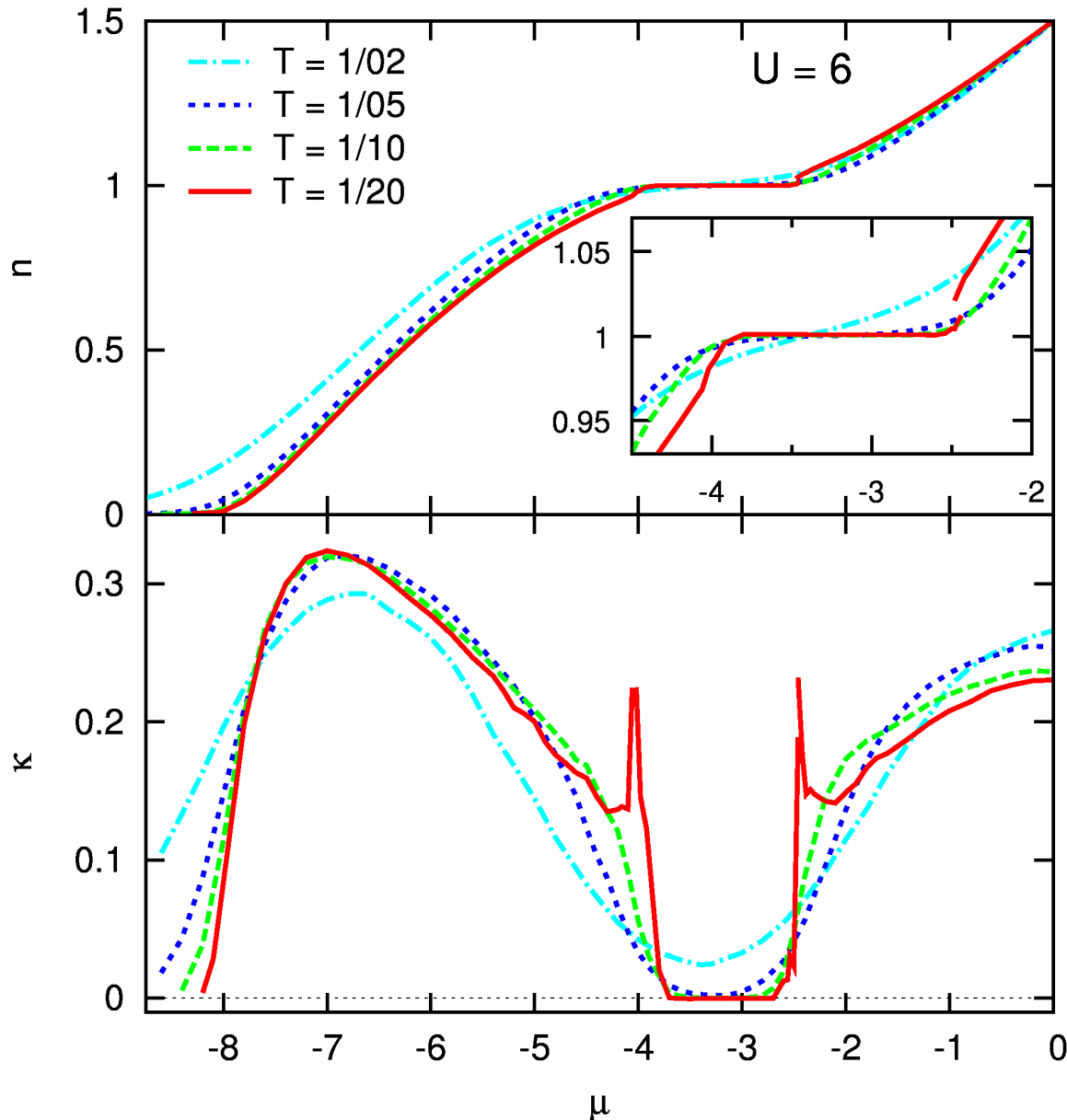
Contrast with SU(4) system:



[E. Gorelik, N. Blümer, PRA(2009)]

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

T dependence of density n and compressibility κ

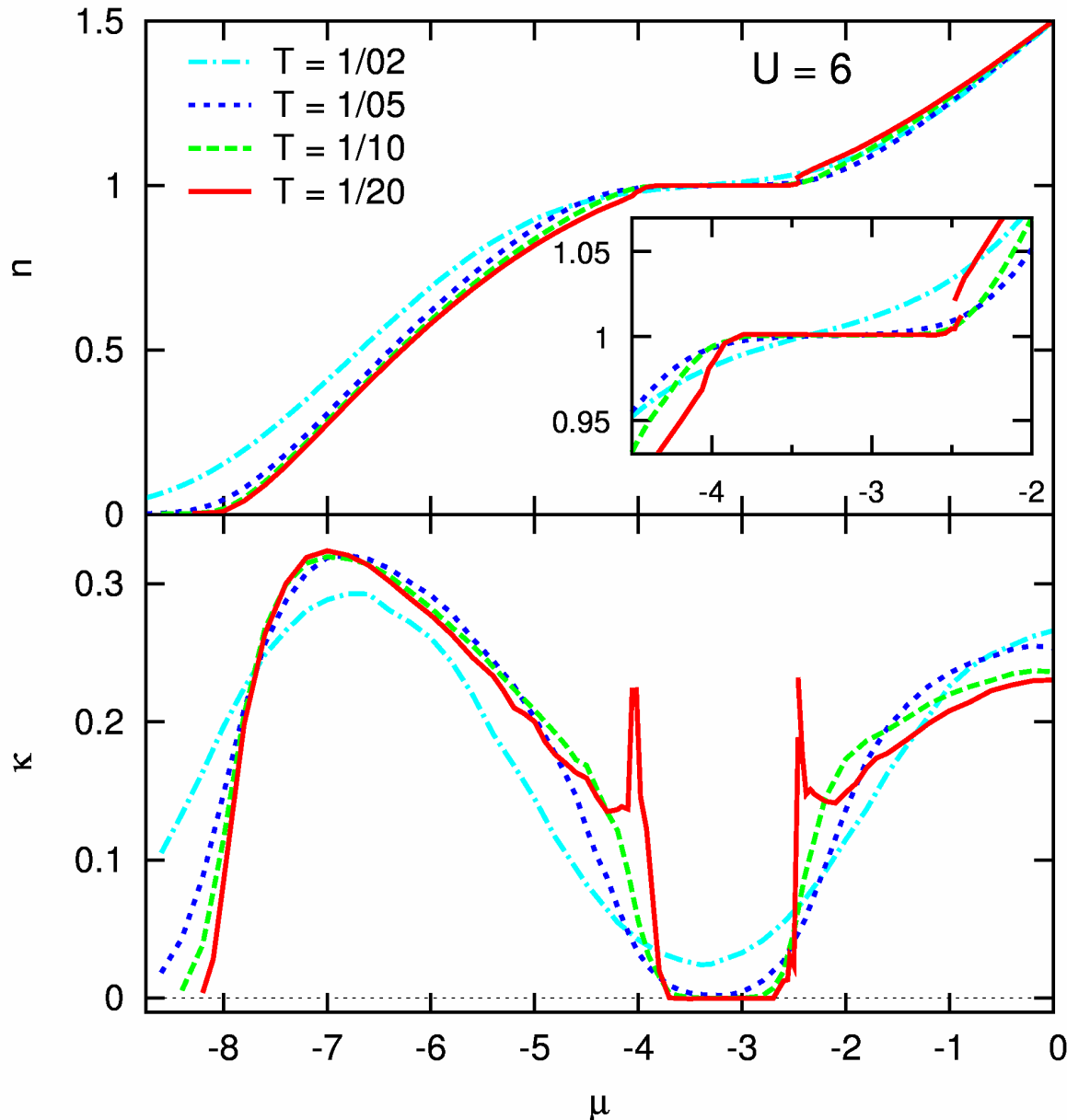


Multigrid HF-QMC results

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

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

T dependence of density n and compressibility κ



Multigrid HF-QMC results

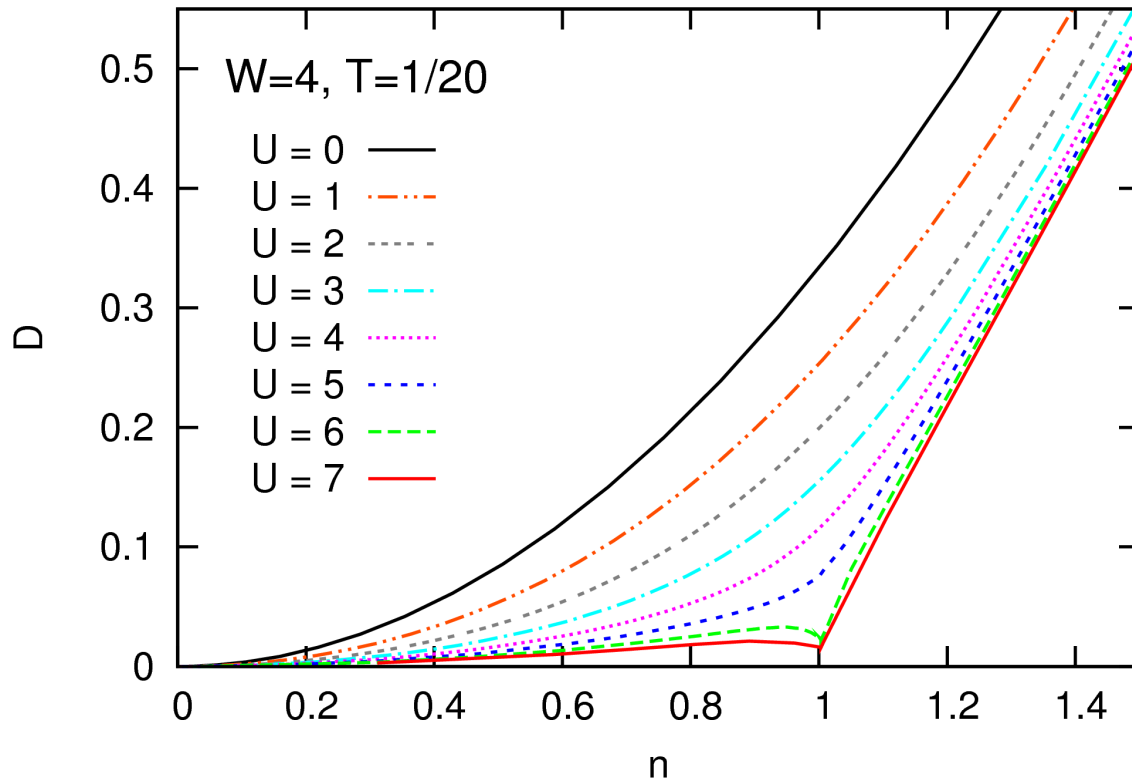
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Important for experiments:

