Néel transition of fermionic atoms in an optical trap: a real-space DMFT study

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Outline

Introduction: SCES, cold atoms on lattices

Approaches for correlated lattice Fermi systems

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

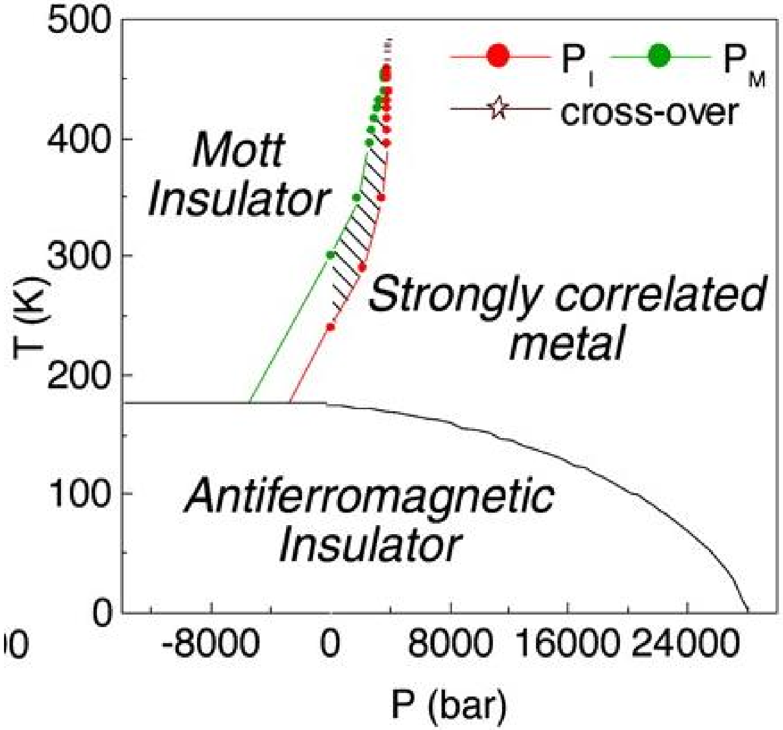
Summary and Outlook

Systems with strong electronic/fermionic correlations

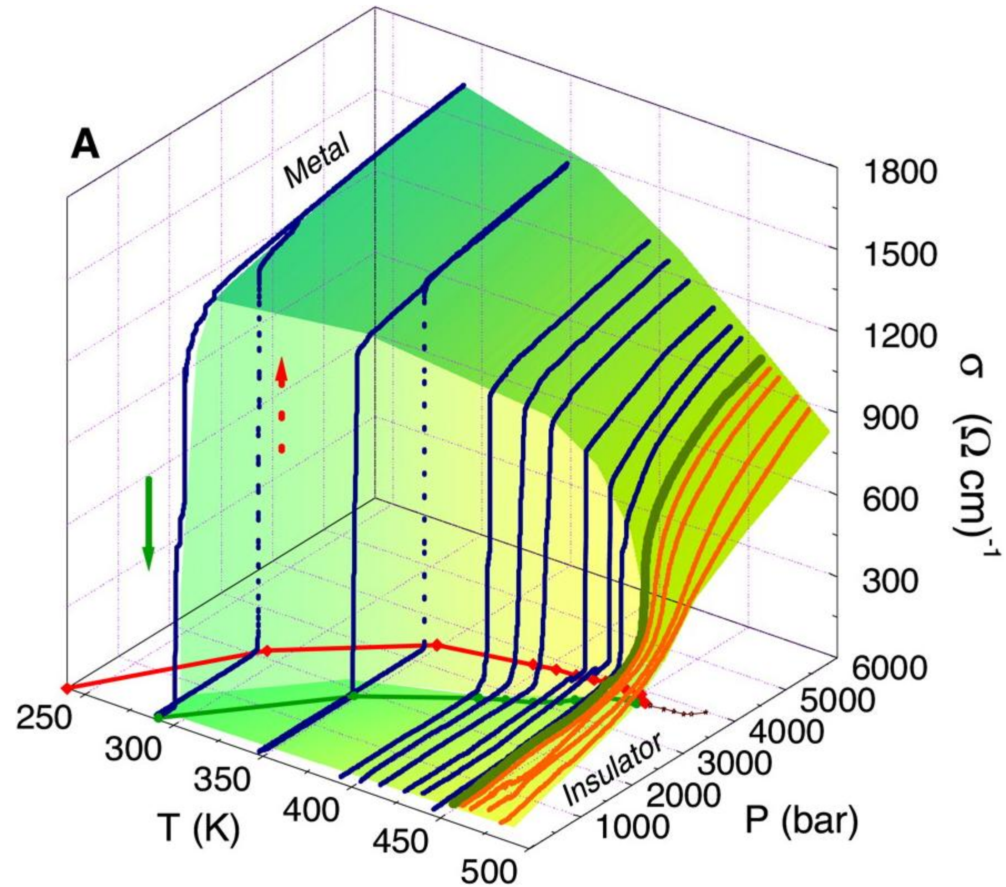
Paramagnetic Mott metal-insulator transition

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

Phase diagram



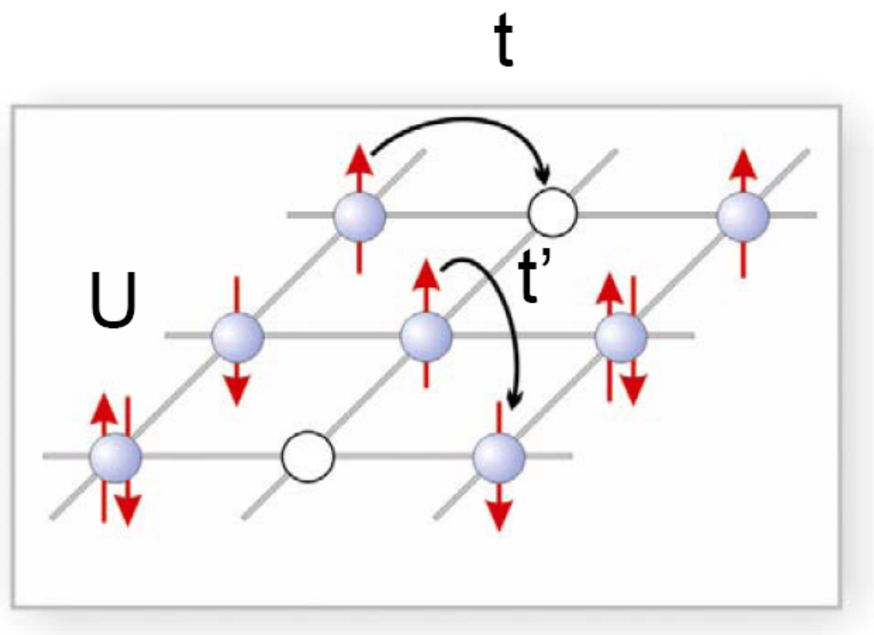
Electrical conductivity



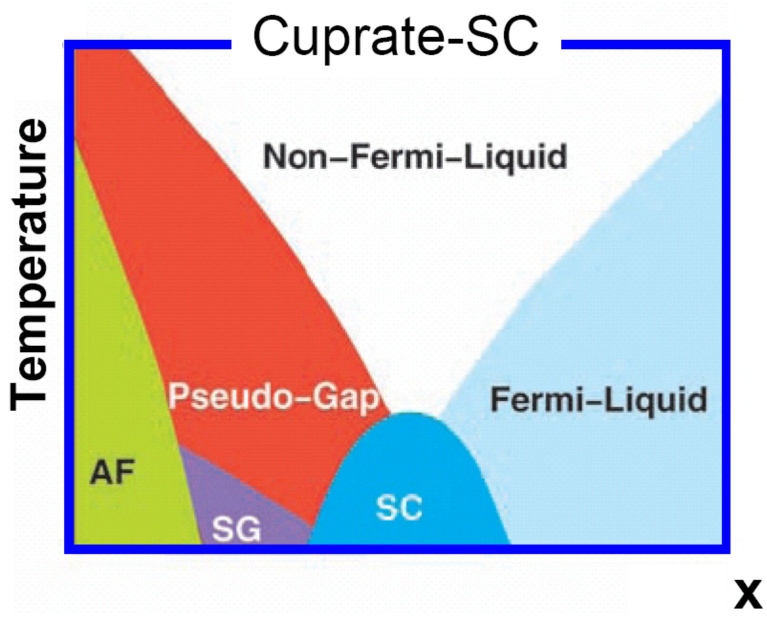
[Limelette et al., Science 302, 89 (2003)]

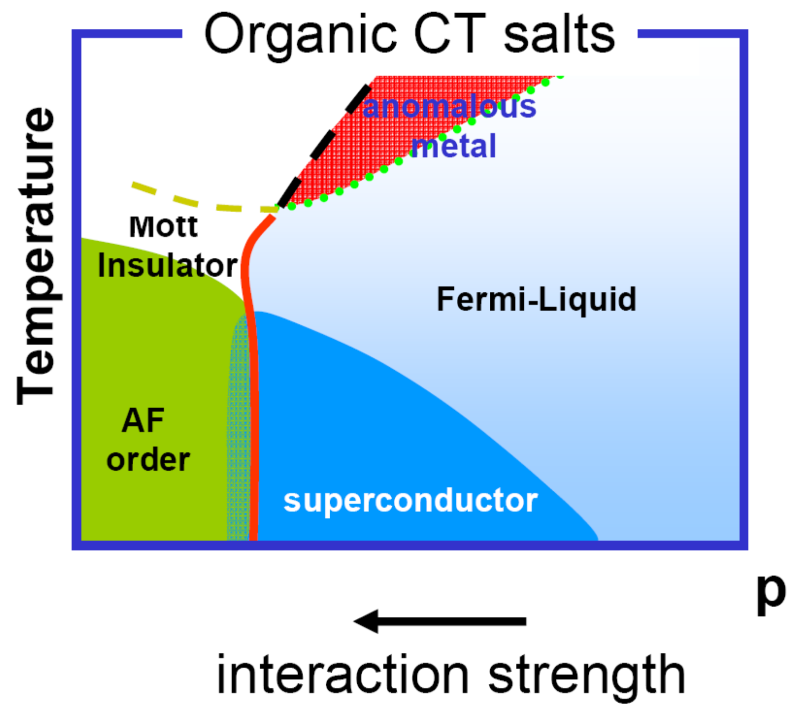
Complex phases of cuprate and organic superconductors

High-T_c physics contained in 2D Hubbard model?



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



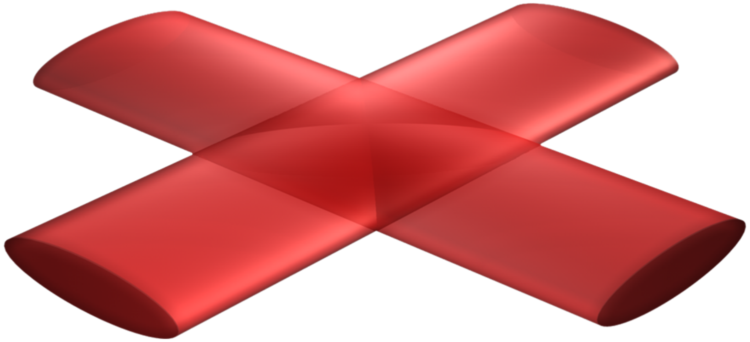


Correlated ultracold quantum gases on optical lattices: basics

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

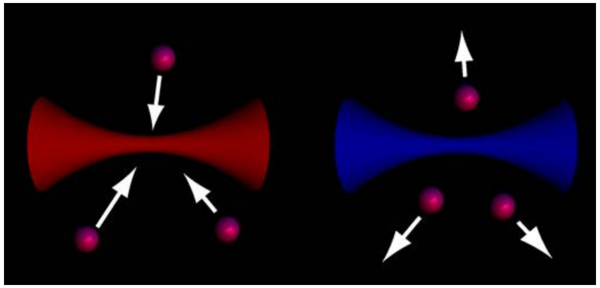
Optical dipole trap (2 beams)

$$V_{\text{dipole}}(\boldsymbol{r}) = -\boldsymbol{d} \cdot \boldsymbol{E}(\boldsymbol{r}) \propto \alpha(\omega_{\text{L}}) \left|\boldsymbol{E}(\boldsymbol{r})\right|^2$$



time-averaged intensity $\left|\boldsymbol{E}(\boldsymbol{r})\right|^2$

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



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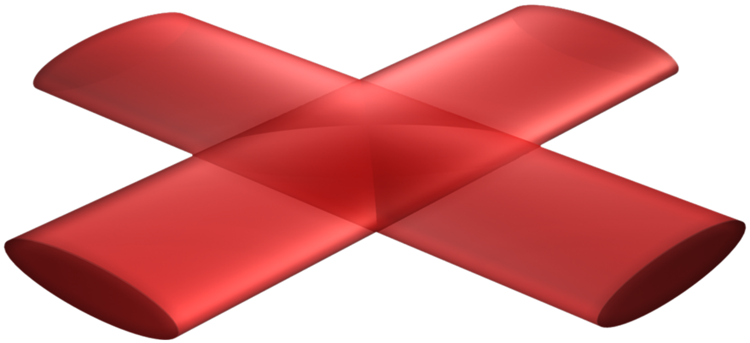

$$V_{\text{dipole}}(\boldsymbol{r}) = -\boldsymbol{d} \cdot \boldsymbol{E}(\boldsymbol{r}) \propto \alpha(\omega_L)\,|\boldsymbol{E}(\boldsymbol{r})|^2$$

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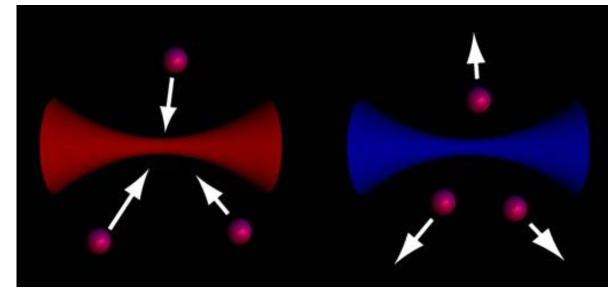
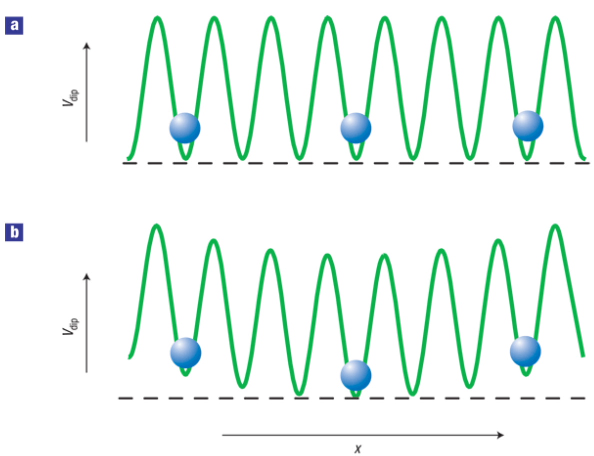


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



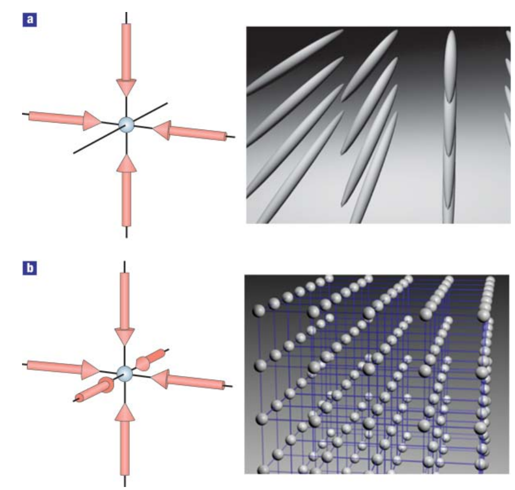
Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