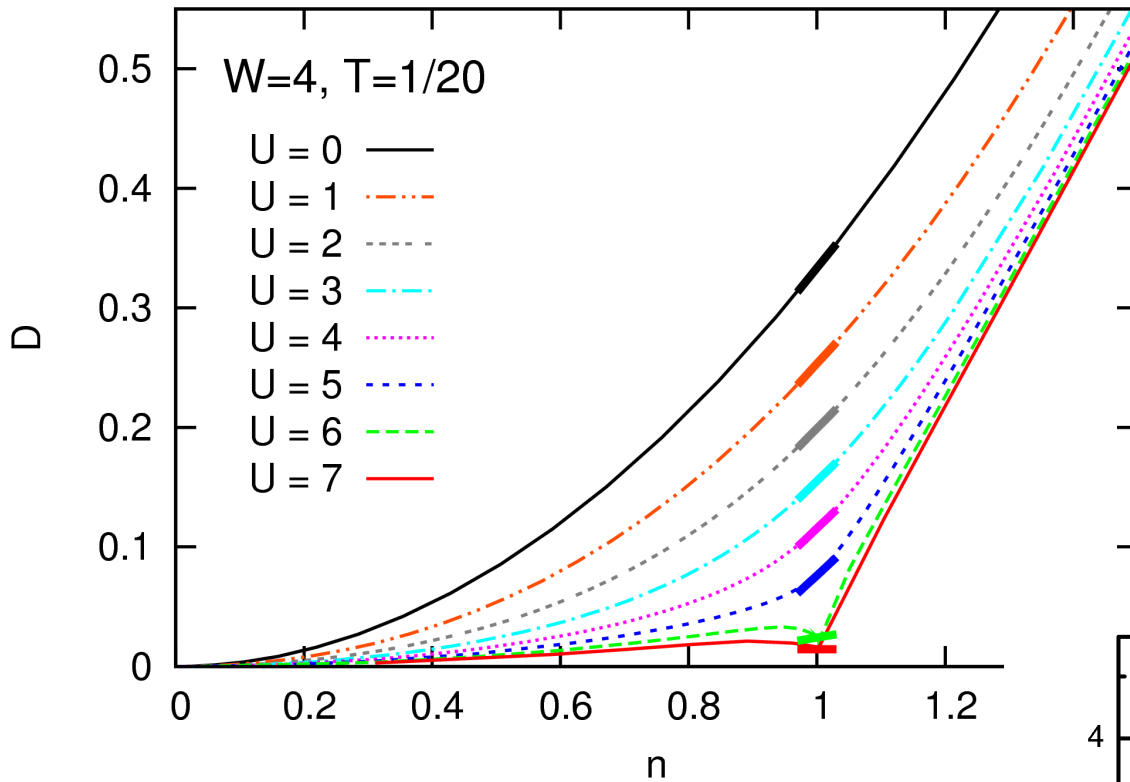
Signatures of Mott transition
persist to high temperatures:

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



3-spin/2-flavor system:

Pair occupancy vs. density



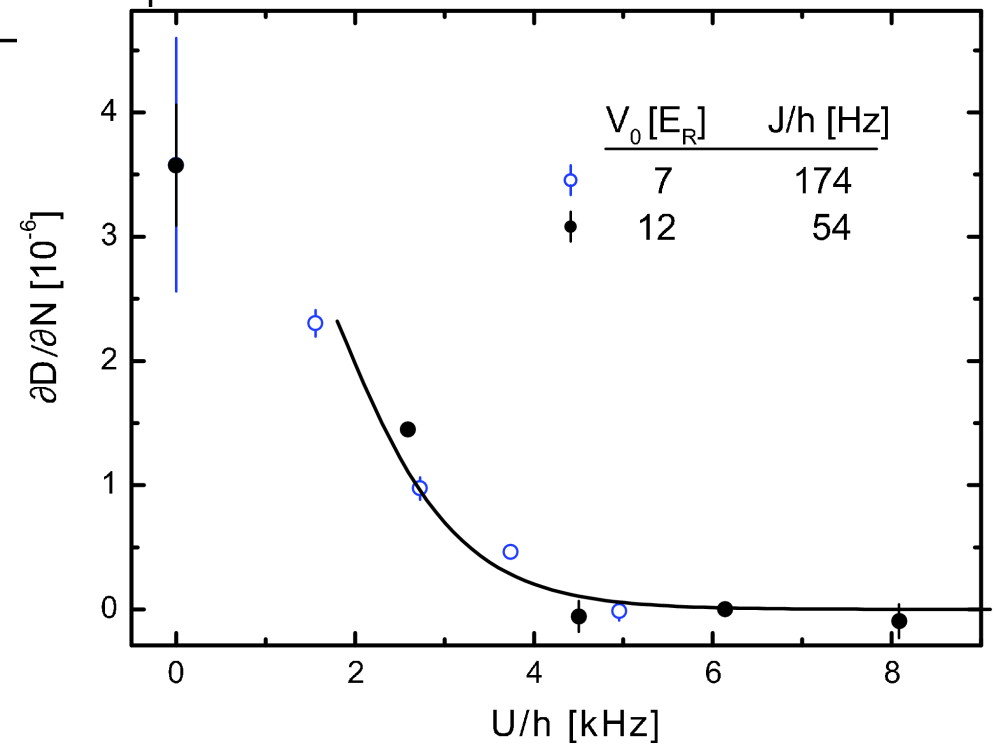
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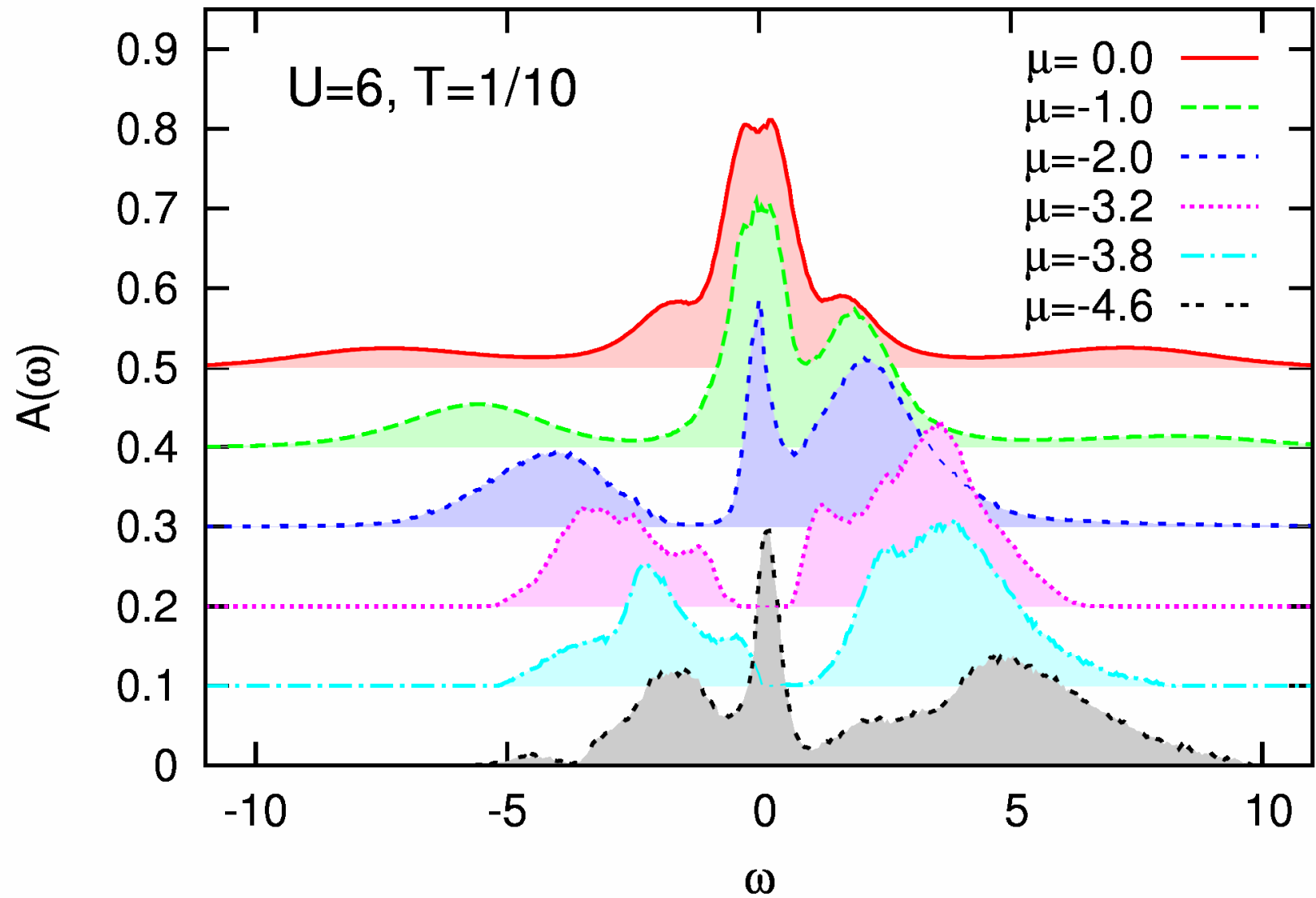
Experiment: 2-spin system

Transition to an incompressible phase

[Jördens et al., Nature (2008)]



Local spectral function



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)

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*

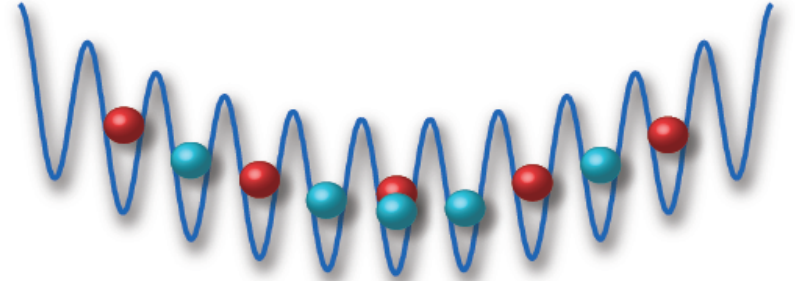
(Received 4 December 2009; published 17 February 2010)

- 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.: $V_i = Vr_i^2$

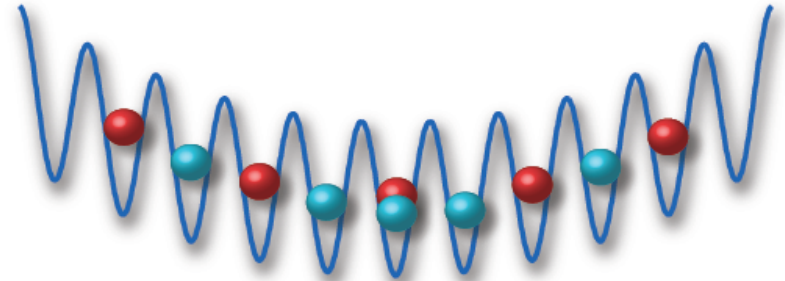
$$H = - \sum_{(ij),\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i n_{i\sigma}$$



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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:

$$\left[G_\sigma(i\omega_n) \right]_{ij}^{-1} = (\mu_\sigma + i\omega_n) \delta_{ij} - t_{ij} - (V_i + \Sigma_{i\sigma}(i\omega_n)) \delta_{ij}$$

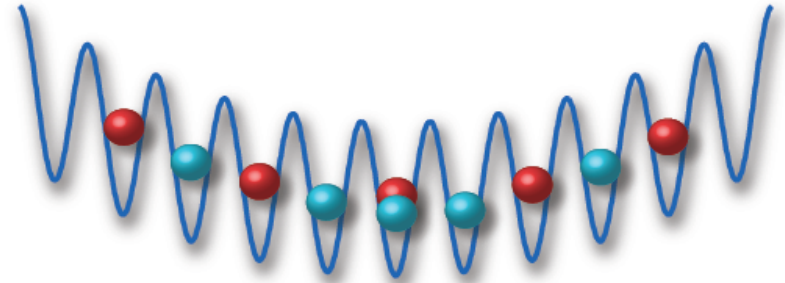
[M. Snoek, I. Titvinidze, C. Toke, K. Byczuk, and W. Hofstetter, *New Journal of Physics* (2008);
R. Helmes, T. A. Costi, and A. Rosch, *PRL* (2008)]