2 pairs of lasers $\rightsquigarrow$ tubes

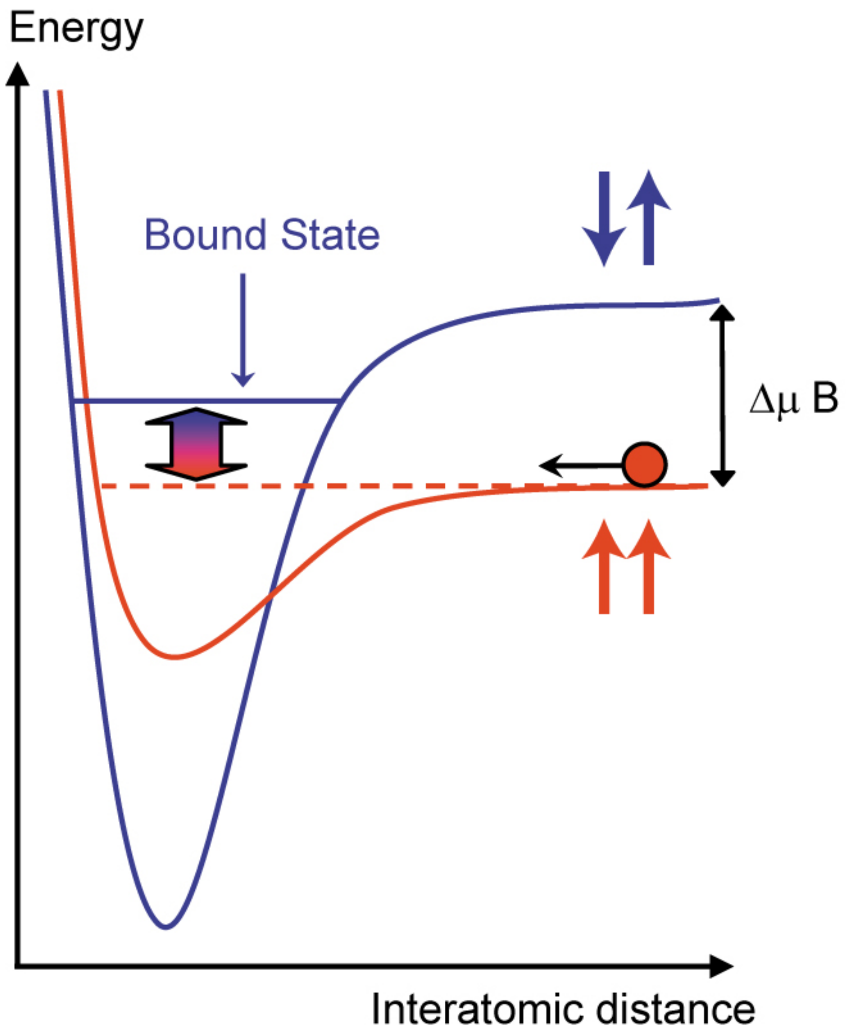
3 pairs of lasers $\rightsquigarrow$ 3D lattice

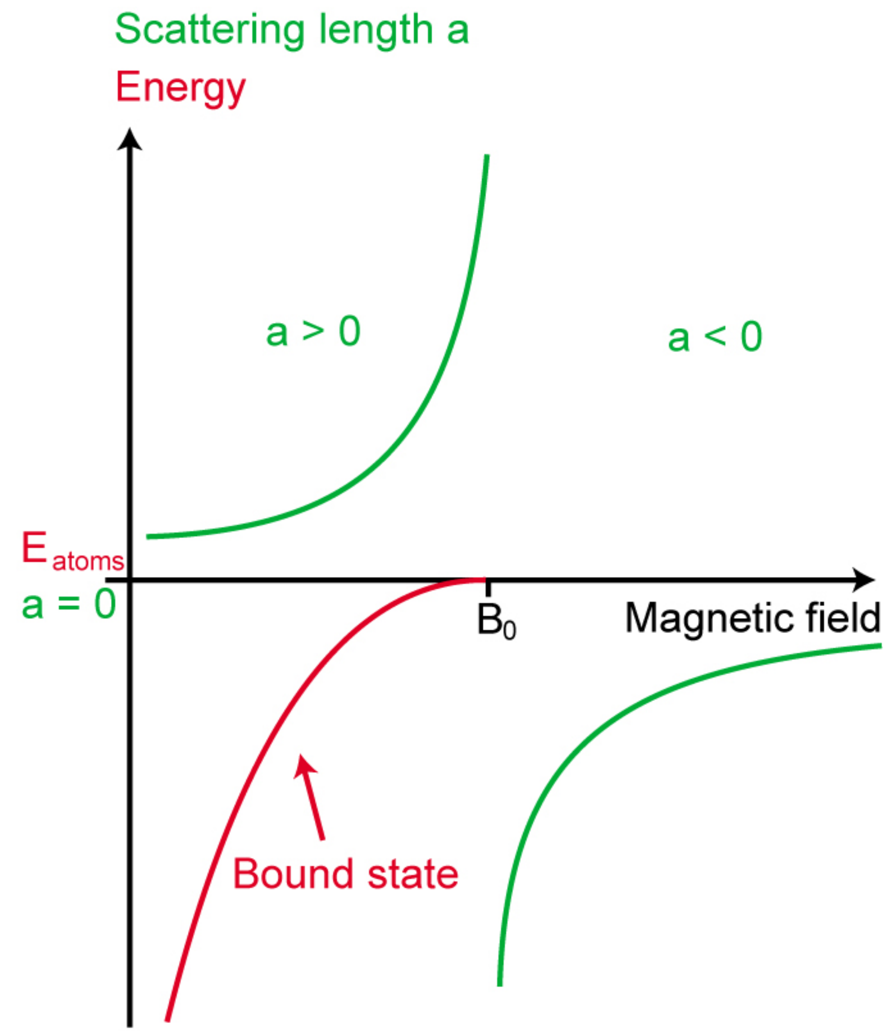
hopping t tunable by laser



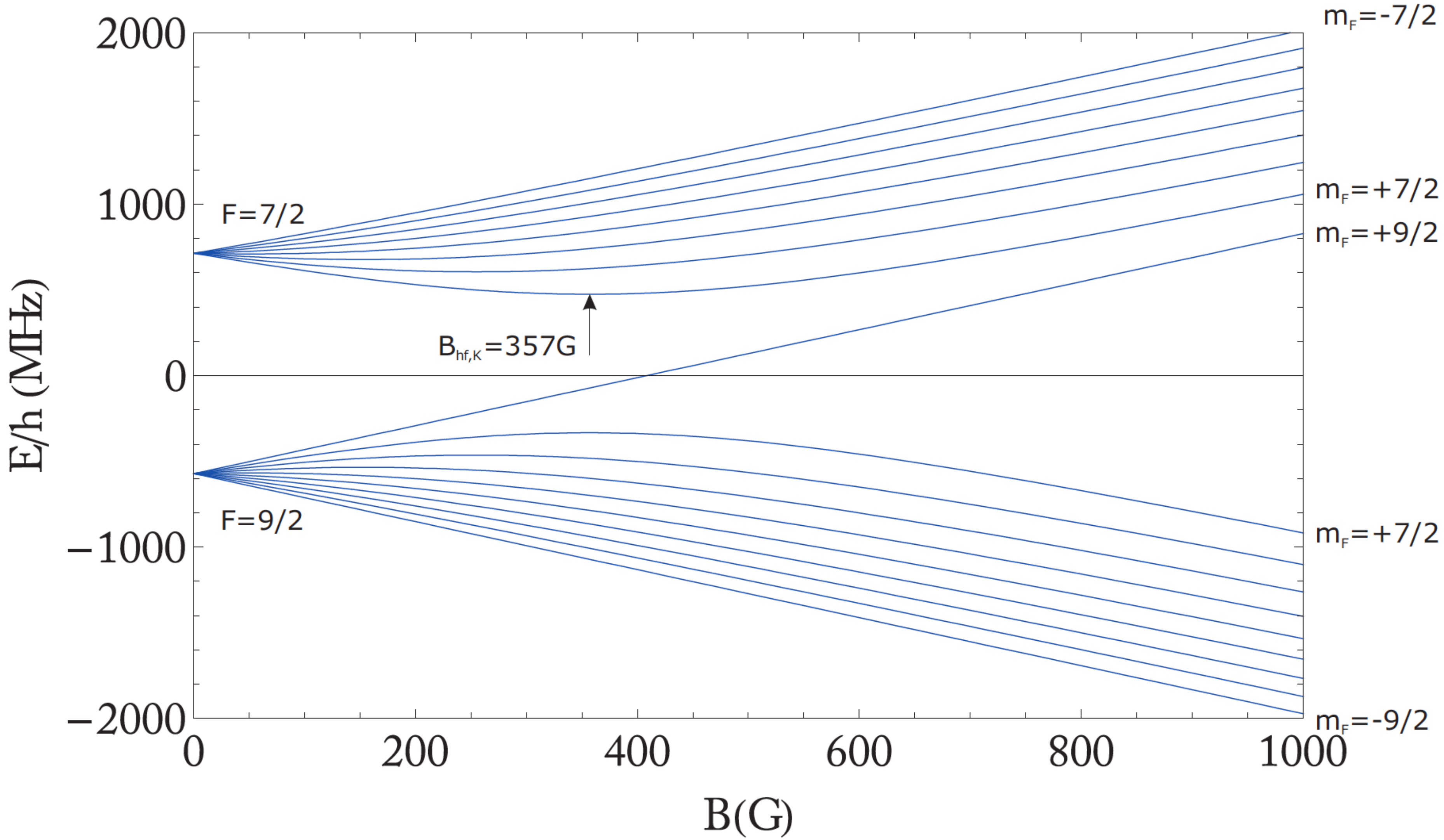
Interactions can be tuned via Feshbach resonances (here in magnetic field ***B***)

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





Large multiplets: reservoir of “flavors”

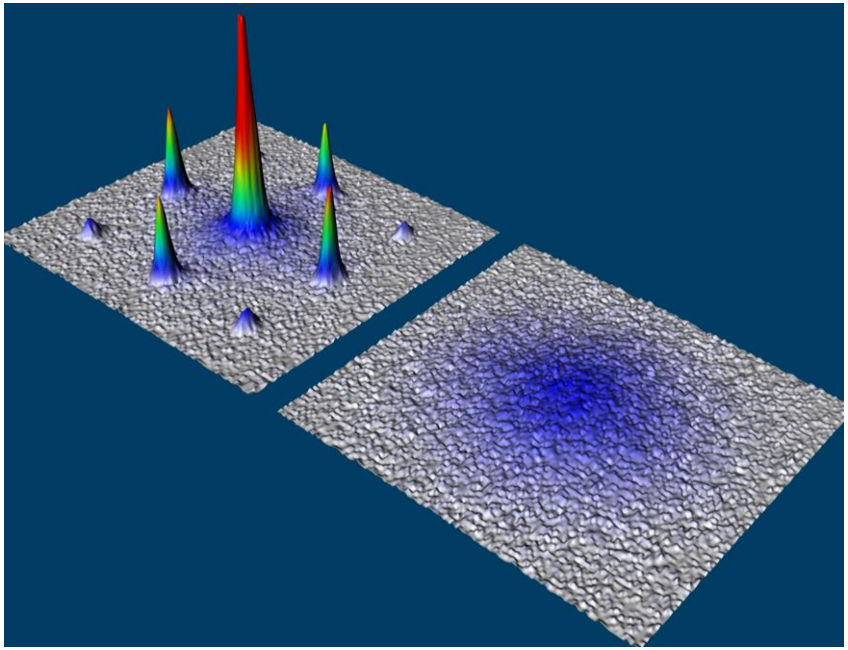


Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

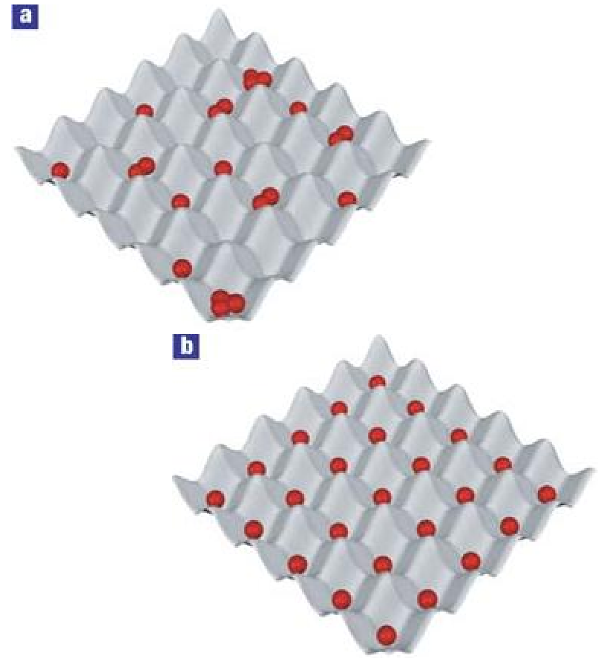
[Tiecke, unpublished]

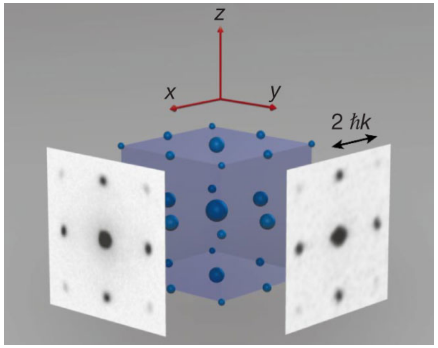
Correlated ultracold quantum gases on optical lattices: bosons

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



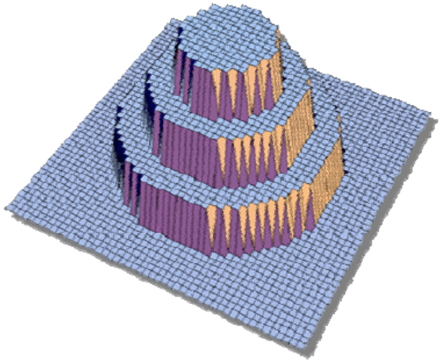
Time-of-flight image – momentum distribution



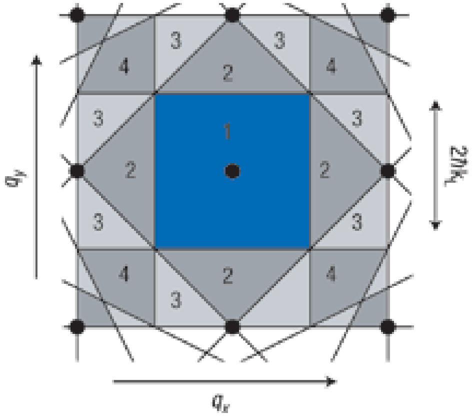


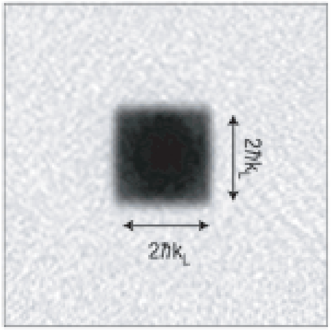
ultracold bosons on optical lattice (Bloch group, 2002)

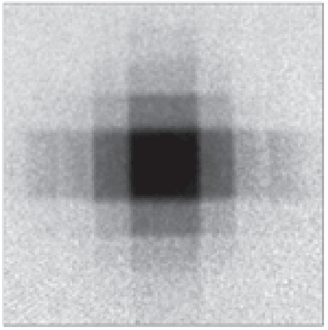
superfluidity destroyed by density constraint at large U;
trapping potential $\rightsquigarrow$ wedding cake structure