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

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

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

All previous implementations: **RDMFT+NRG**

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

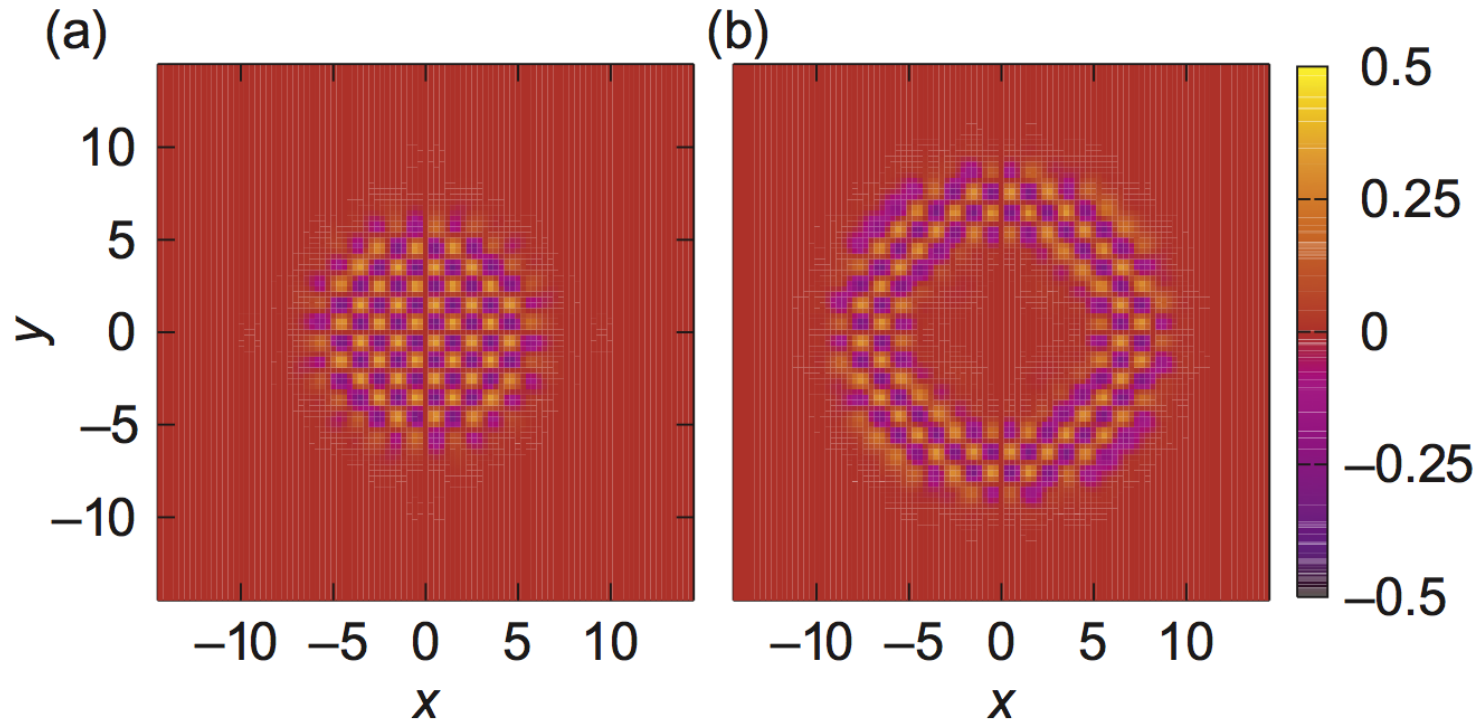
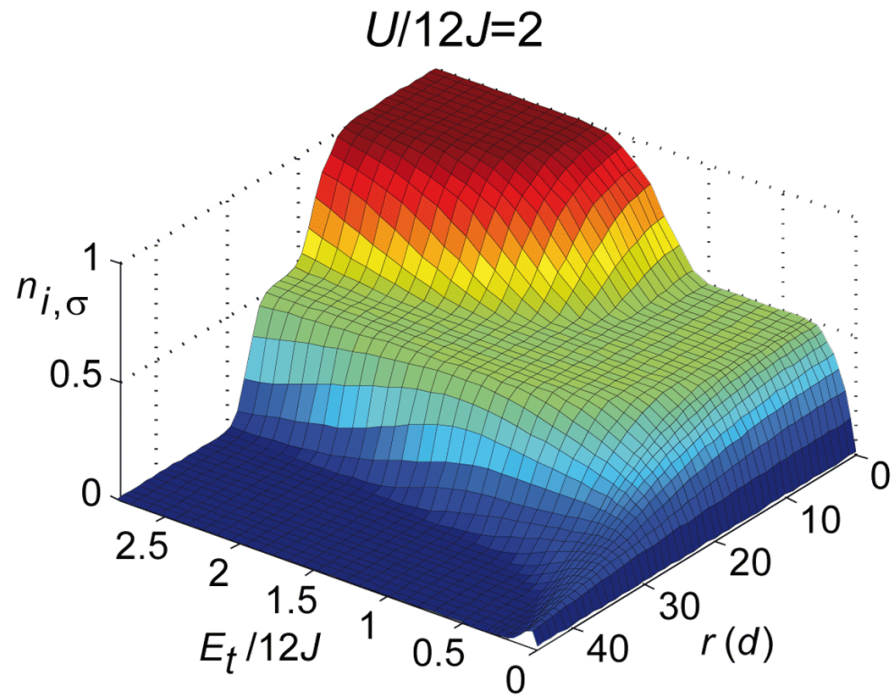


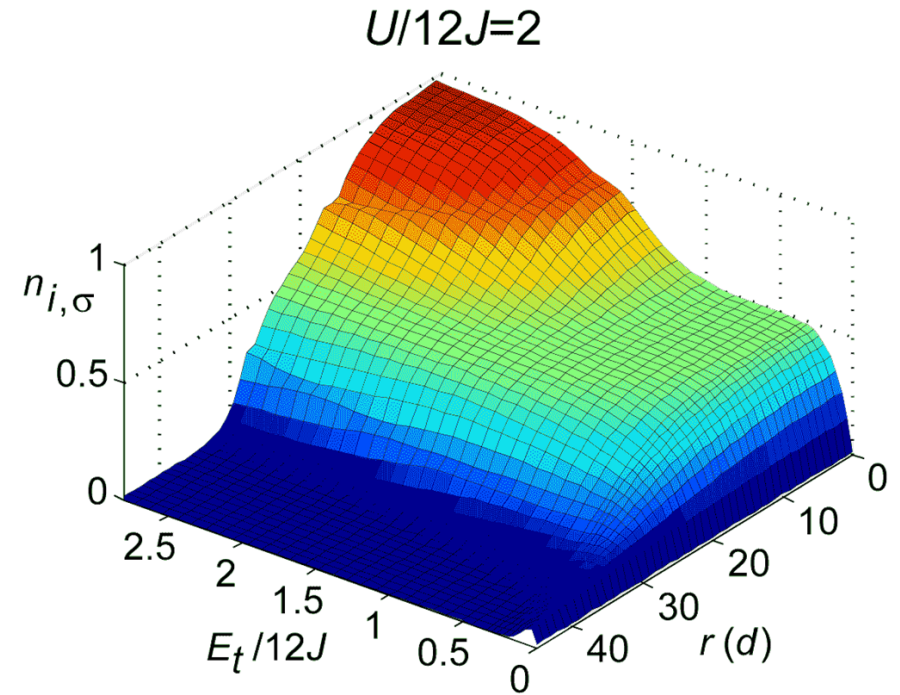
Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_{\uparrow} = \mu_{\downarrow} = 5$; (b) $V = 0.2$ and $\mu_{\uparrow} = \mu_{\downarrow} = 15$. Energies are expressed in units of the hopping parameter J .

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

But: NRG problematic at elevated temperatures



$$T = 0.07t$$

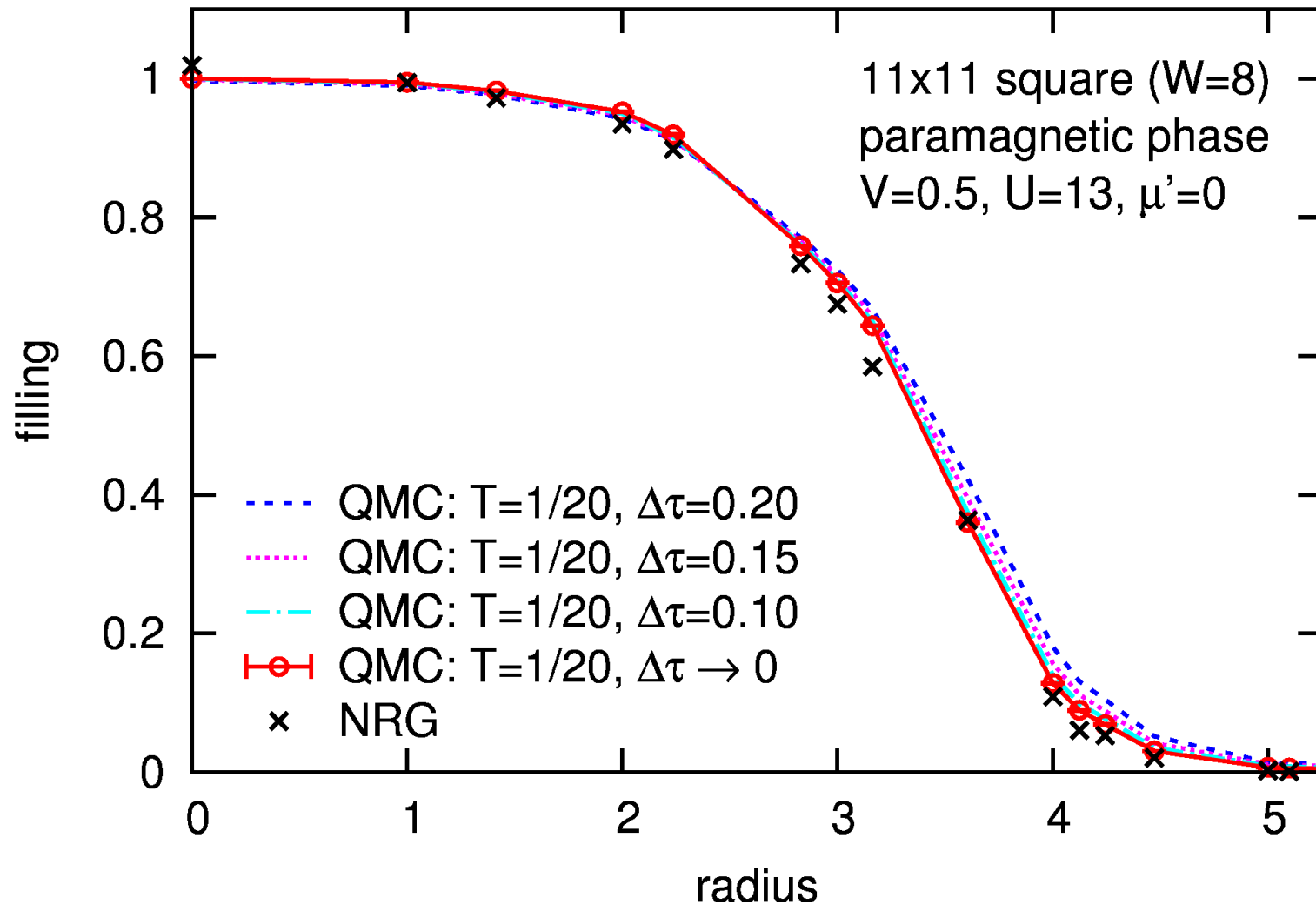


$$T = 0.15t$$

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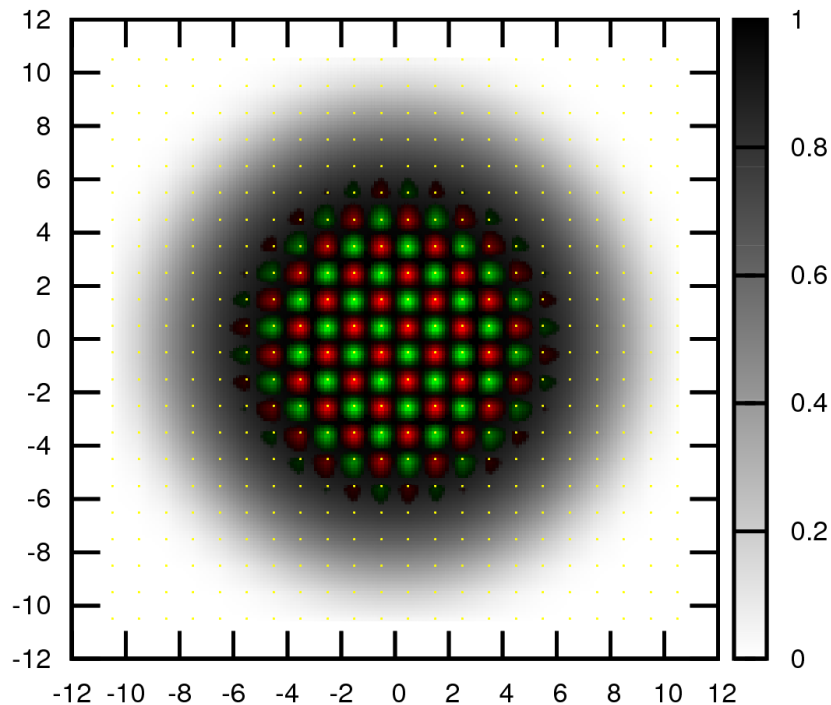
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Practical (dense inversion, fully parallel): $\lesssim 10000$ sites \rightsquigarrow need smart strategies



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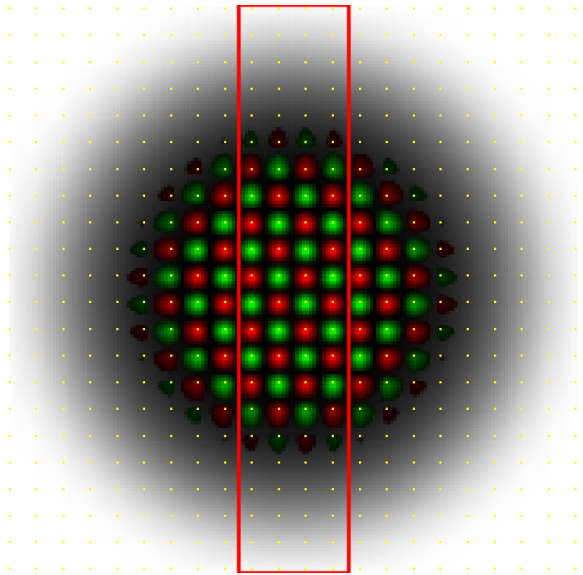
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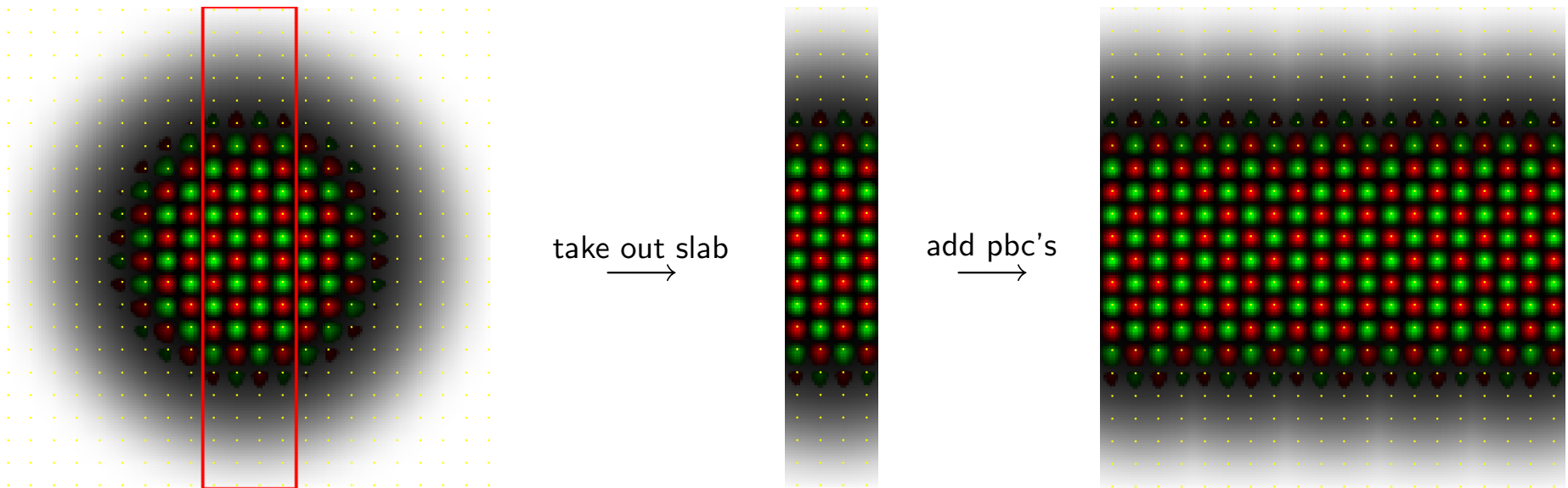
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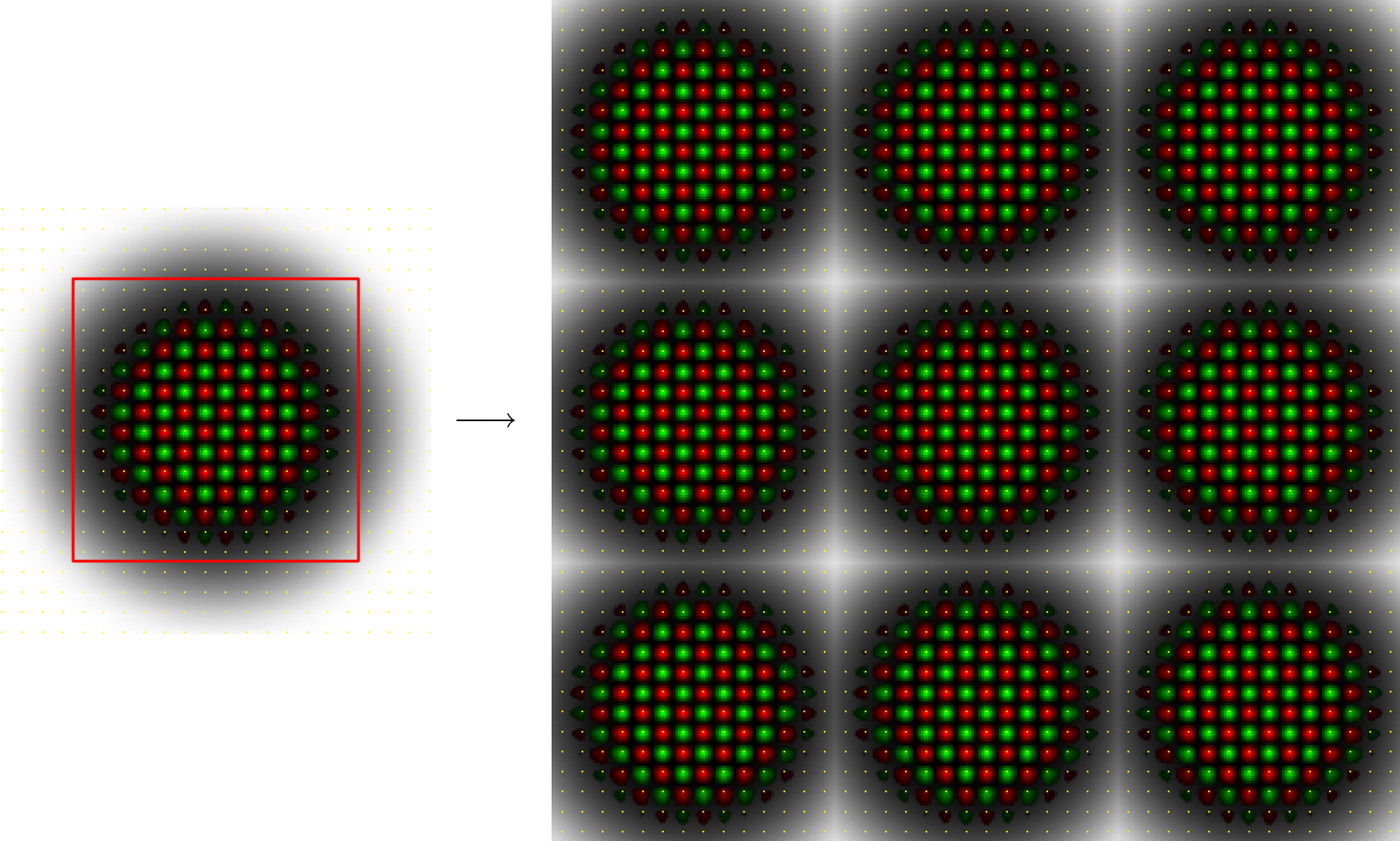
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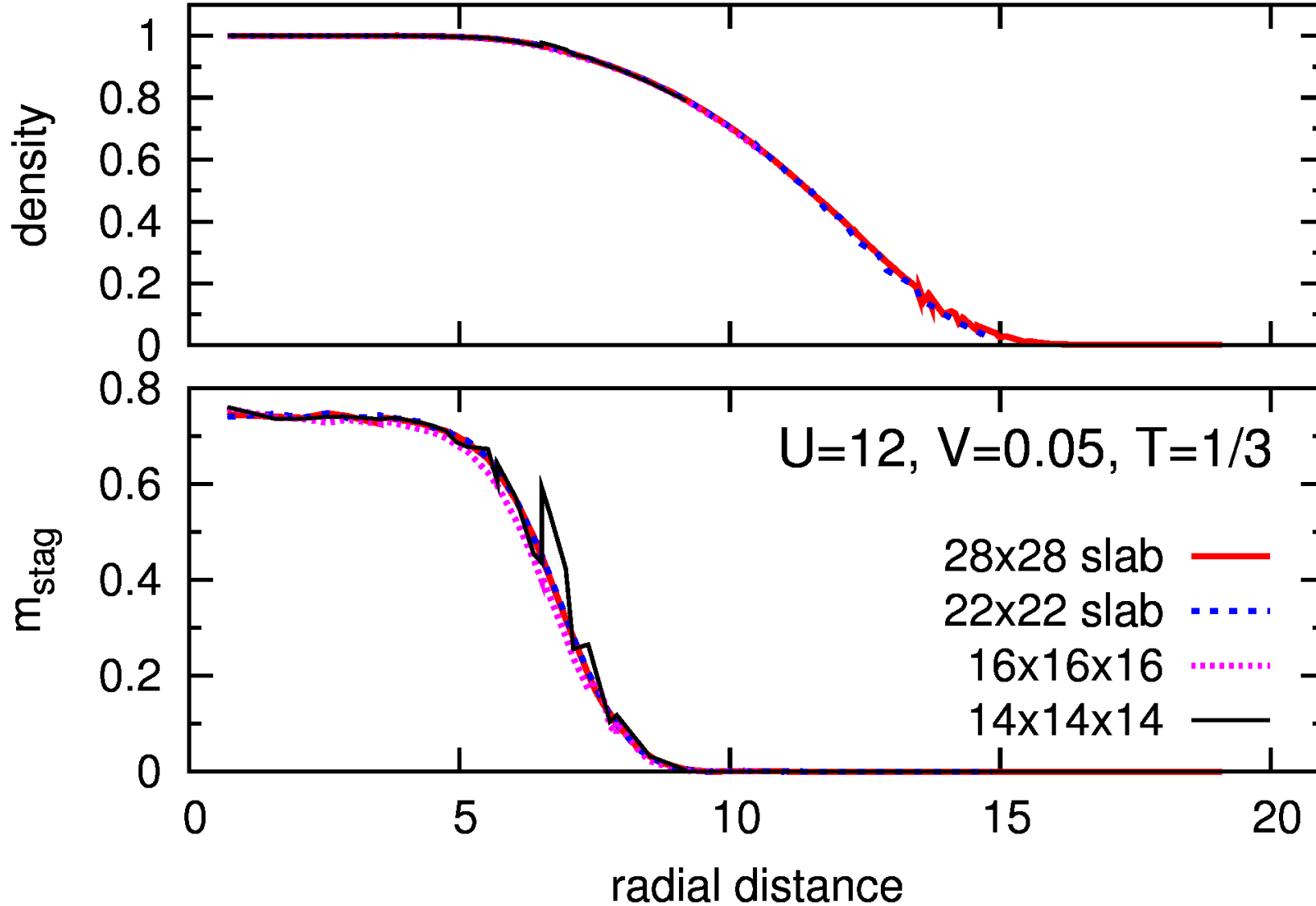
In practice: cylindrical potential (equivalent layers)