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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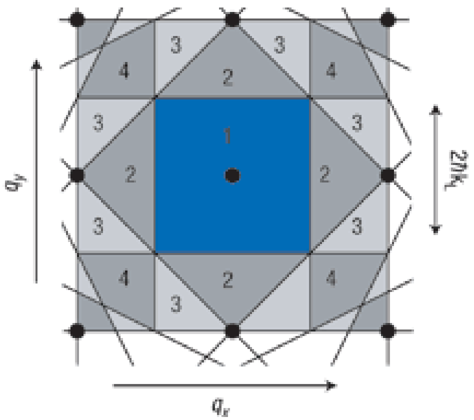

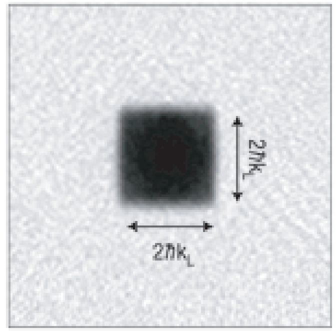

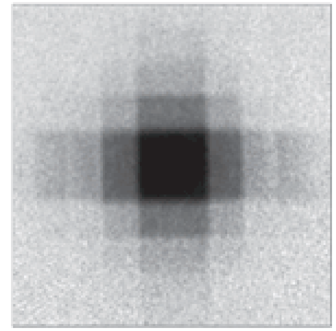

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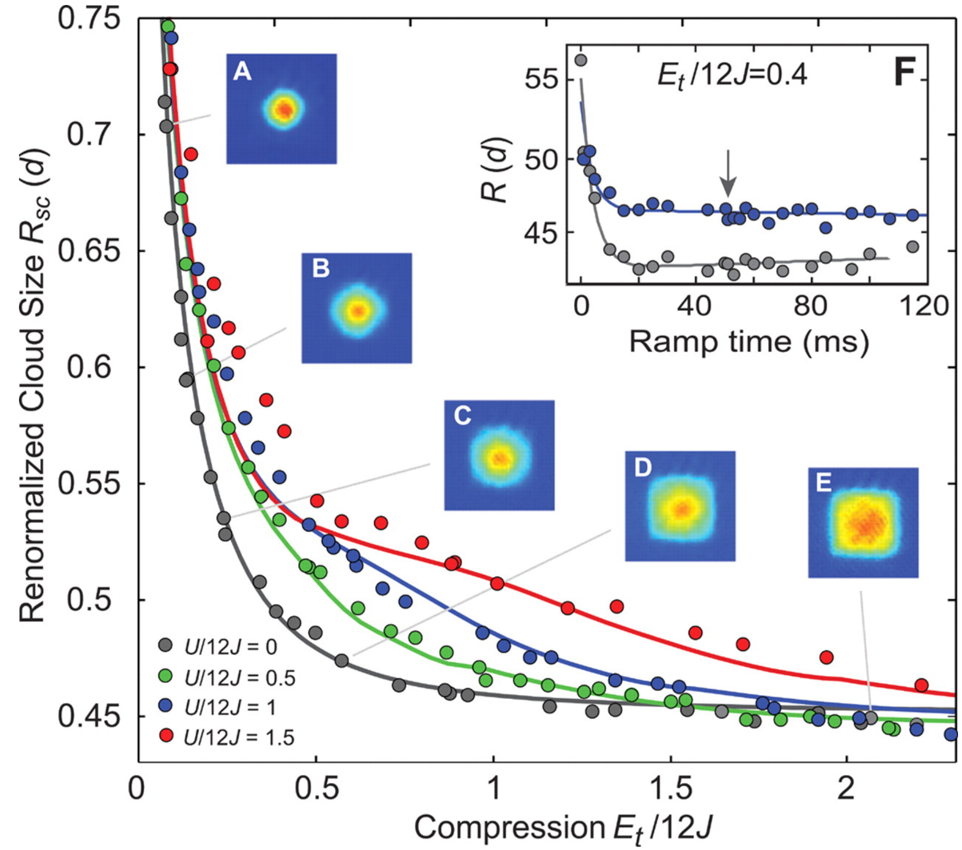
Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

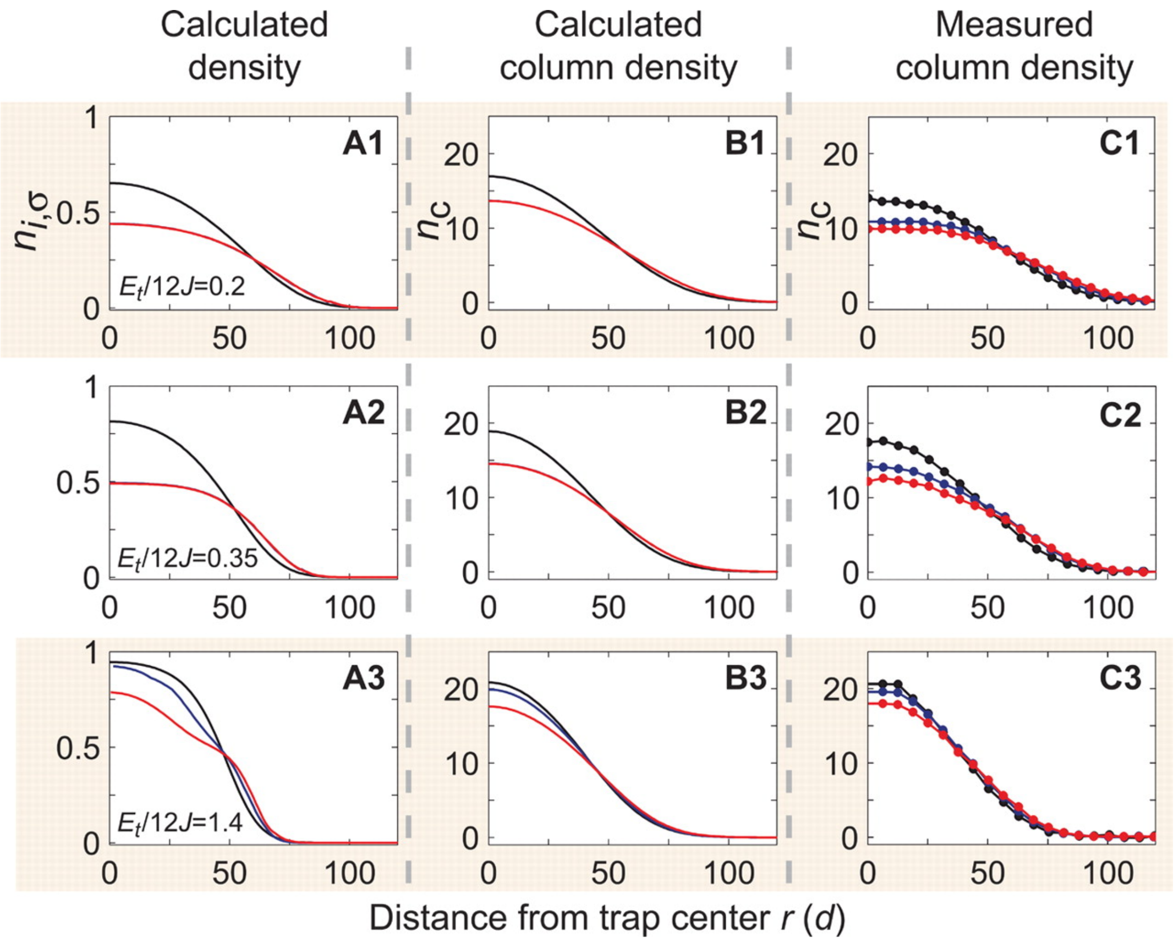
Detection method: measure cloud diameter vs. trap strength

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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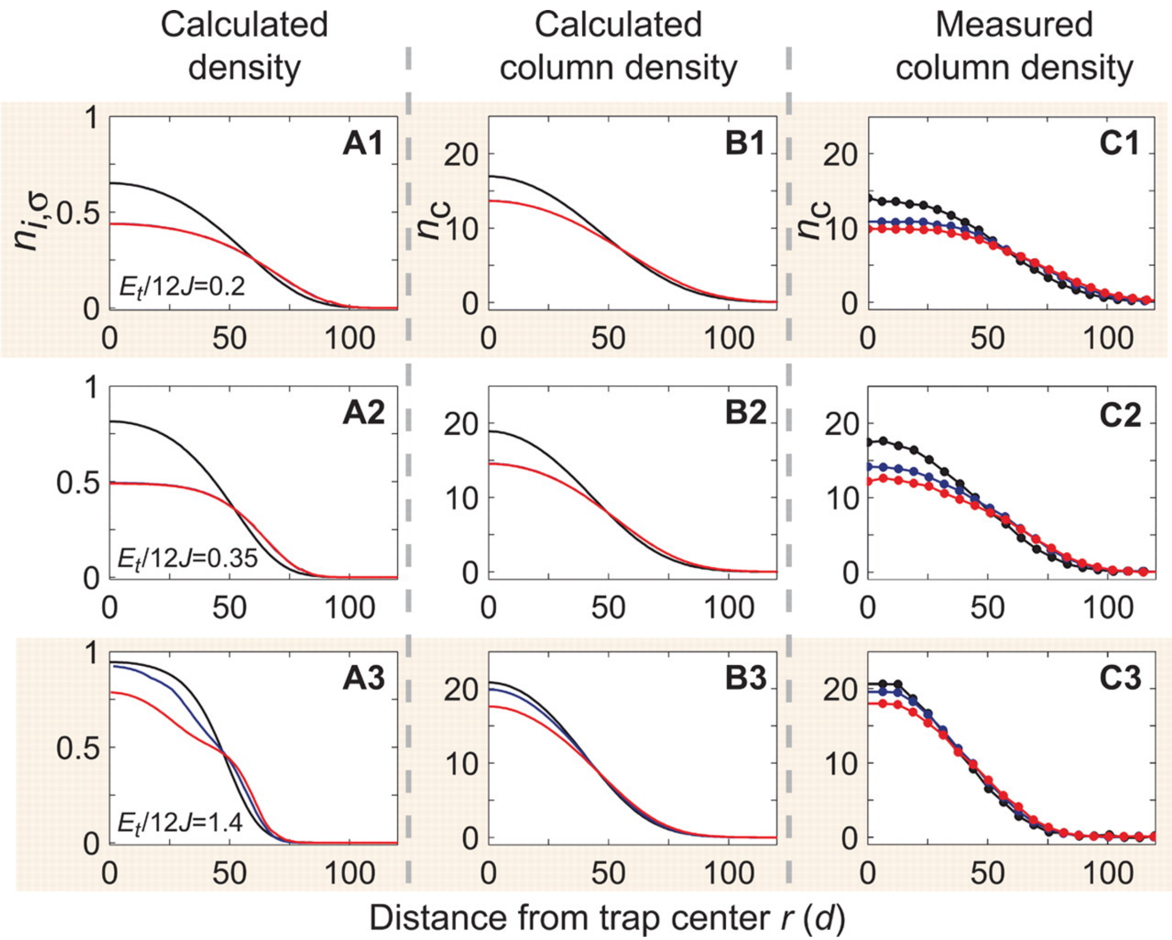

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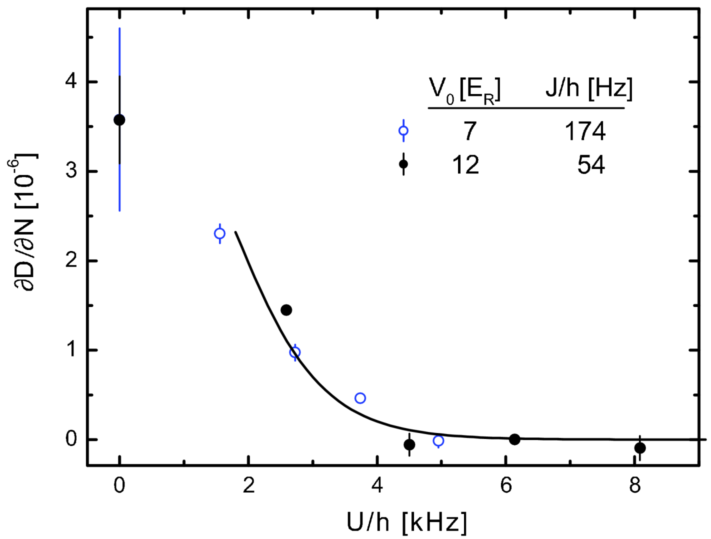

[Jördens et al., Nature (2008)]

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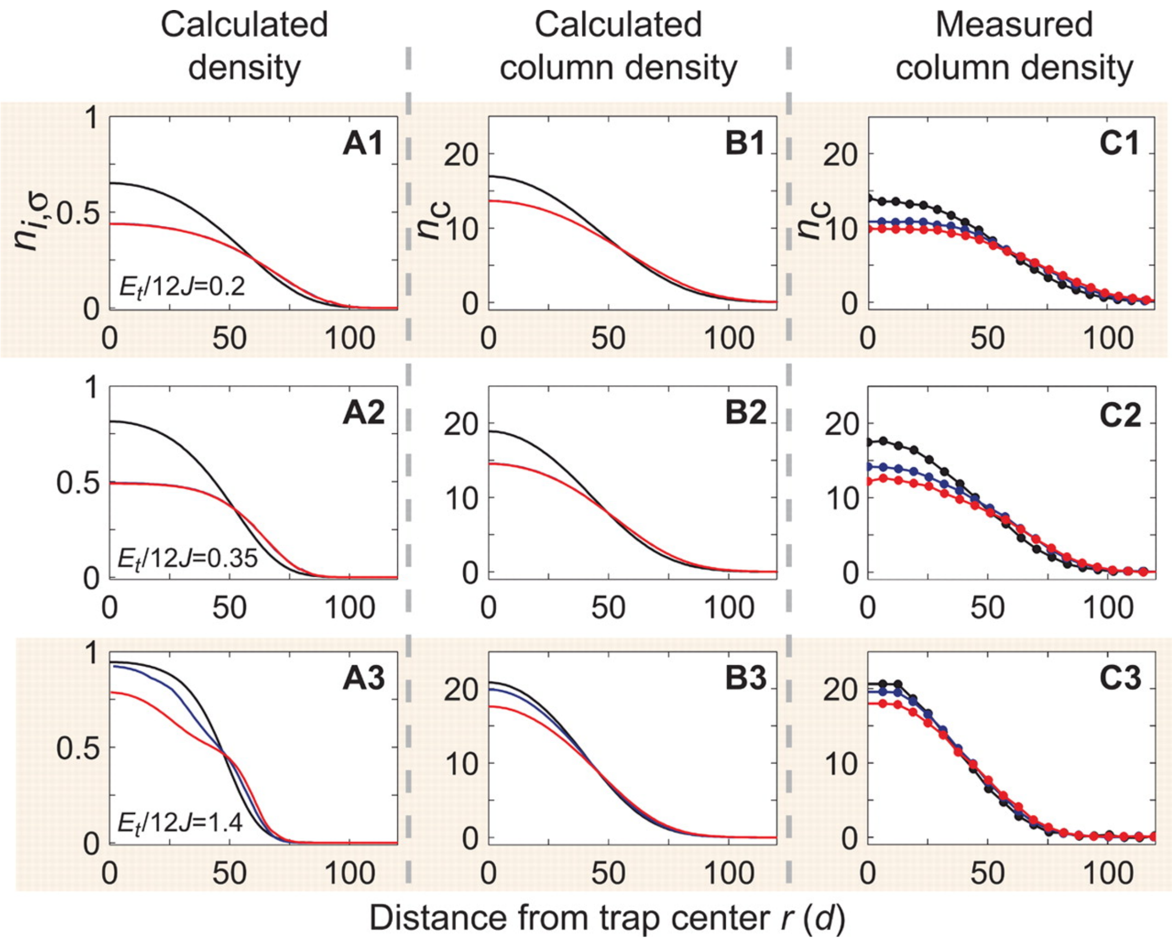