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



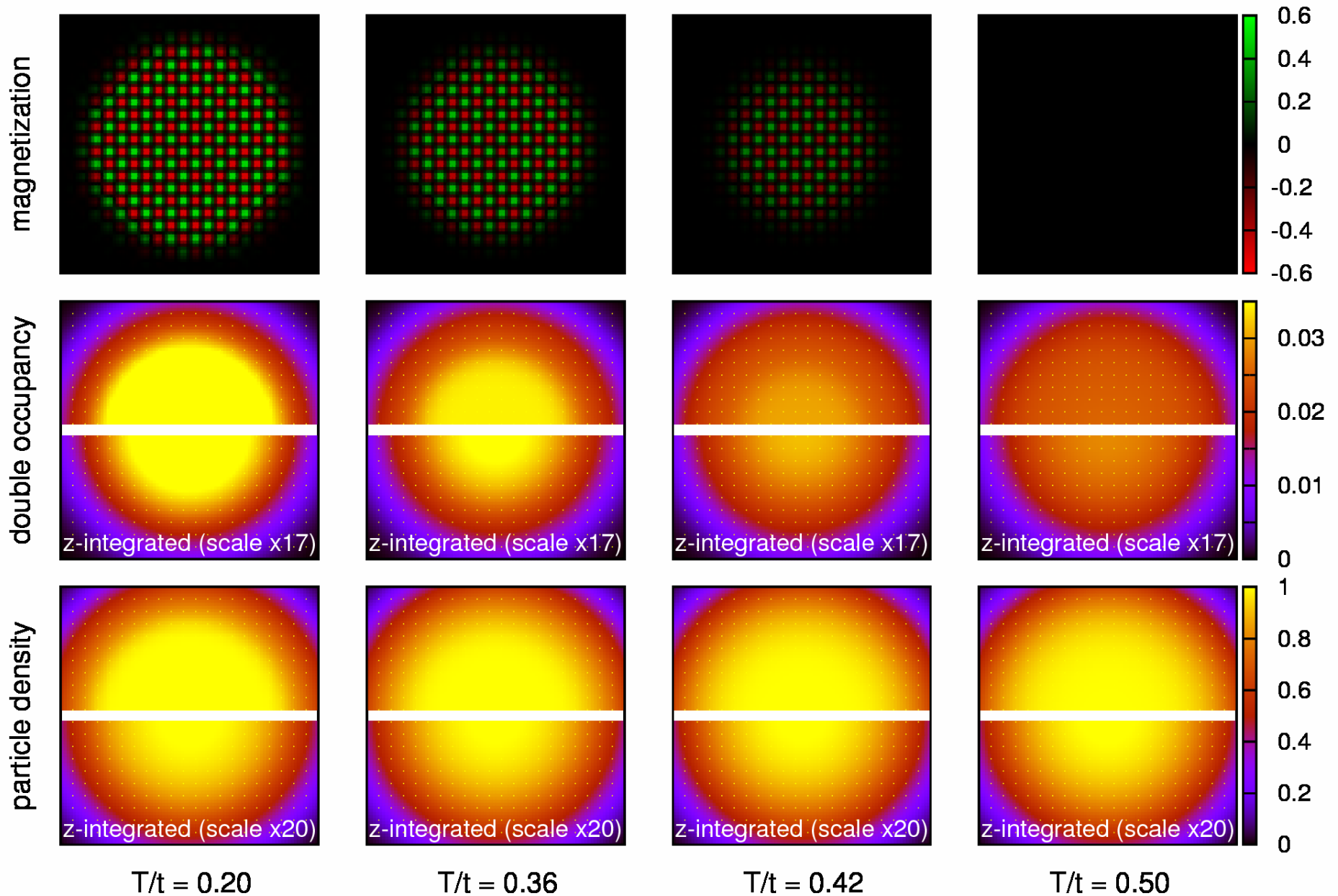
Most efficient: slab calculation focussing on AF core (with pbc)

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

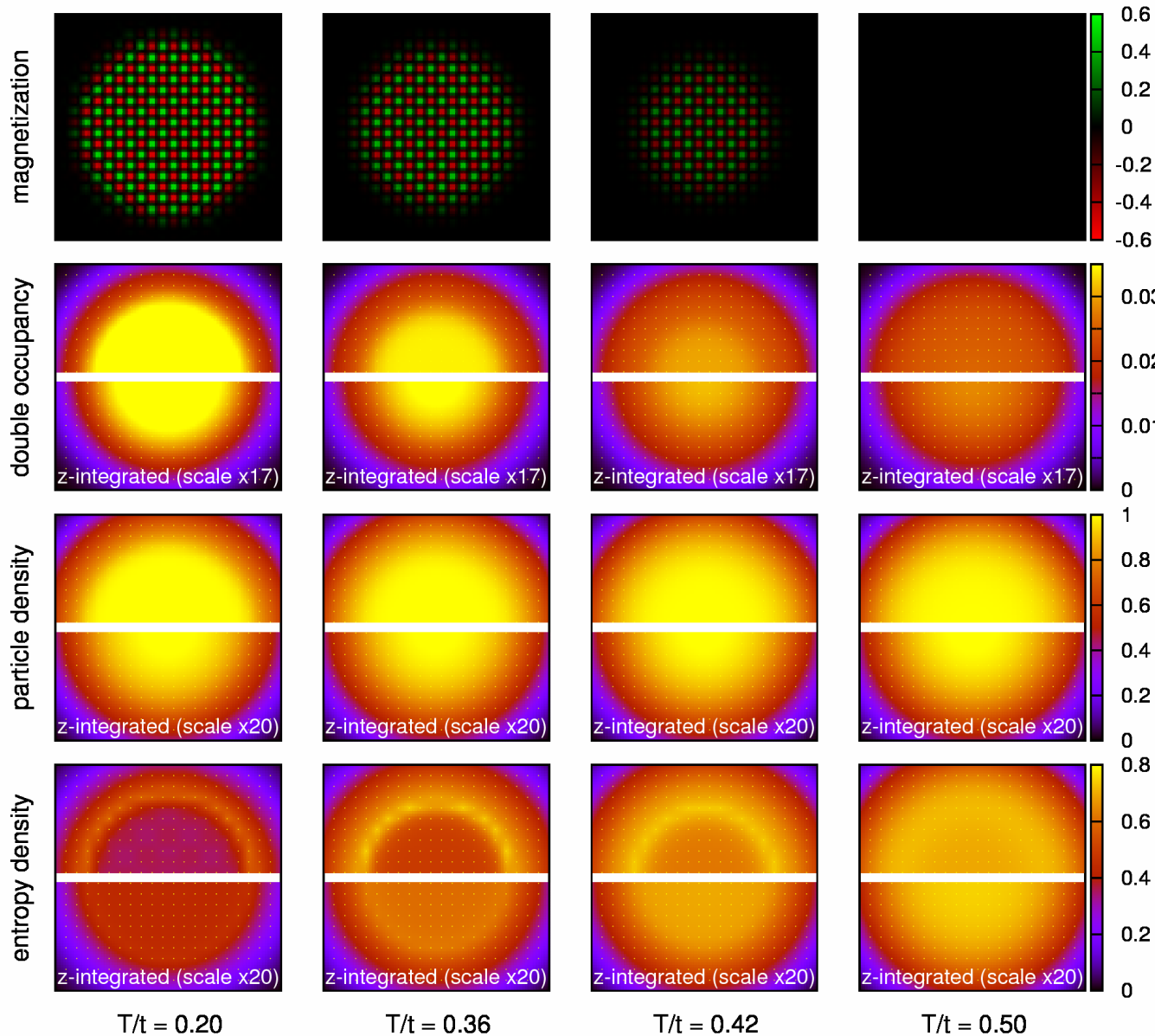


Significant deviations only if core touches boundaries!

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)

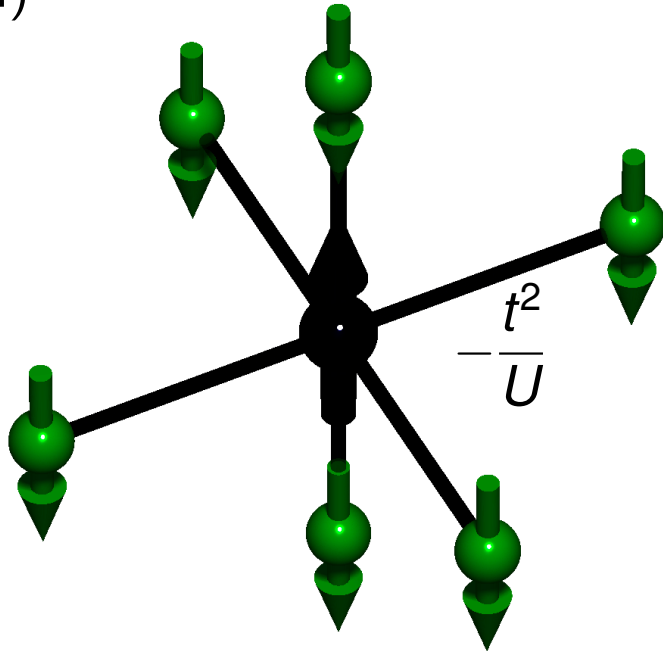
Entropy

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

Enhanced double occupancy: a signature of AF order

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

(a)

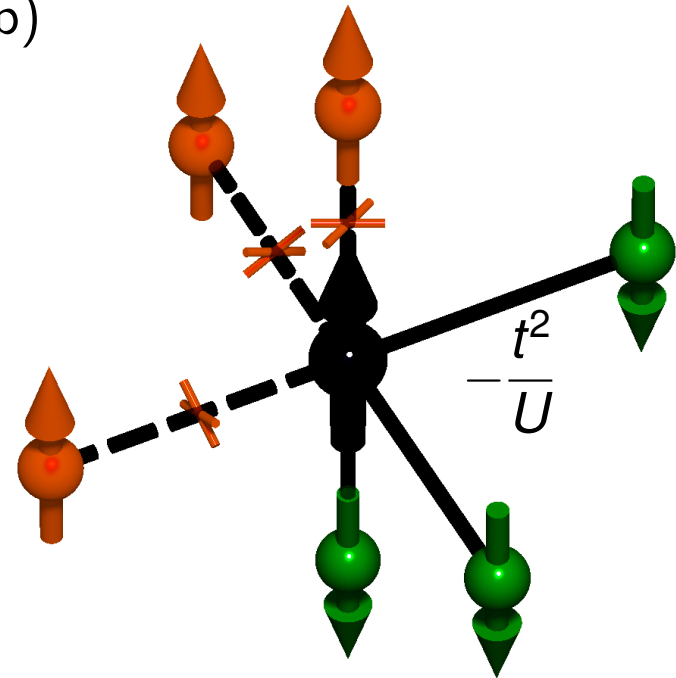


AF state:

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

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

(b)



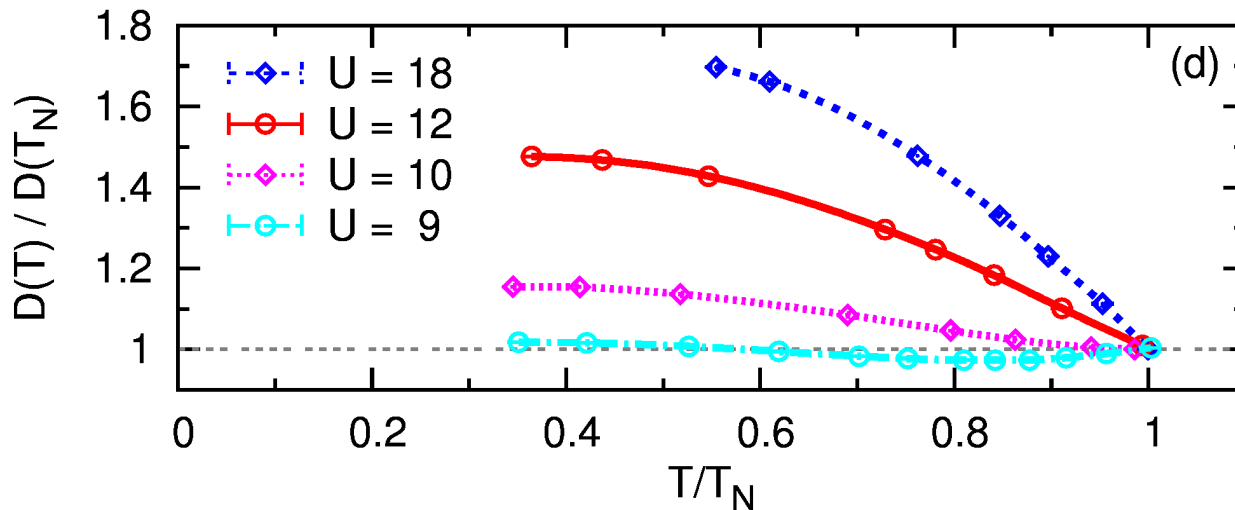
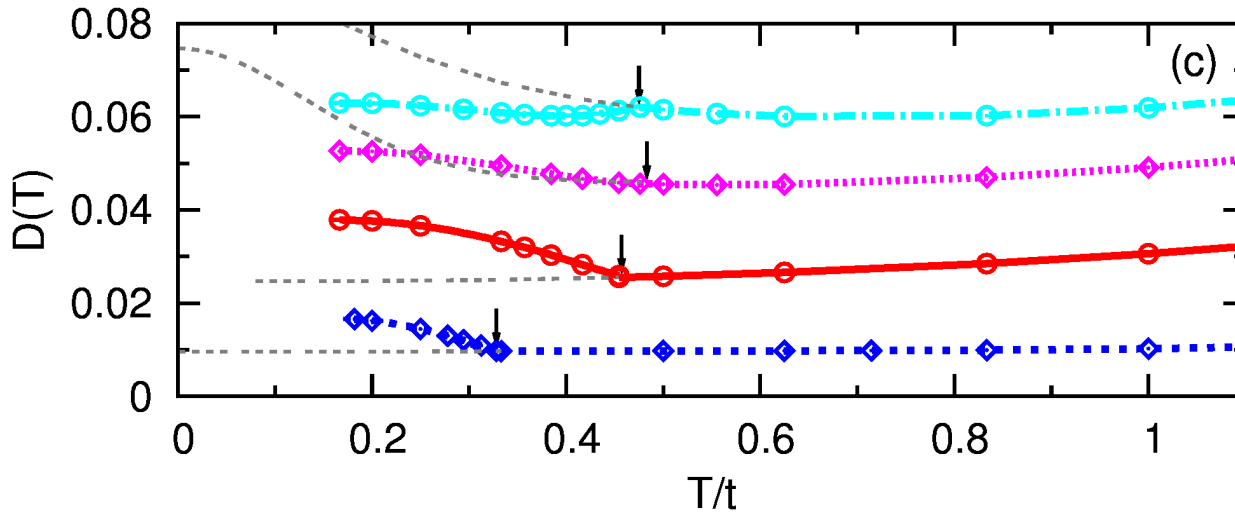
Paramagnetic state:

1/2 of the neighboring sites
are forbidden for hopping

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

By $D = dE/dU$ (at $T = 0$), the argument implies $D_{\text{AF}}/D_{\text{p}} \xrightarrow{U \rightarrow \infty} 2$.

DMFT-QMC estimates of D at half filling



AF \Rightarrow

enhanced D at $U \gtrsim 10t$

arrows: Néel temperatures

thin lines: metastable paramagnetic phase.

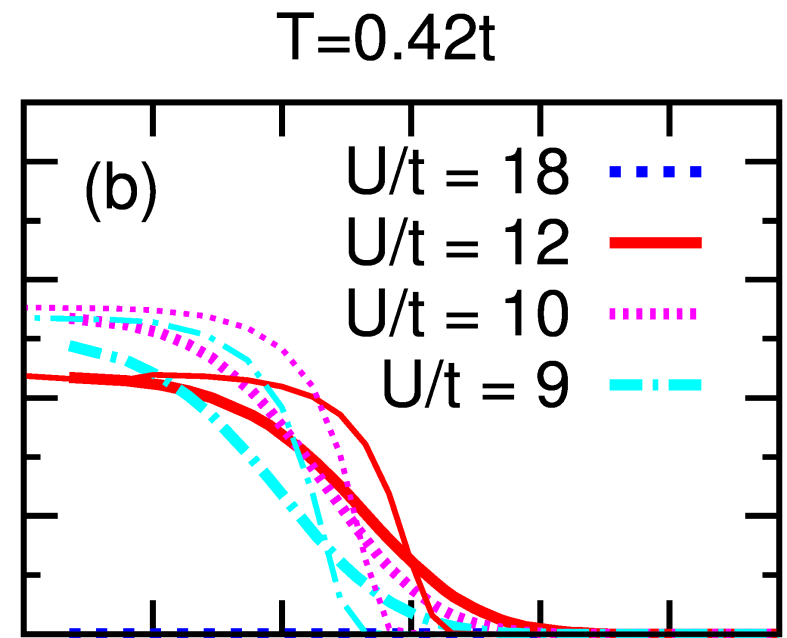
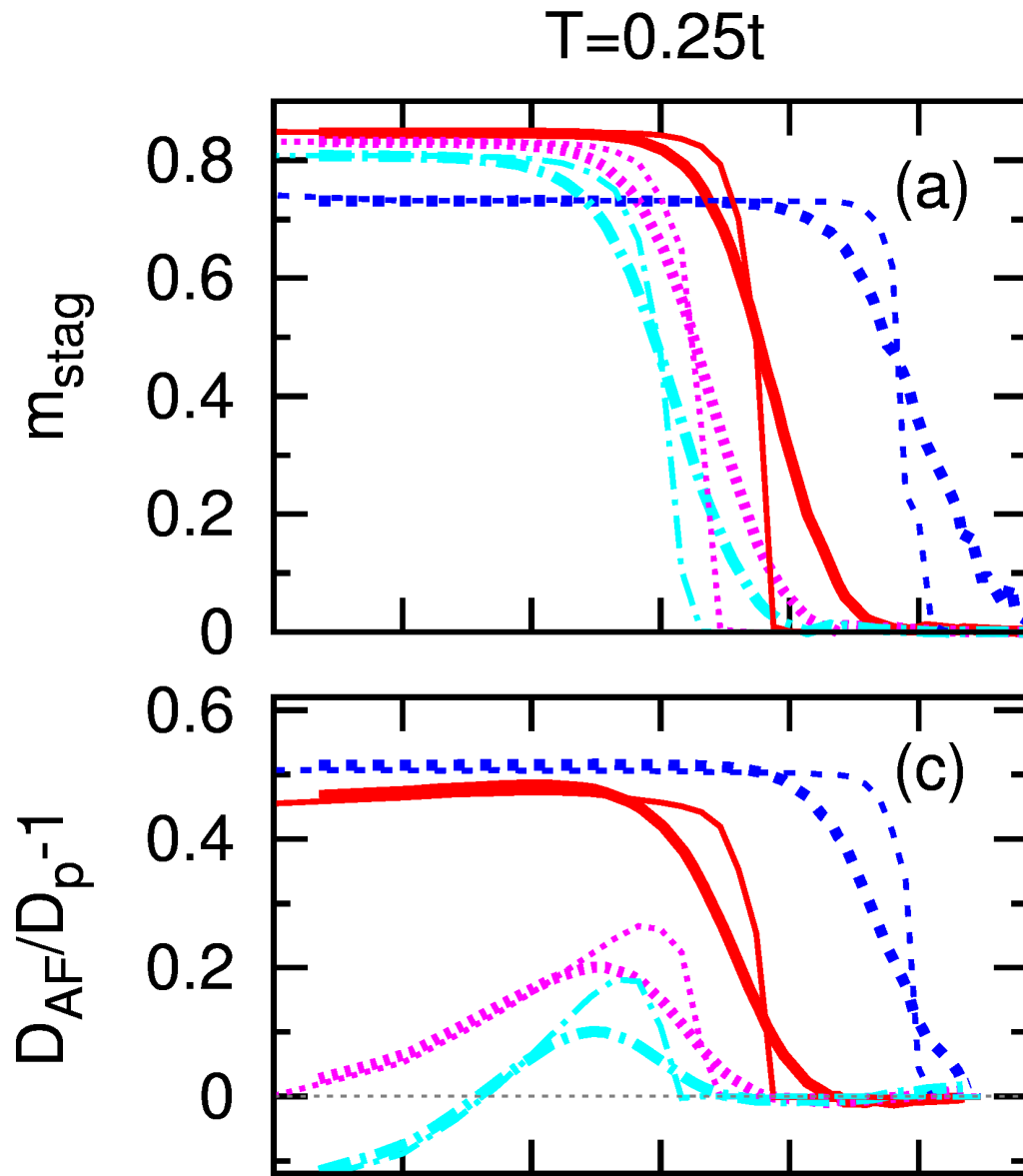
Data scaled to values of critical point:

relative enhancement

$$D/D(T_N) \xrightarrow{U \rightarrow \infty} 2$$

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

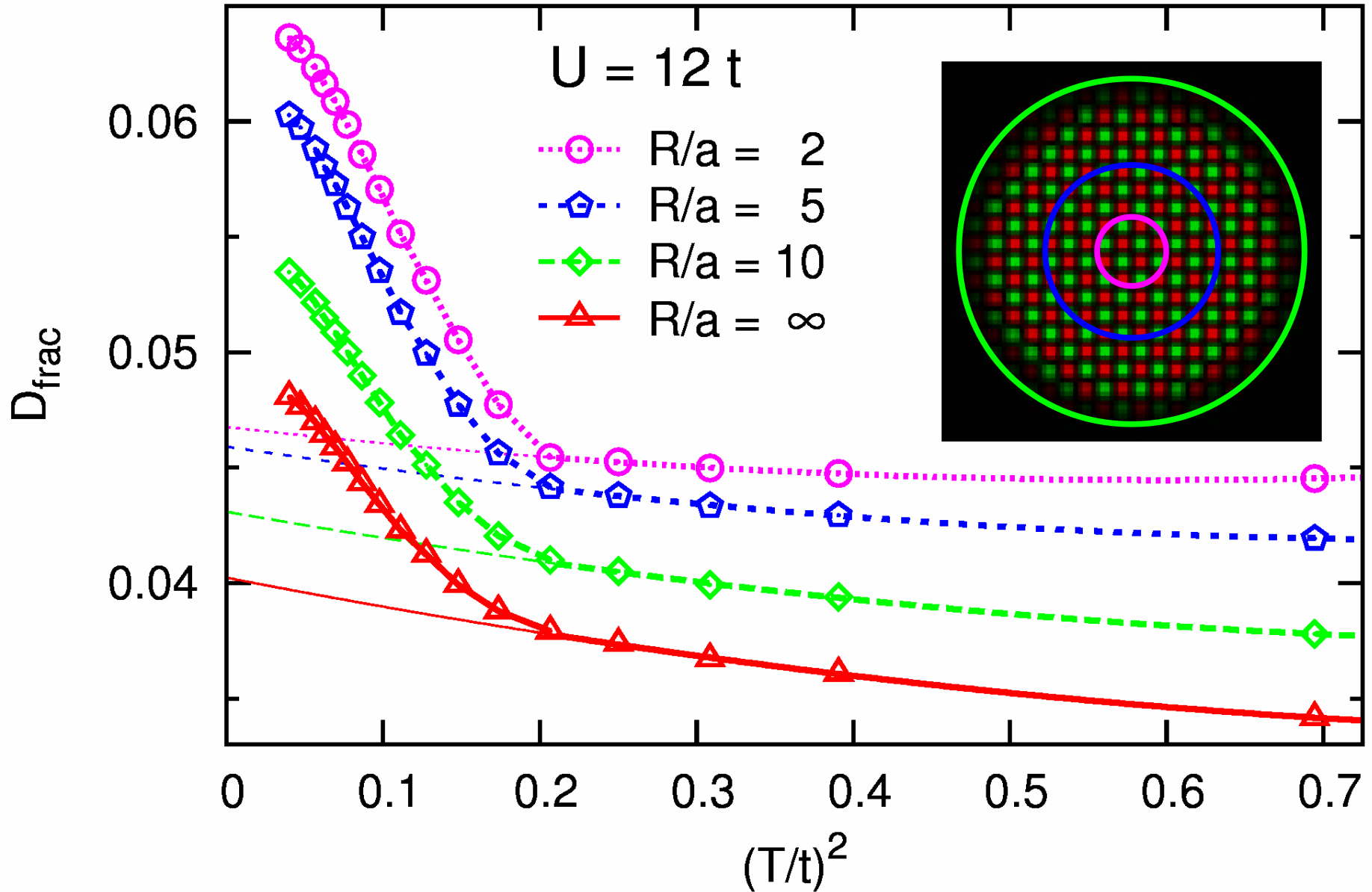
Radial dependence of m_{stag} and D : RDMFT calculations ($V = 0.05t$)