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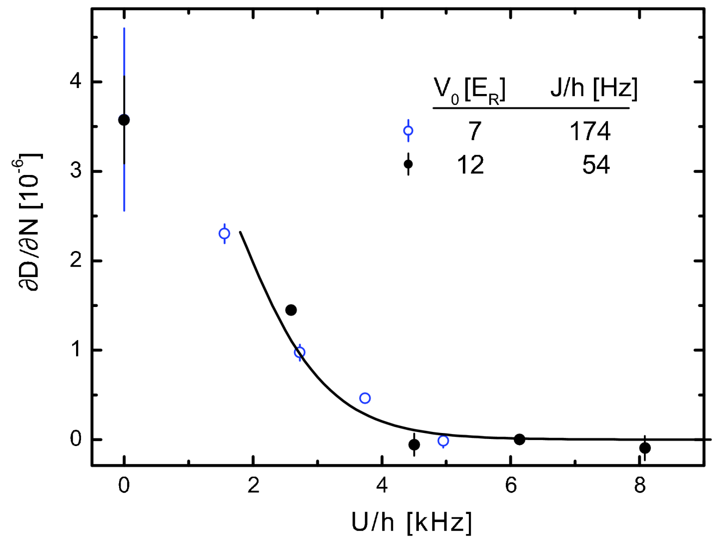
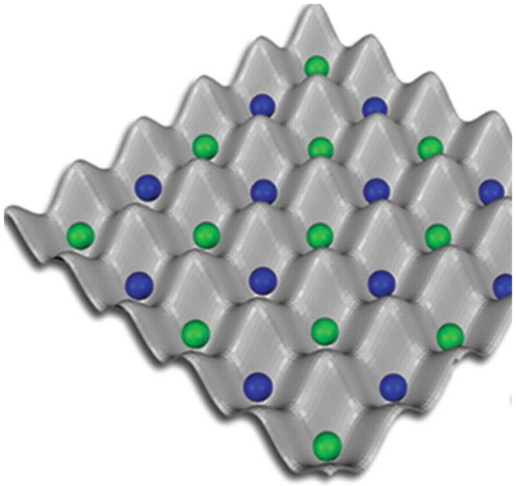


[Jördens et al., Nature (2008)]

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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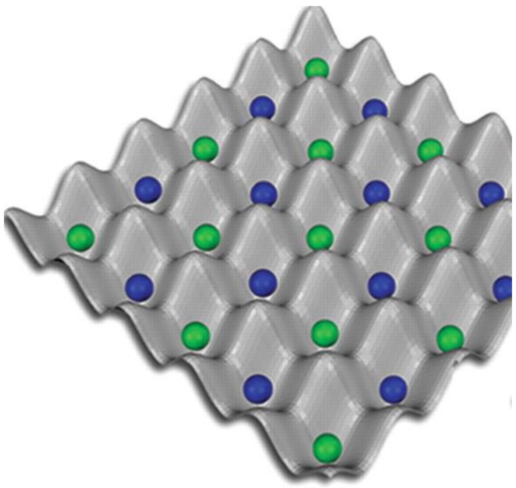

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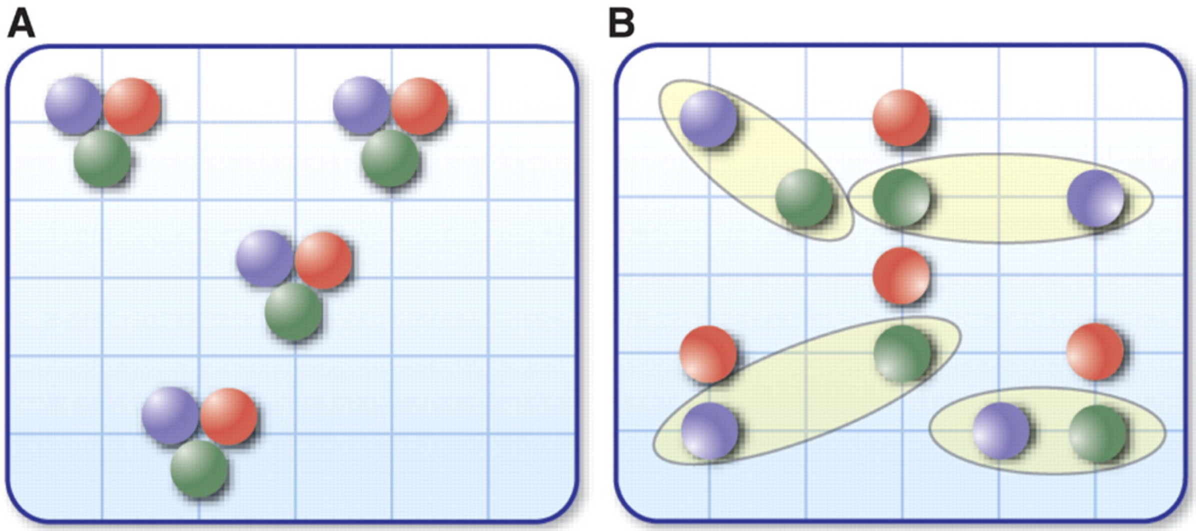
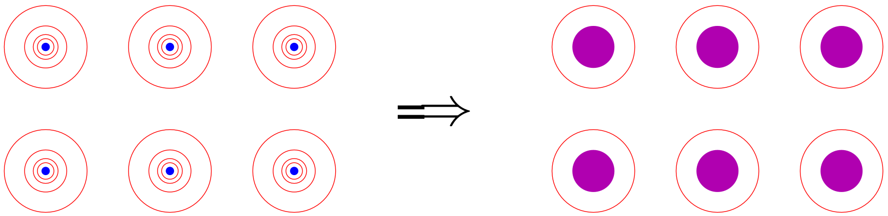
Multiflavor phenomena, e.g. trions versus color superconductivity



Approaches for correlated lattice Fermi systems

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

reduction to valence electrons ↓



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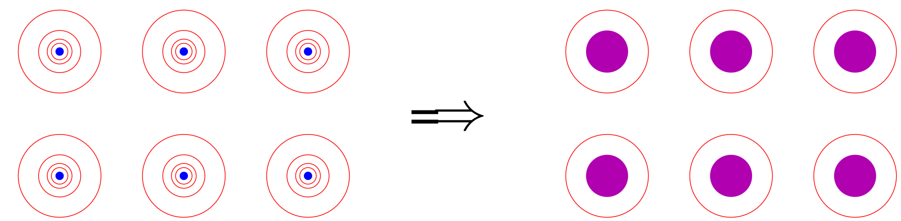

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occupation number formalism ↓ Wannier orbitals

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

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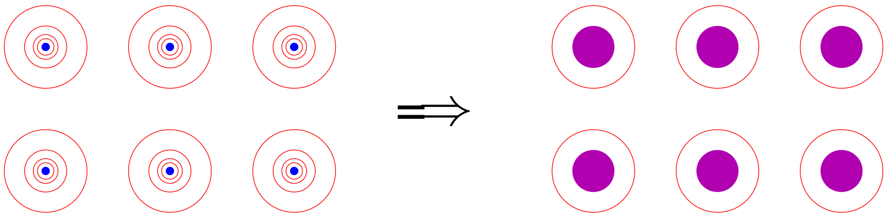

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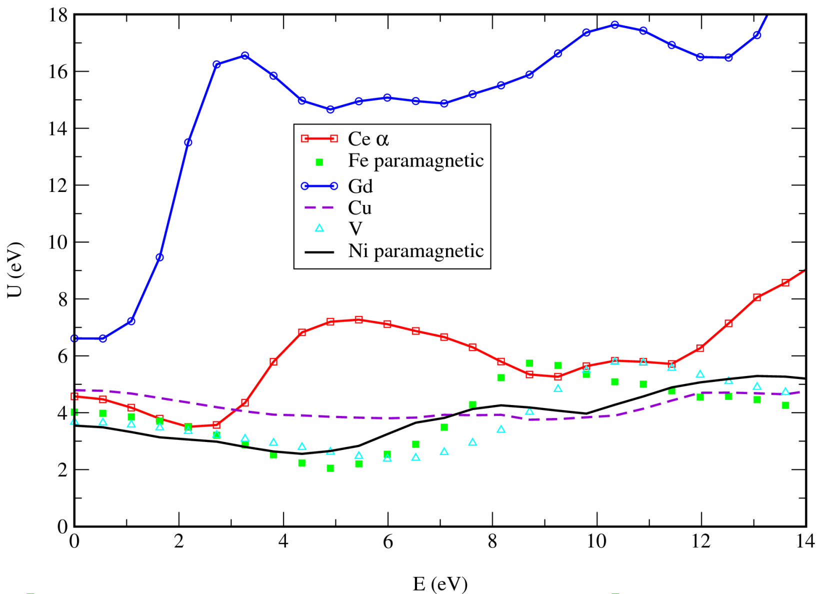
elated lattice Fermi systems



[Aryasetiawan et al, PRB 2006]

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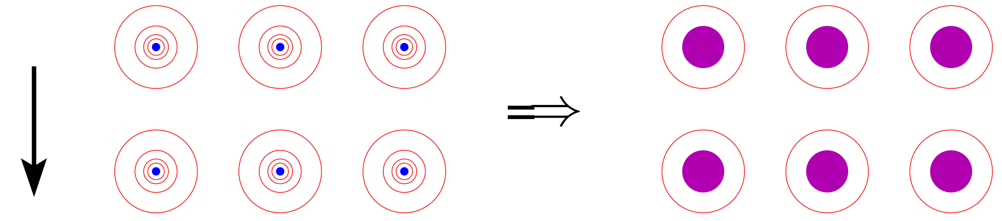
rons



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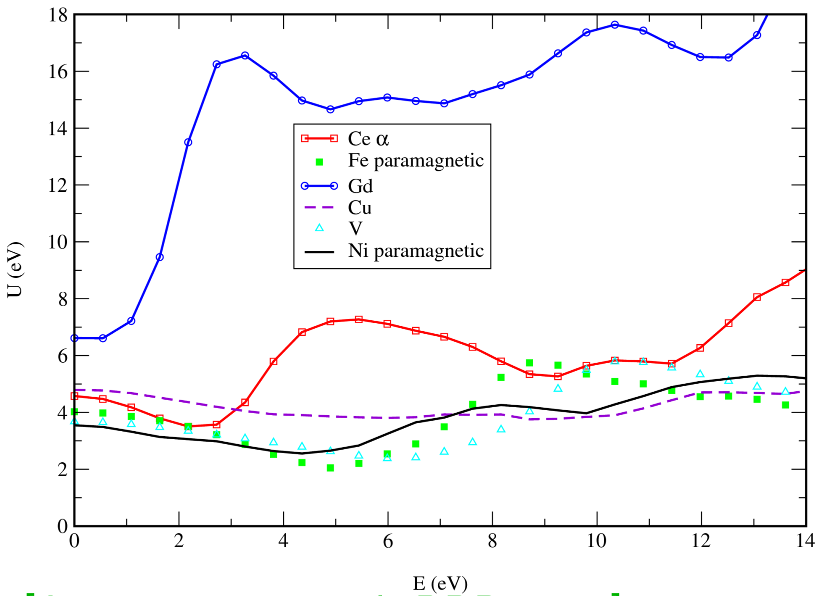

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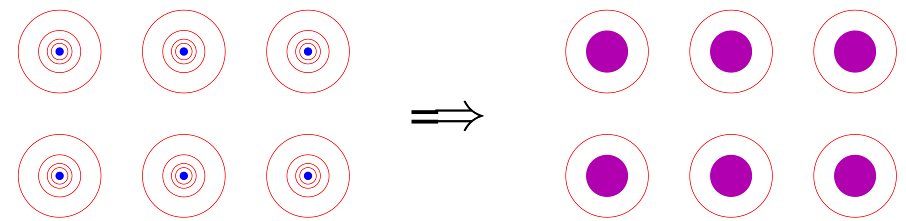

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Note: no core states in quantum gas case!

Approaches for Hubbard-type models

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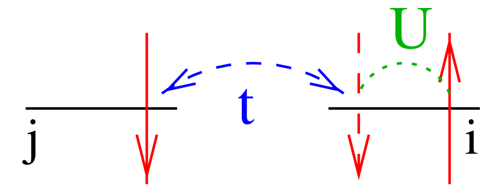
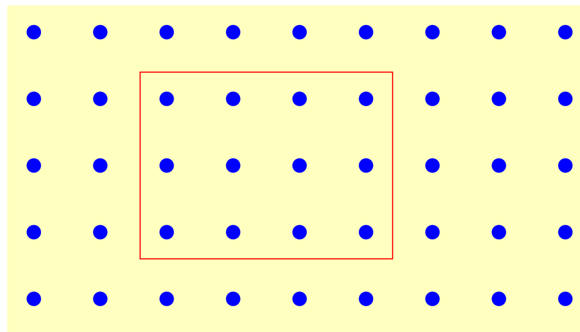


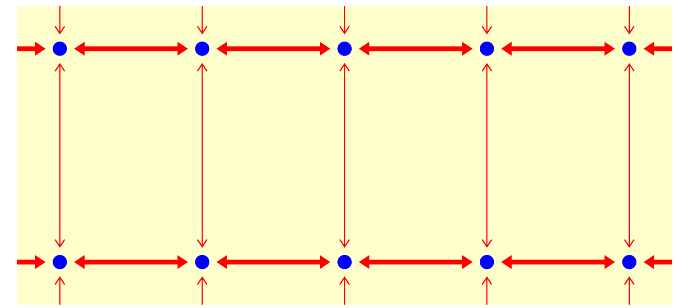
Perturbation theory

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

finite clusters: ED, QMC



$d \longrightarrow 1$: Bethe ansatz, DMRG



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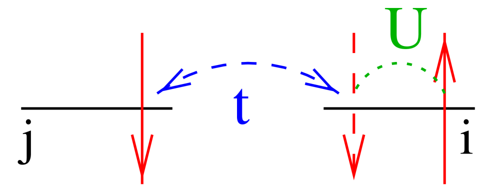

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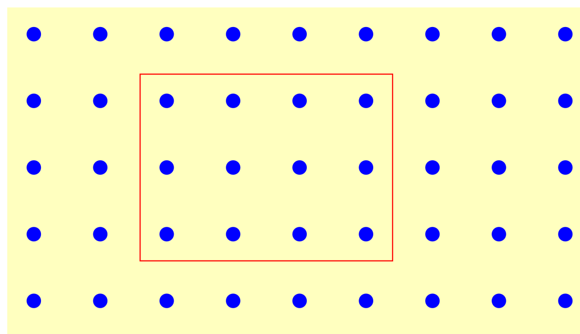

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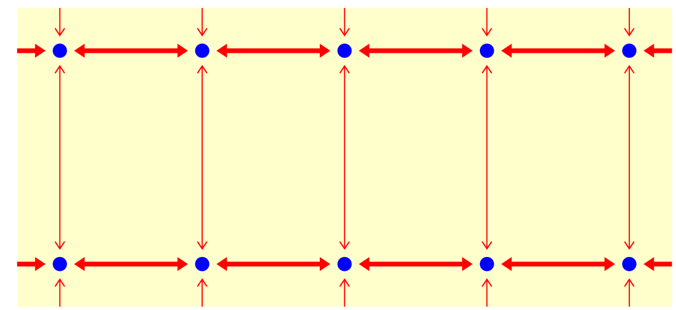
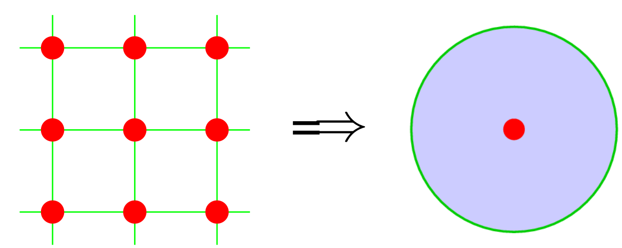


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

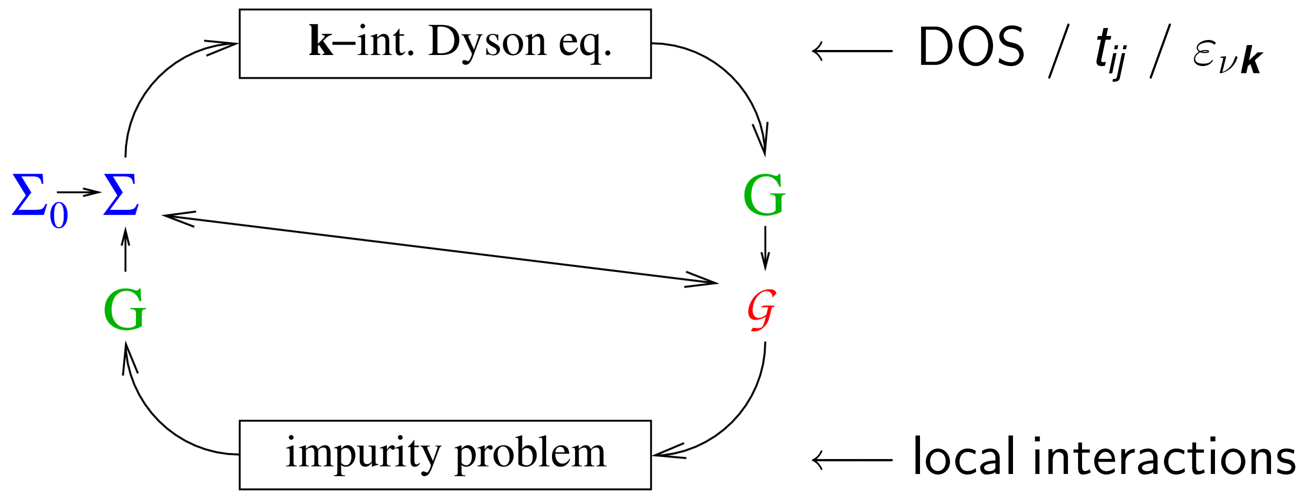
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

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



Iterative solution of DMFT equations

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



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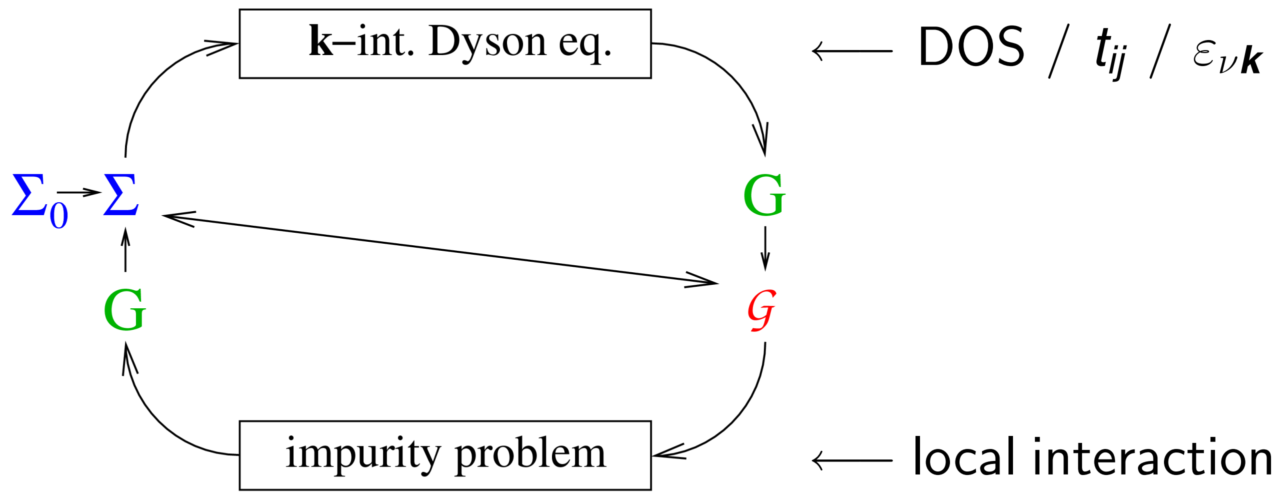
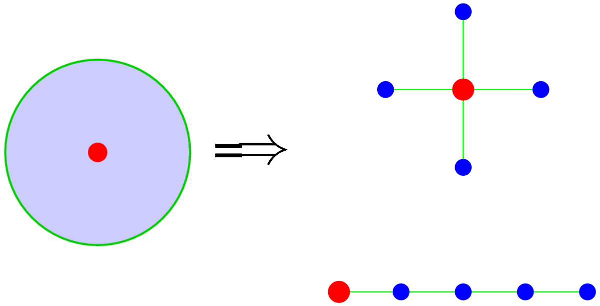


Impurity solver:

- 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)]

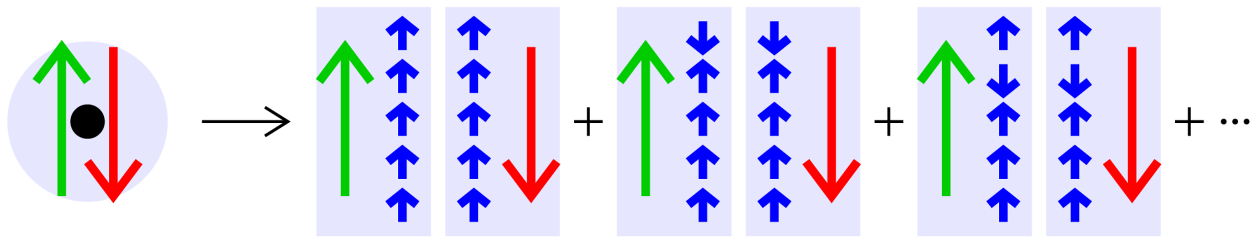
Green function G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

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

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

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

(iii) Hubbard-Stratonovich transformation



Wick theorem:

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

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

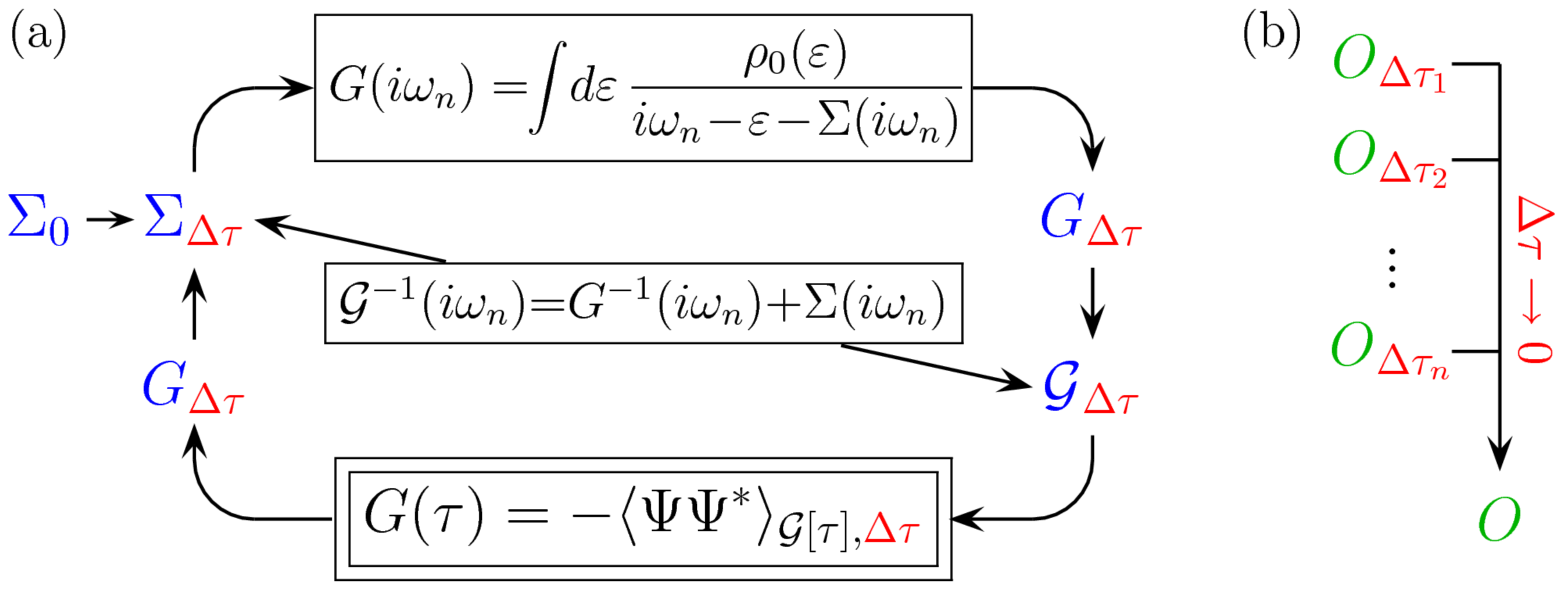
+ numerically exact, + no sign problem, − effort scales as T^{-3}

(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



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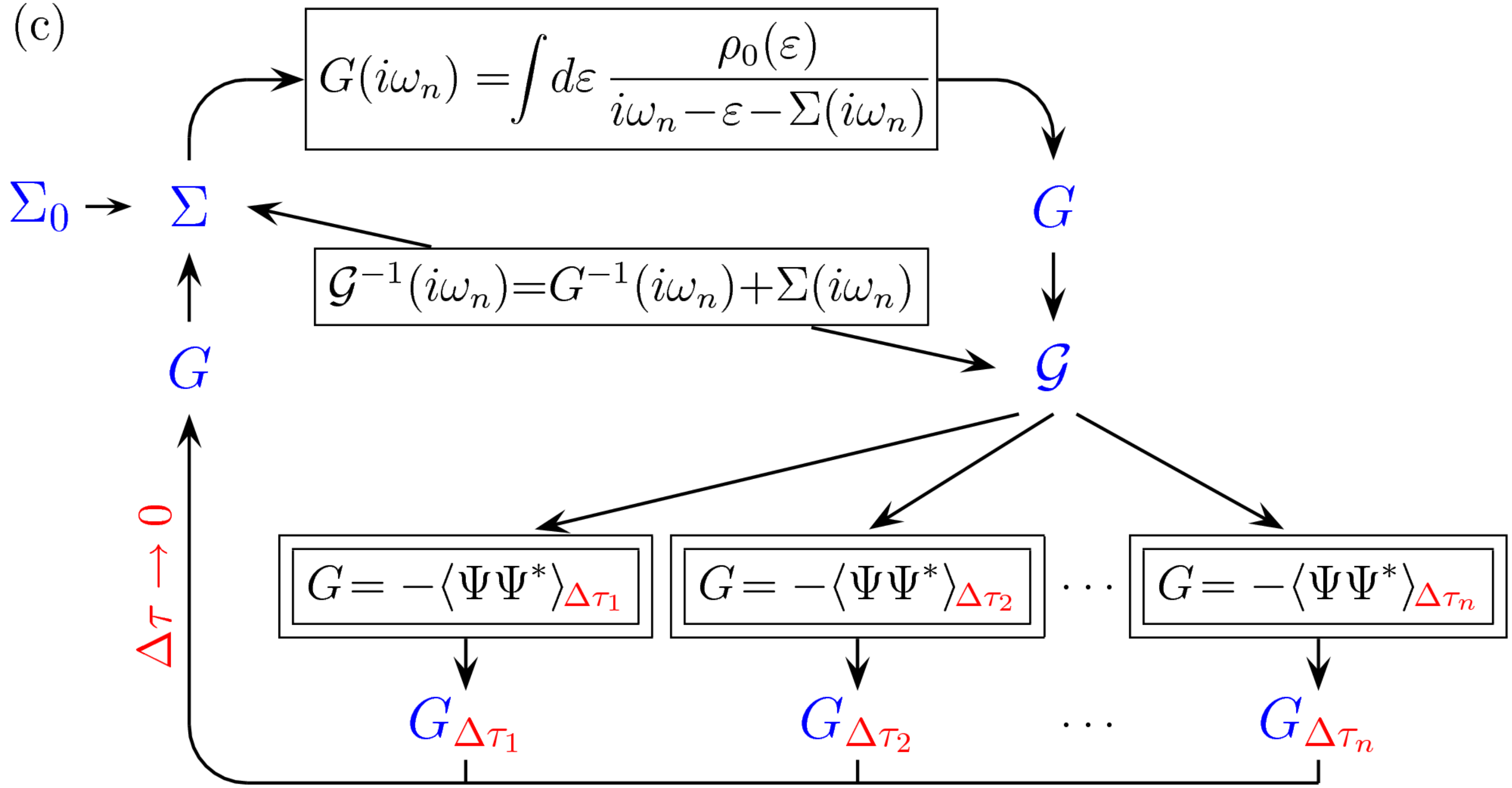
(c)

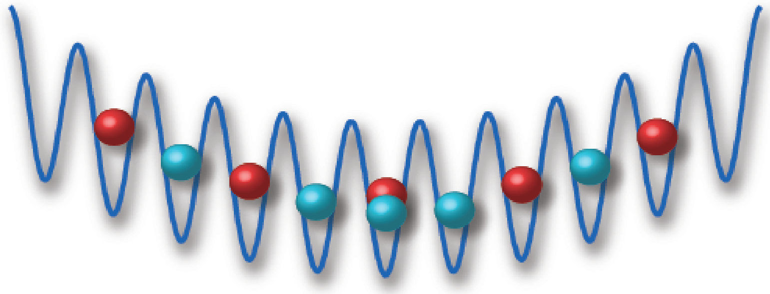


(c) Multigrid HF-QMC: internal elimination of Trotter error

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

Antiferromagnetic order at finite T in an optical trap

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



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

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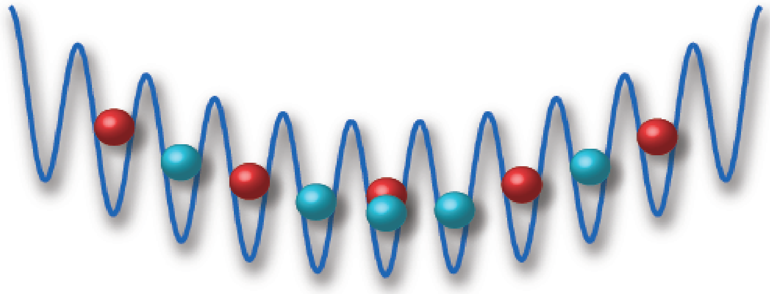

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Real-space DMFT: use local self-energy in inhomogeneous system

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

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

[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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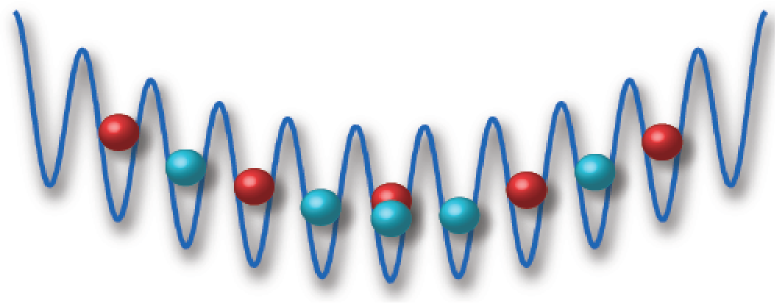

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Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