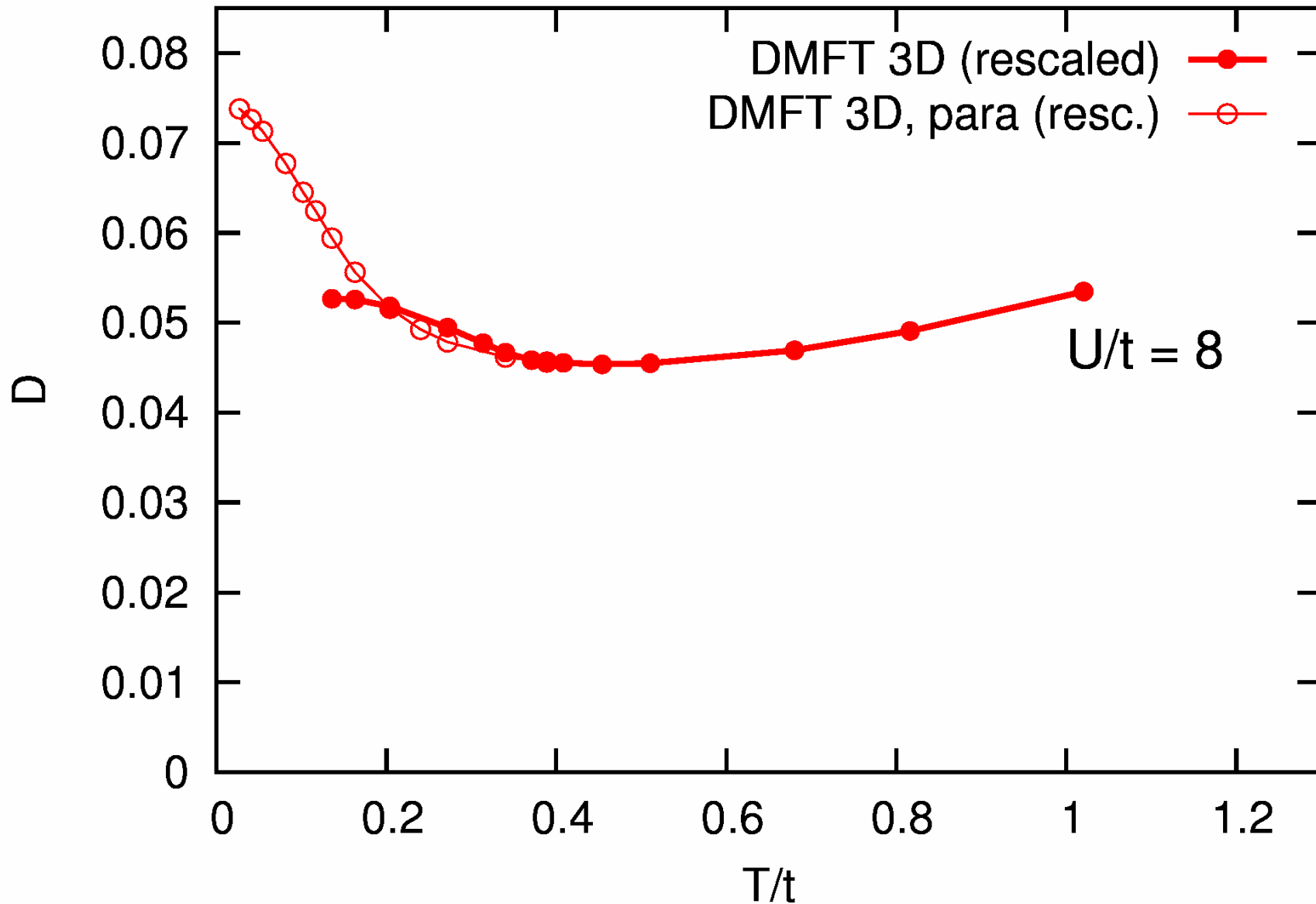
Strong proximity effects
beyond LDA (thin lines)

significant enhancement of D
only at strong coupling

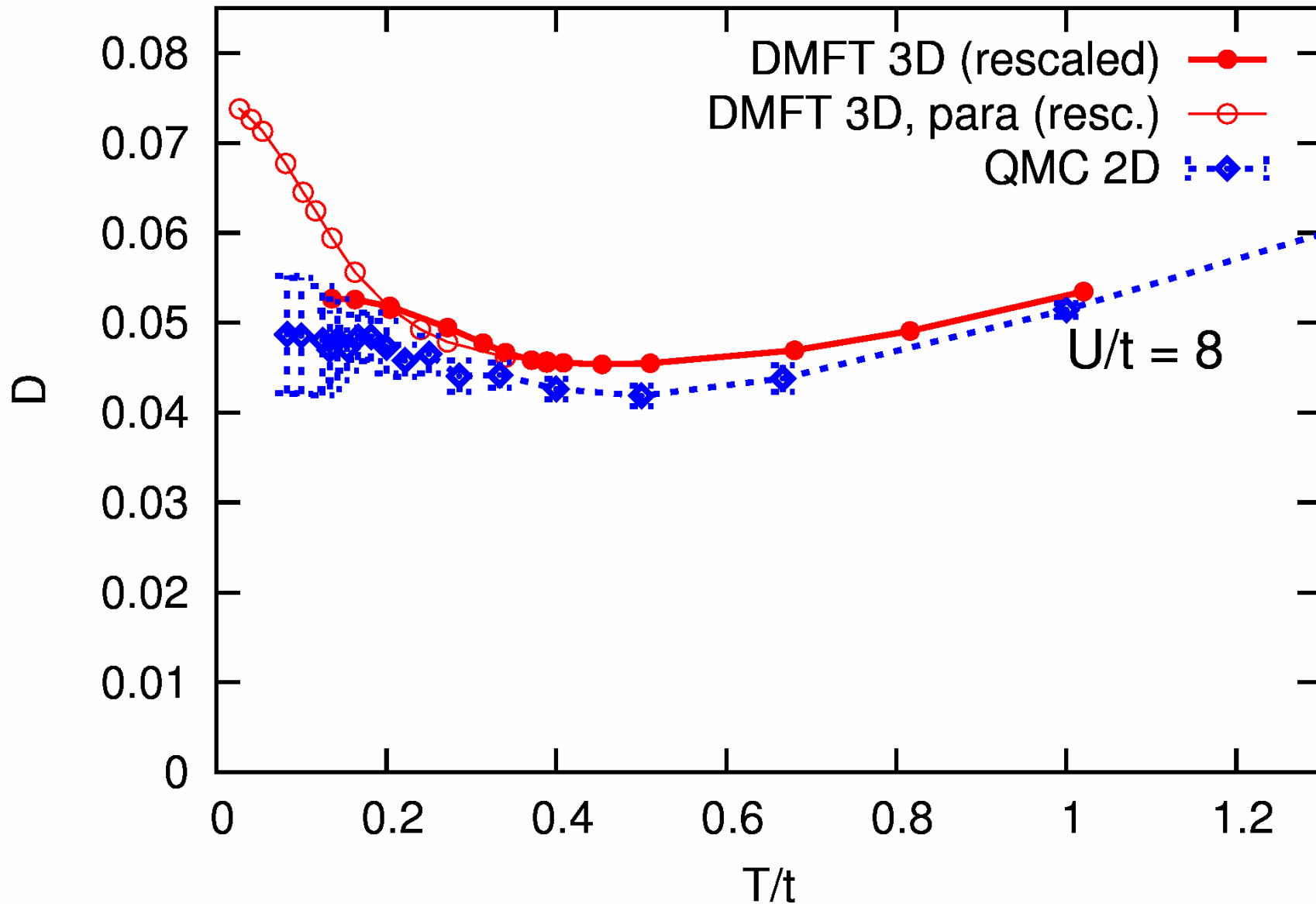
Néel transition visible in integrated quantities? Yes!



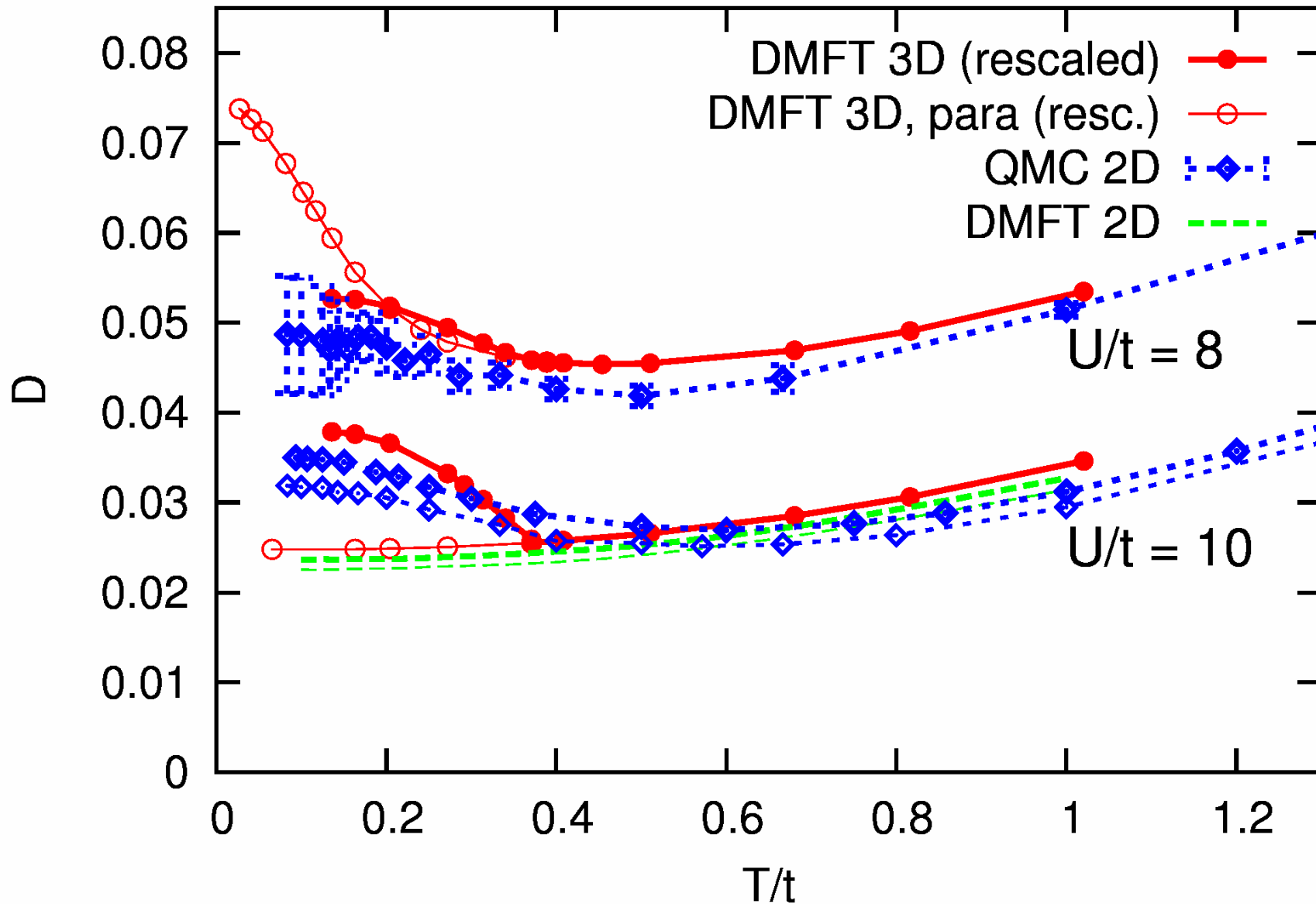
How realistic is DMFT? Extreme test case: 2 dimensions (square)