All previous implementations: RDMFT+NRG

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

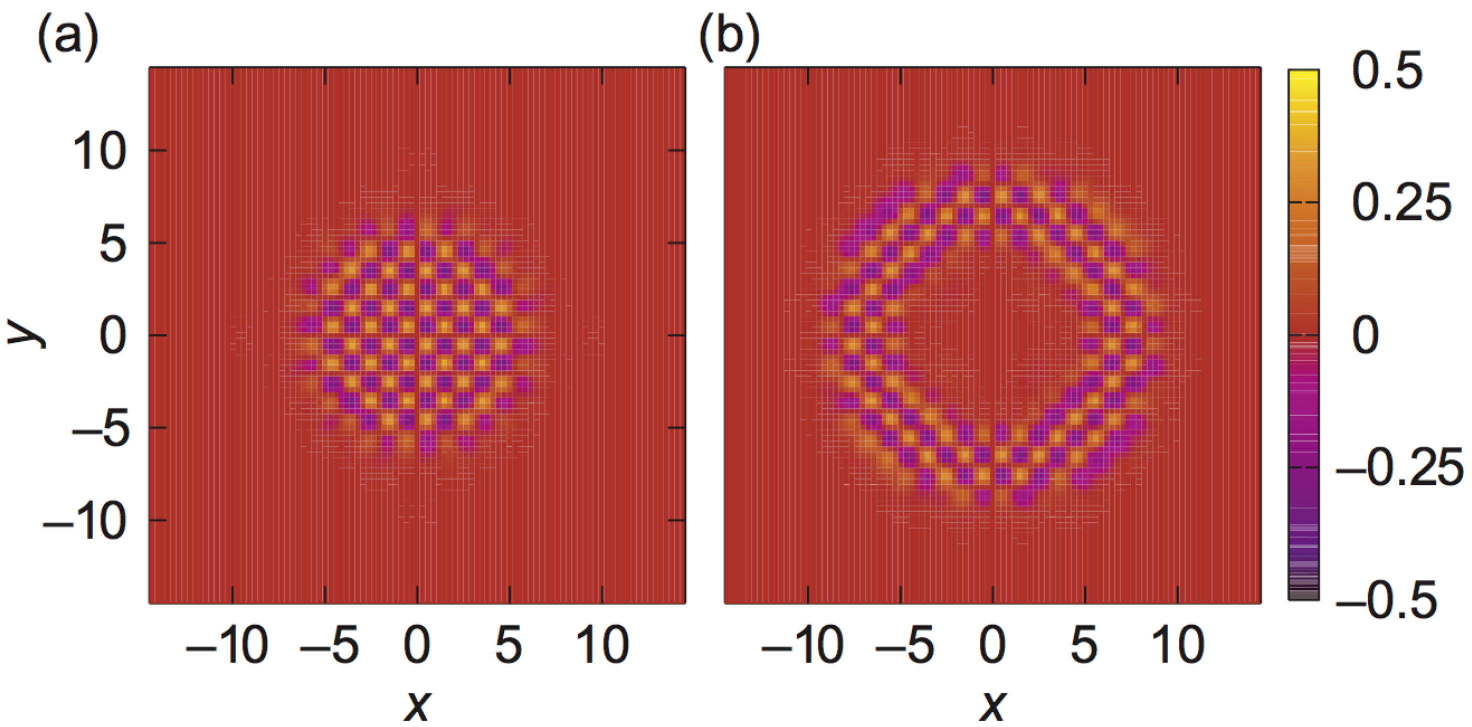
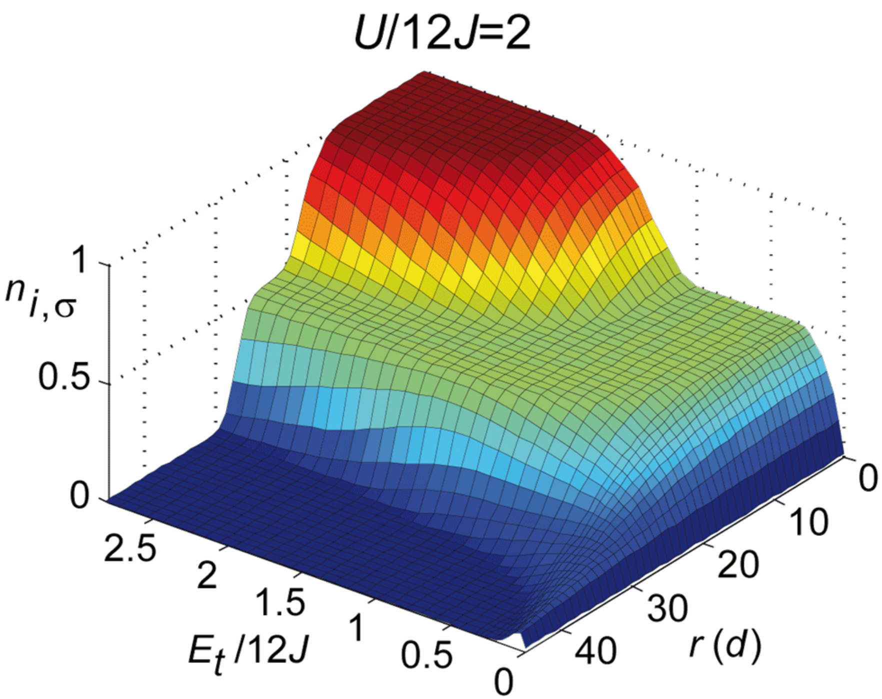


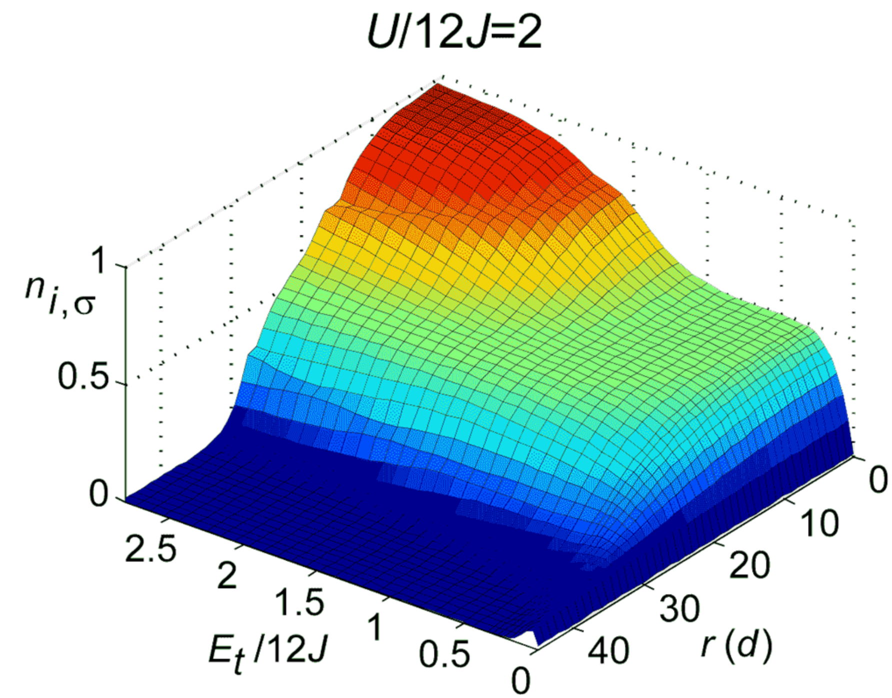
Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_\uparrow = \mu_\downarrow = 5$; (b) $V = 0.2$ and $\mu_\uparrow = \mu_\downarrow = 15$. Energies are expressed in units of the hopping parameter J.

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

But: NRG problematic at elevated temperatures



$T = 0.07t$

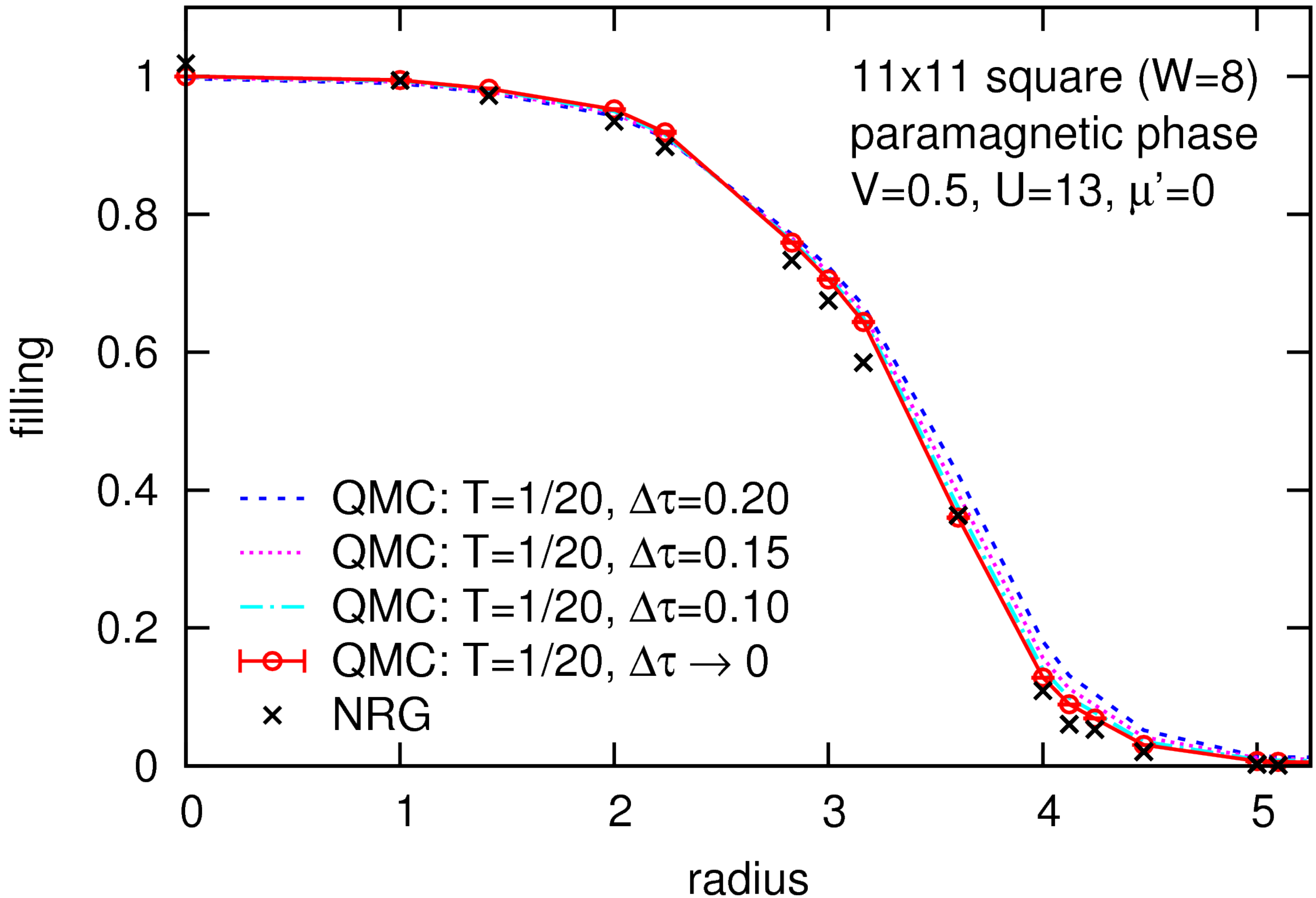


$T = 0.15t$

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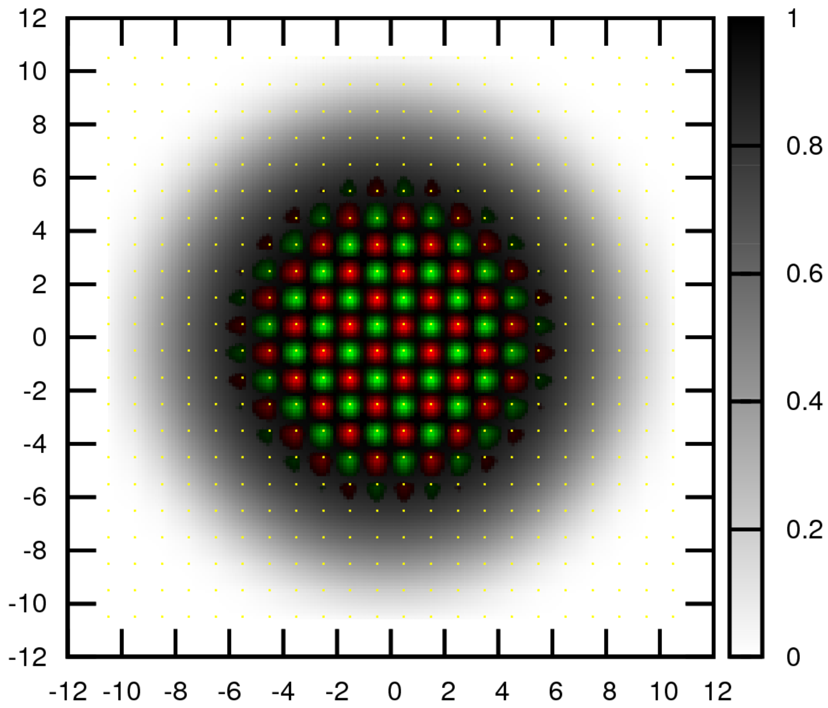
Practical (dense inversion, fully parallel): $\lesssim$ 10000 sites $\rightsquigarrow$ need smart strategies



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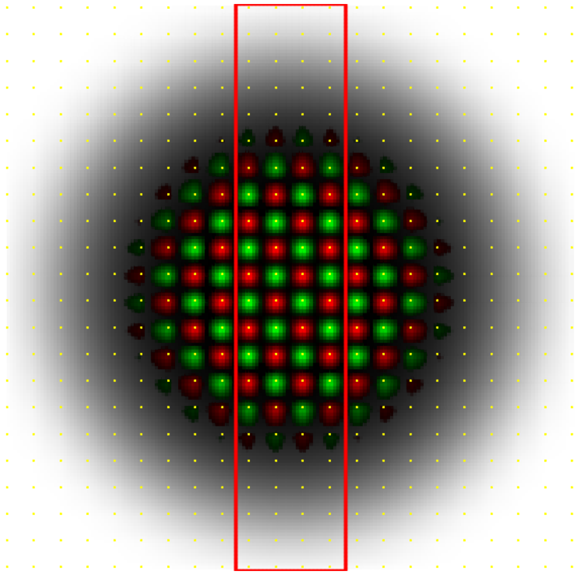

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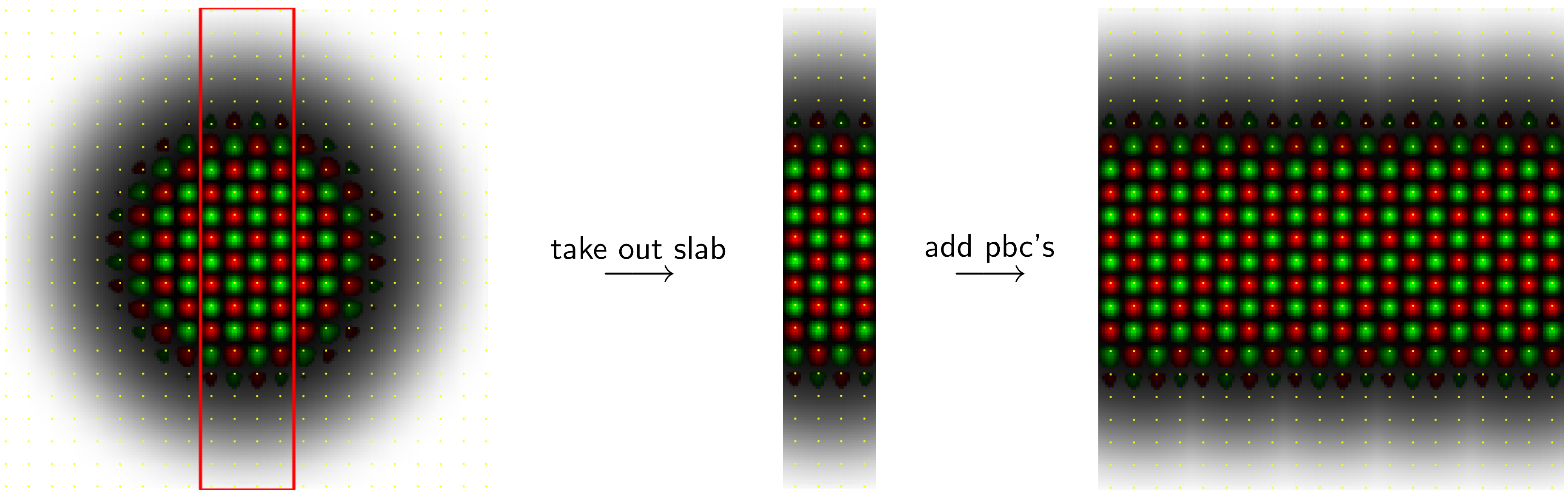
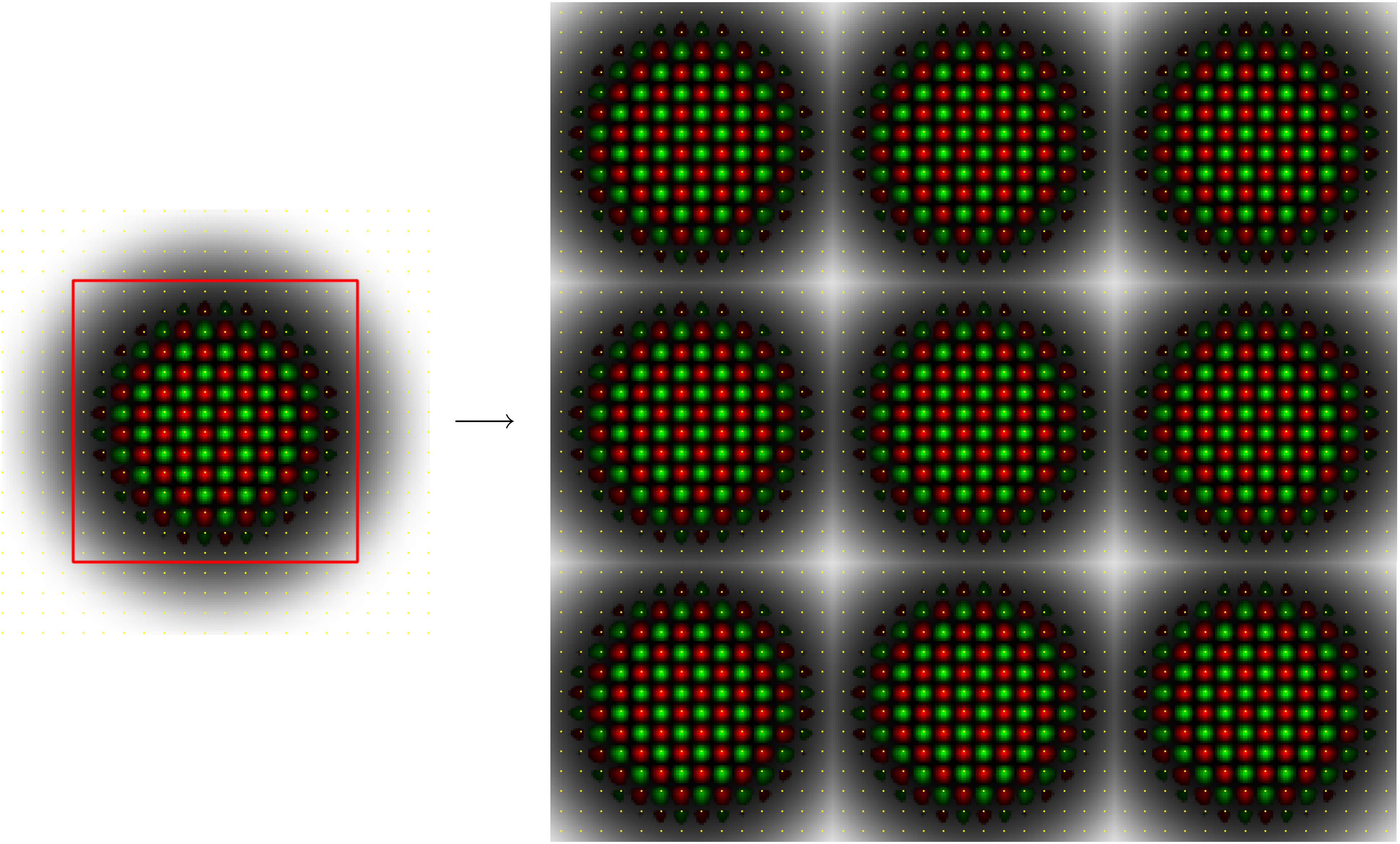


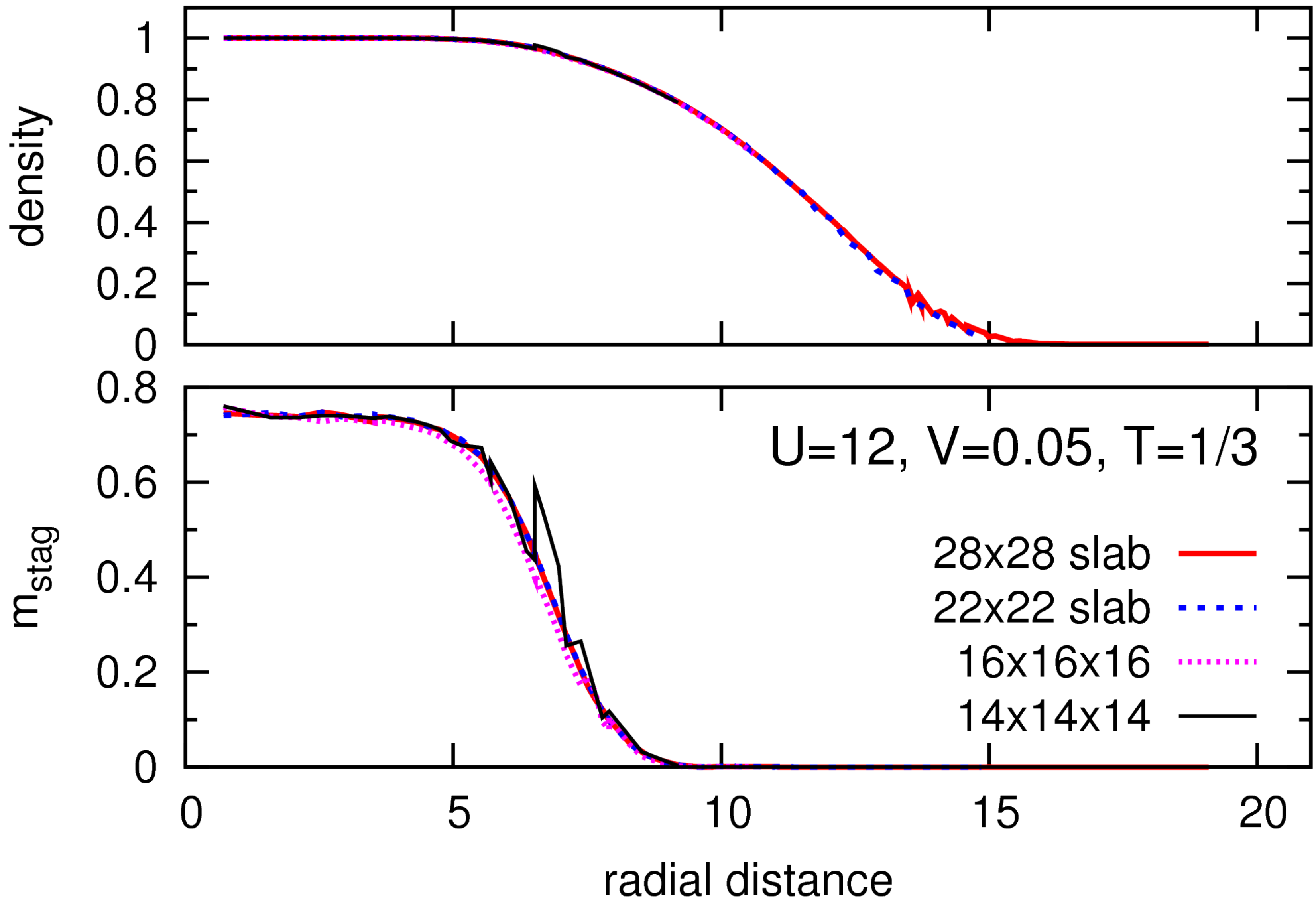
In practice: cylindrical potential (equivalent layers)

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



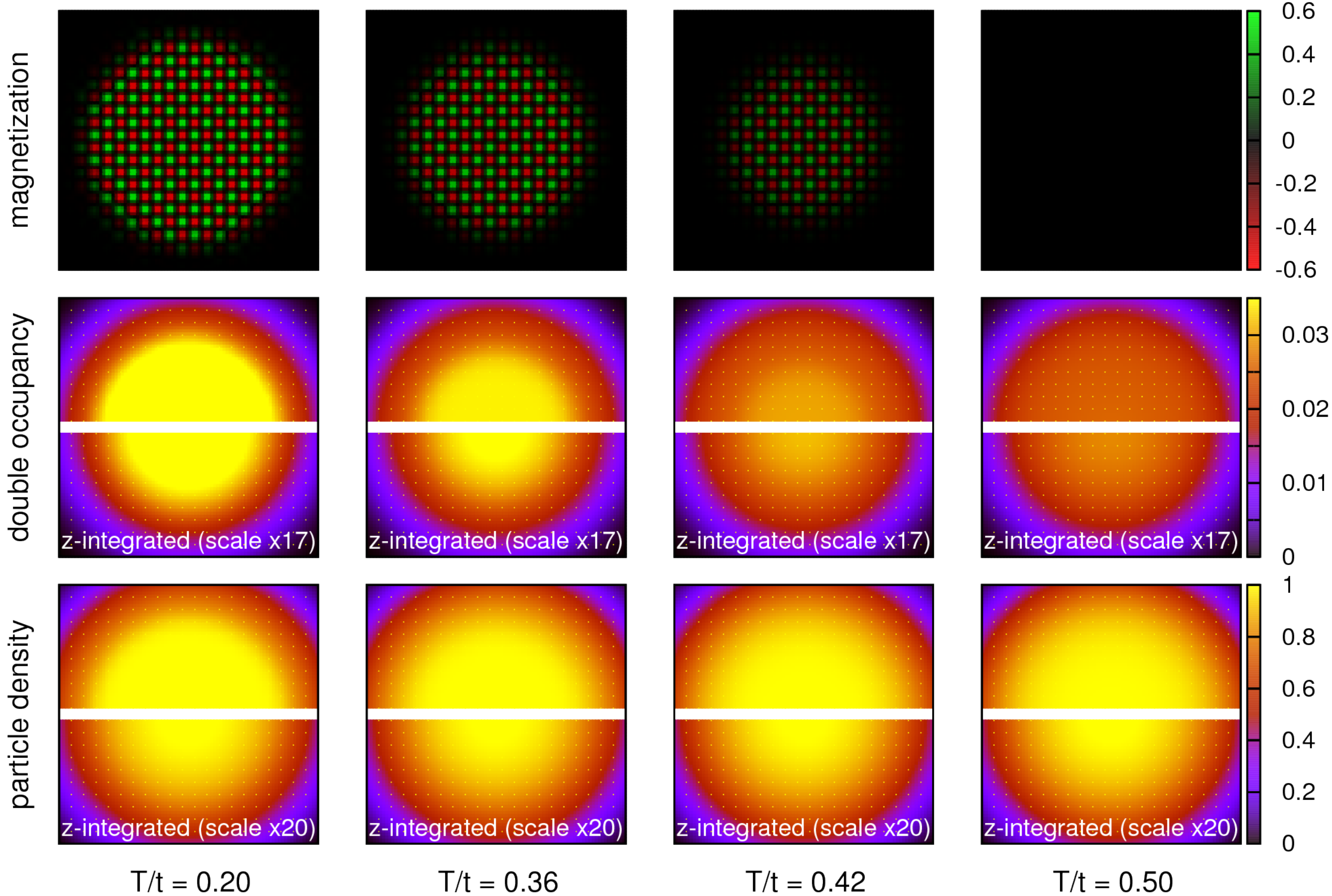
Most efficient: slab calculation focussing on AF core (with pbc)

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



Significant deviations only if core touches boundaries!

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



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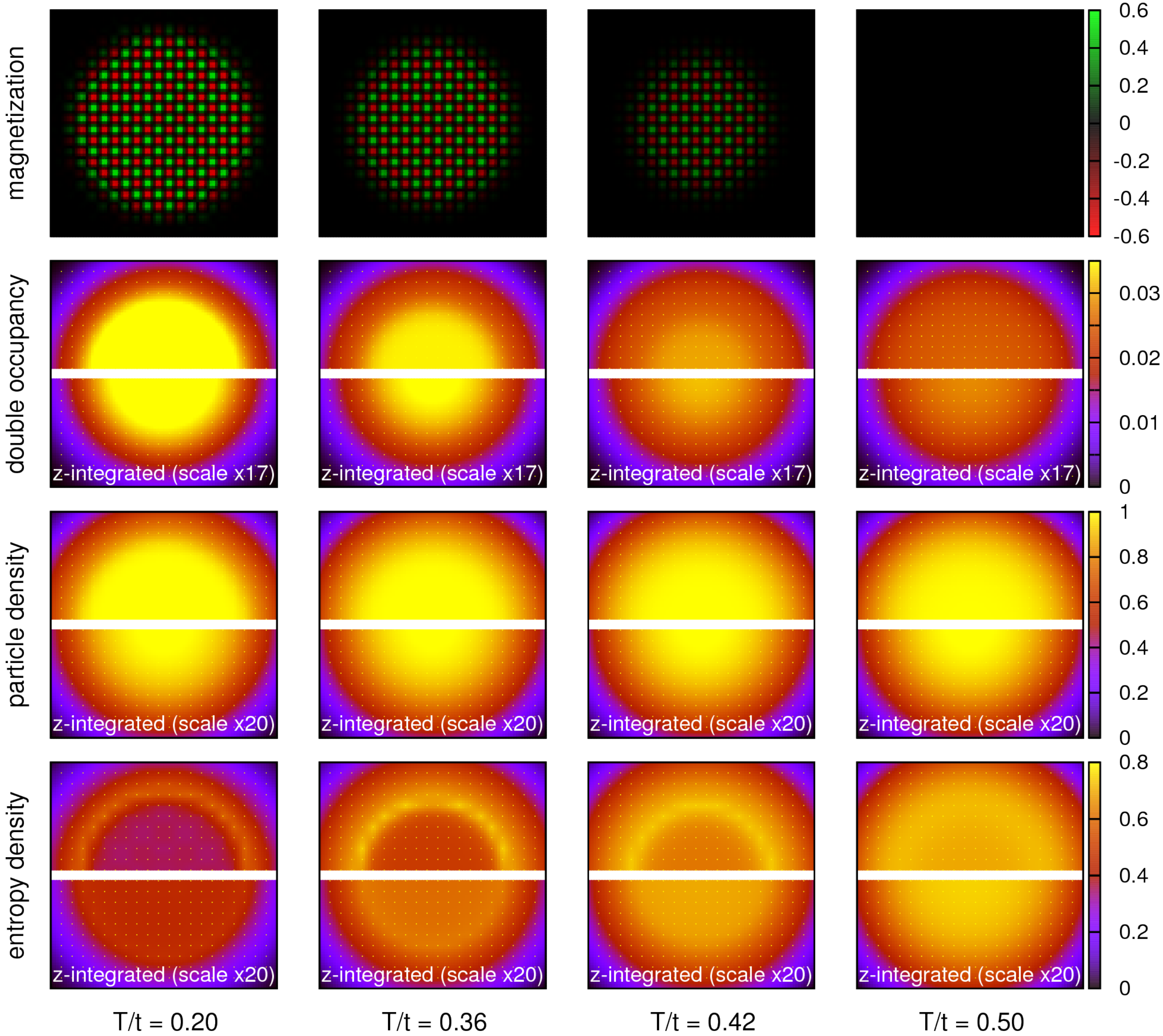