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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

DMFT surprisingly accurate in low dimensions

[E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, N. Blümer, [arXiv:1004.4857](https://arxiv.org/abs/1004.4857)]

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: U. Schneider, I. Bloch and Hofstetter

and DFG (TR49)

General method development: new initiative DFG-FG 1346

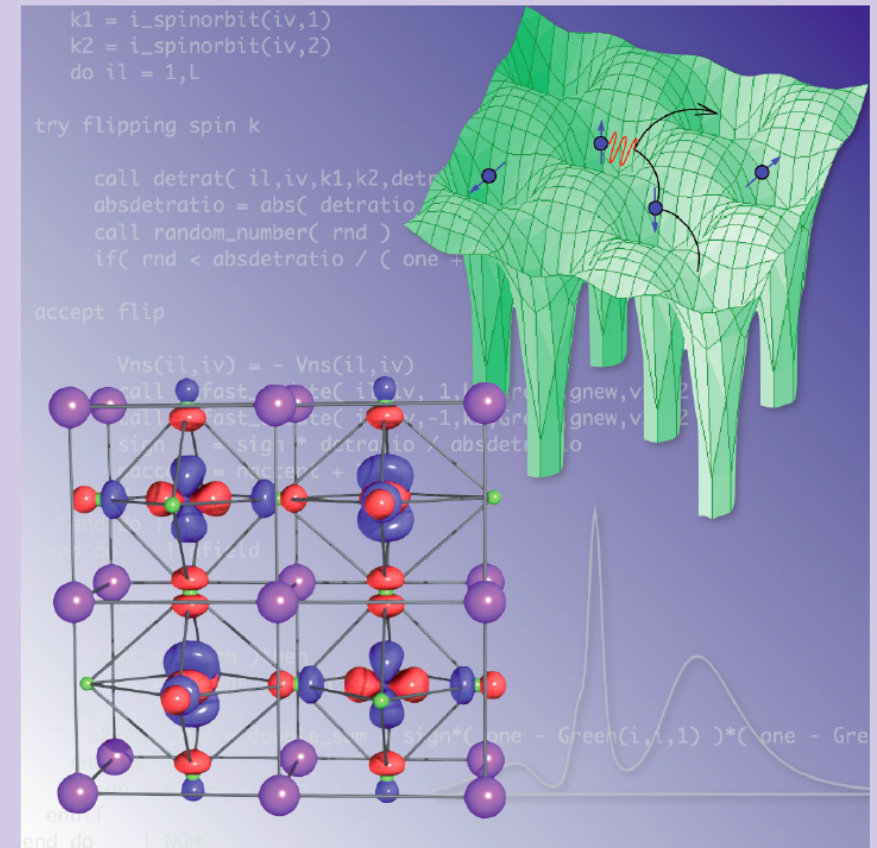
Positive evaluation on 2010/04/15+16,
senate decision on 2010/06/30.

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**

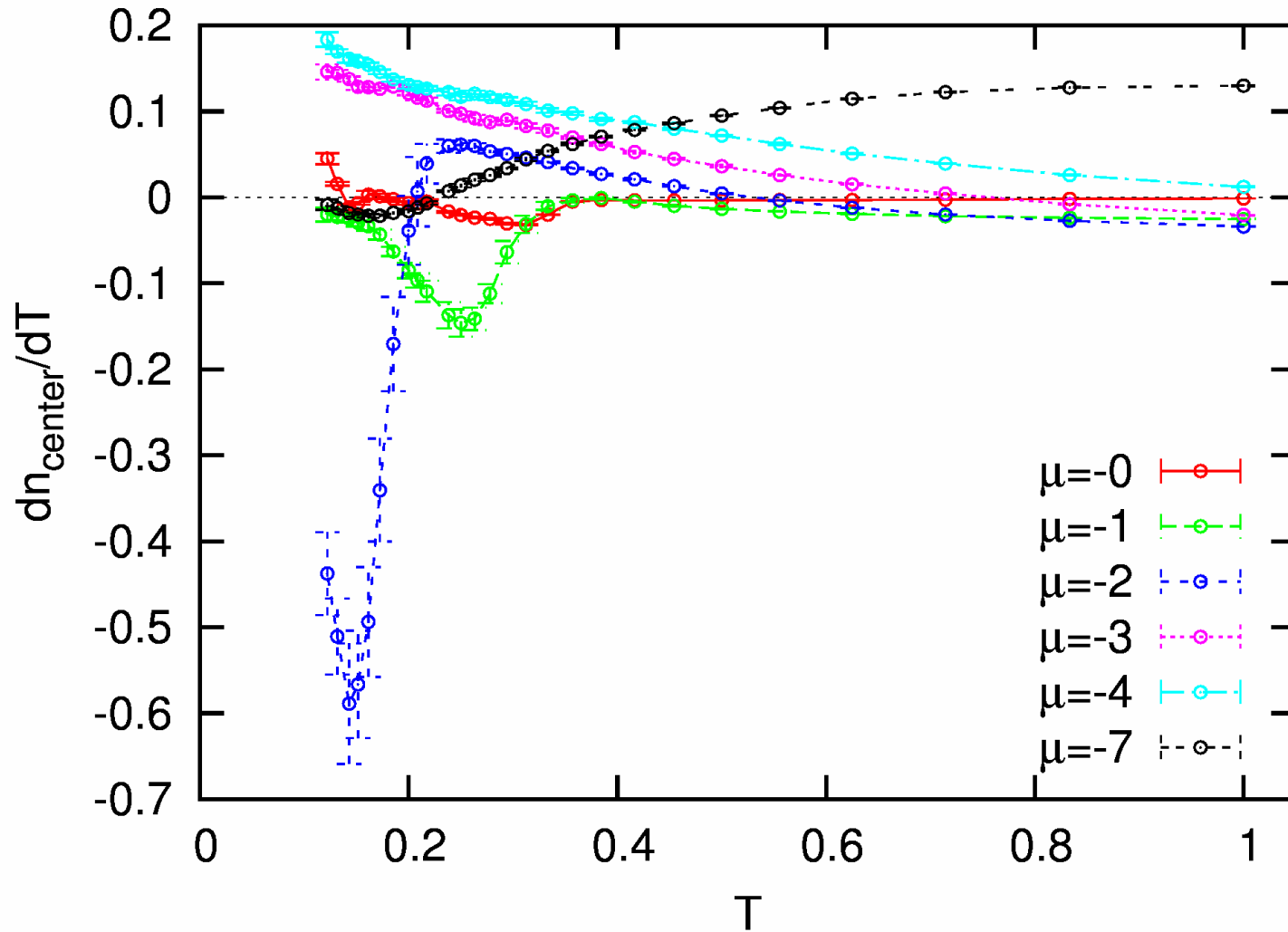
P7: GW+DMFT (Held, Toschi, Kresse)

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



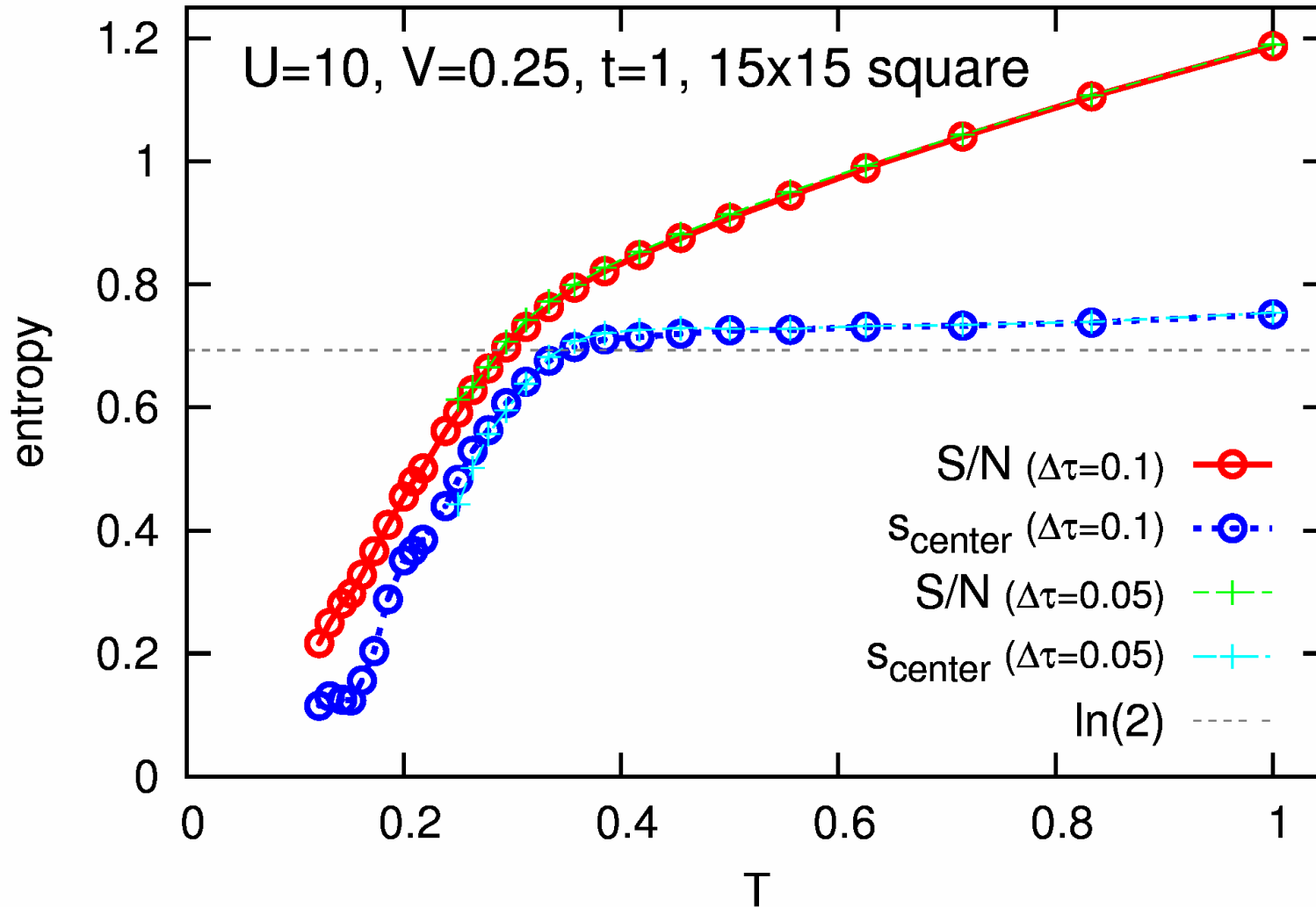
Dieter Vollhardt, University of Augsburg (Spokesperson)
Alexander Lichtenstein, University of Hamburg (Co-Spokesperson)

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!