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

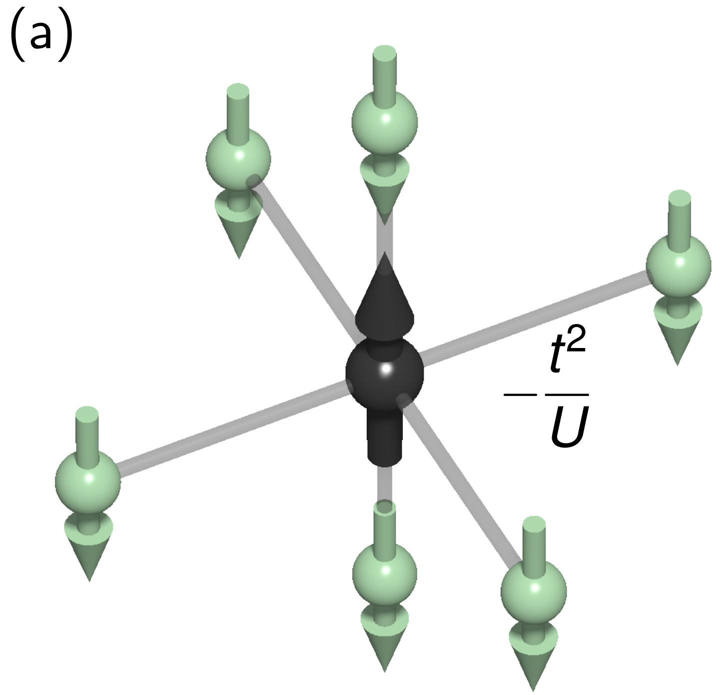
$\sim$ 6000 atoms (naively $\sim 30^3 = 27000$ sites needed)

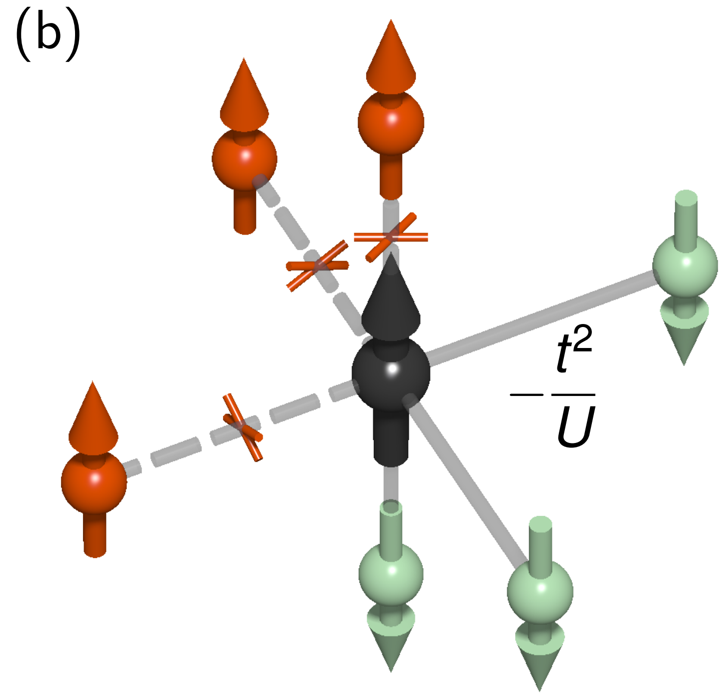
Entropy

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

Enhanced double occupancy: a signature of AF order

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





AF state:

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

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

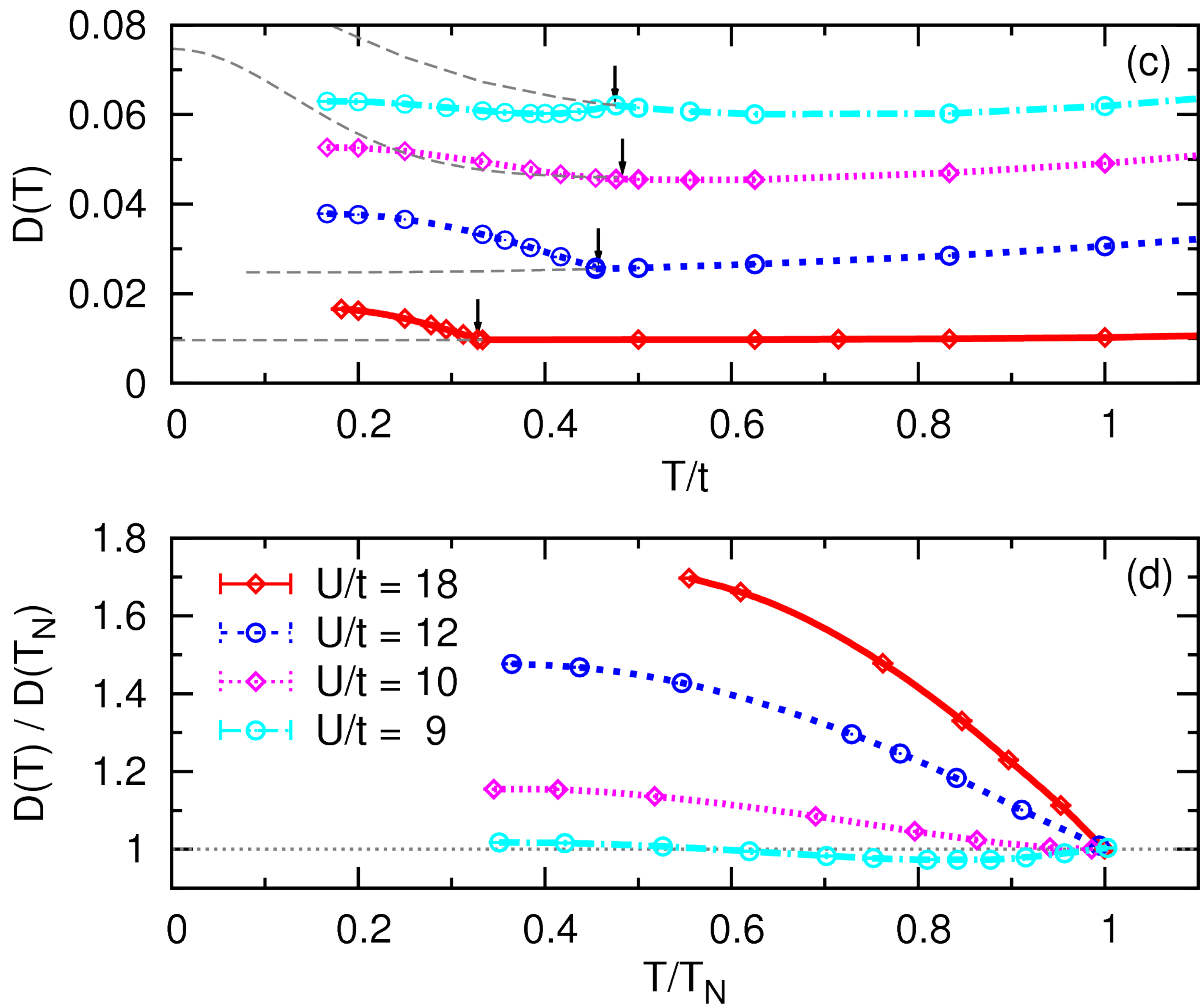
Paramagnetic state:

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 $D_{\mathbf{AF}}/D_{\mathbf{p}} \overset{U\to\infty}{\longrightarrow} 2$.

DMFT-QMC estimates of D at half filling



AF $\Rightarrow$

enhanced D at $U \gtrsim 10t$

arrows: Néel temperatures

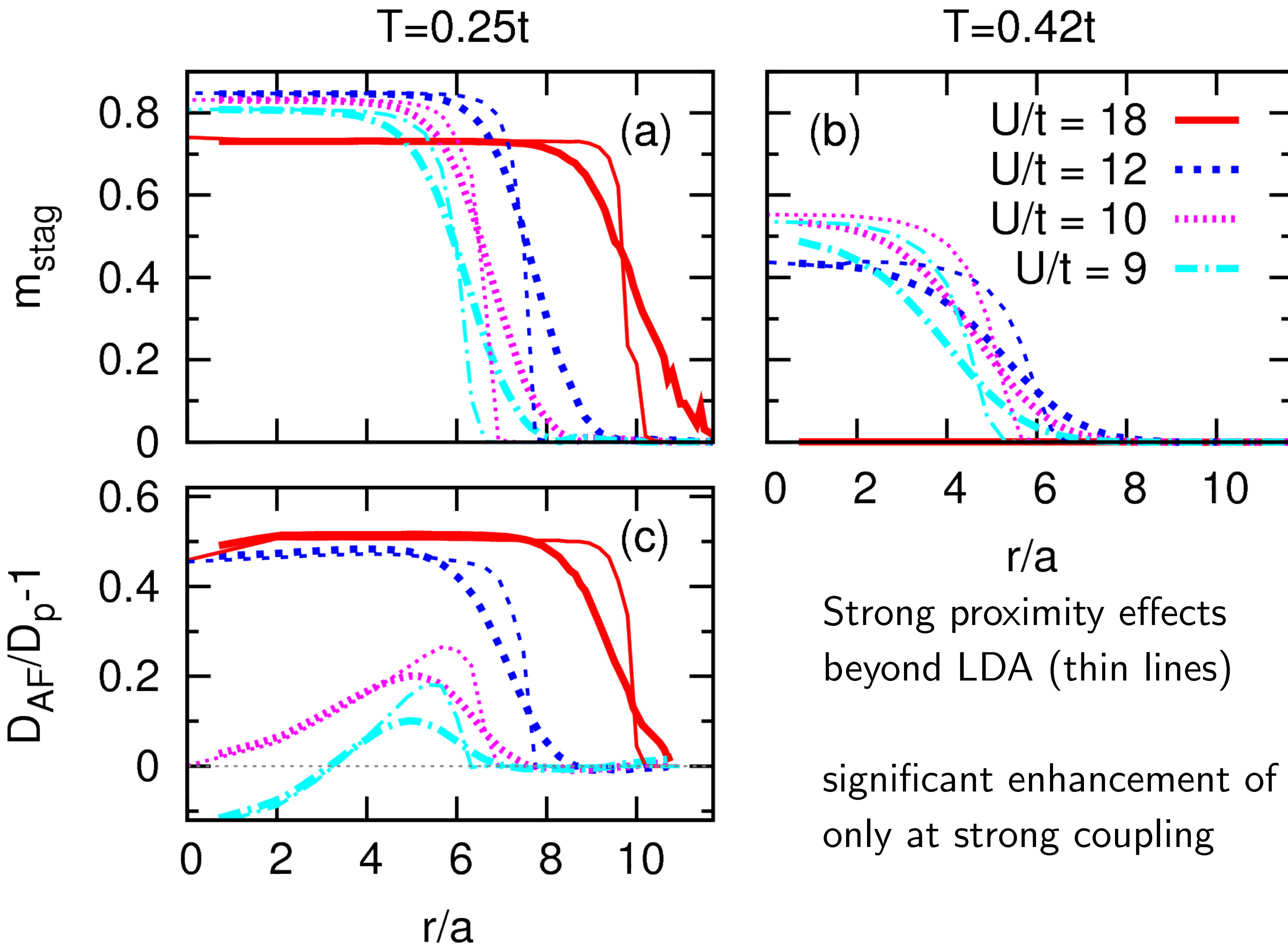
thin lines: metastable paramagnetic phase.

Data scaled to values of critical point:

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

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

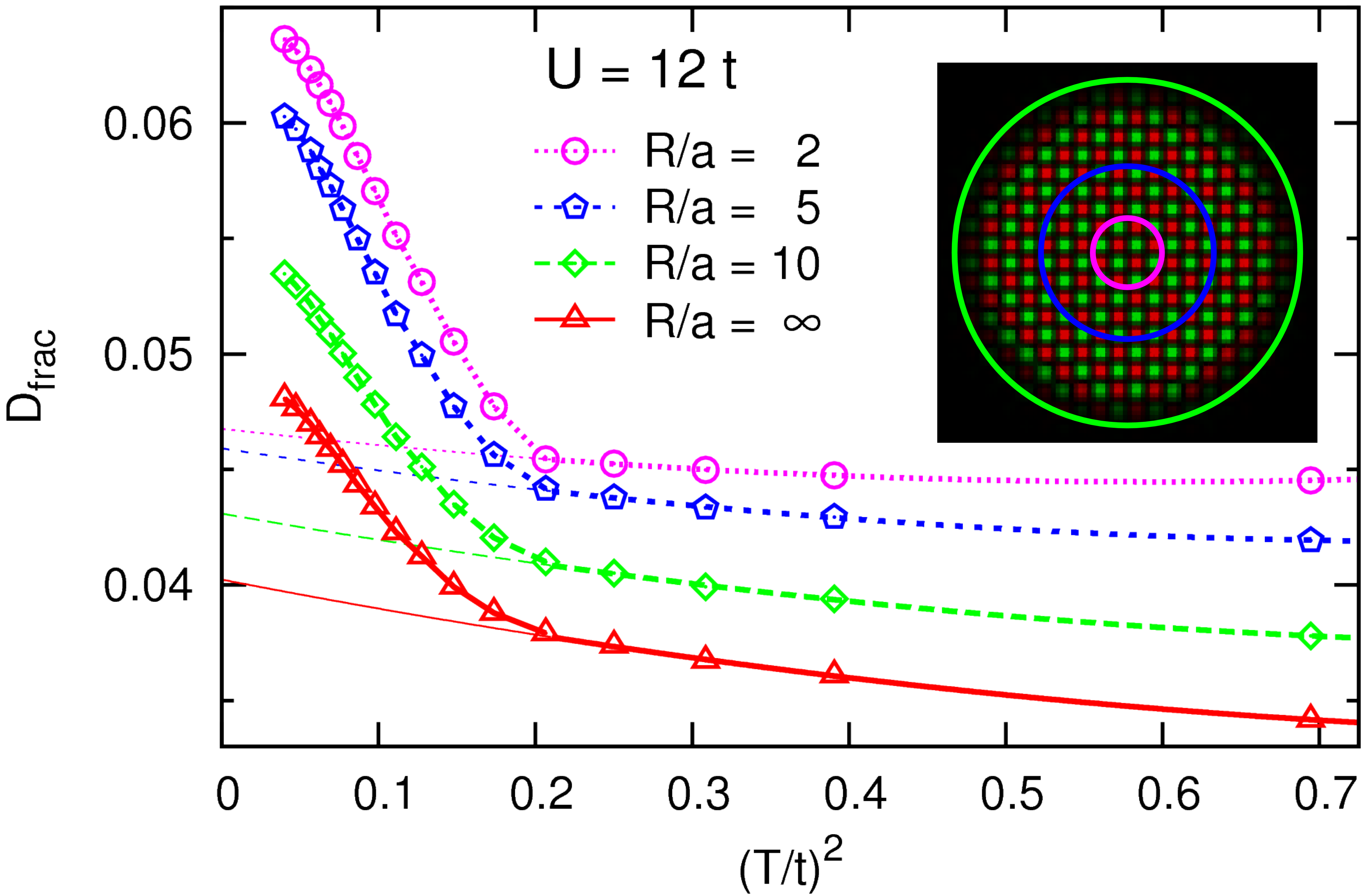
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



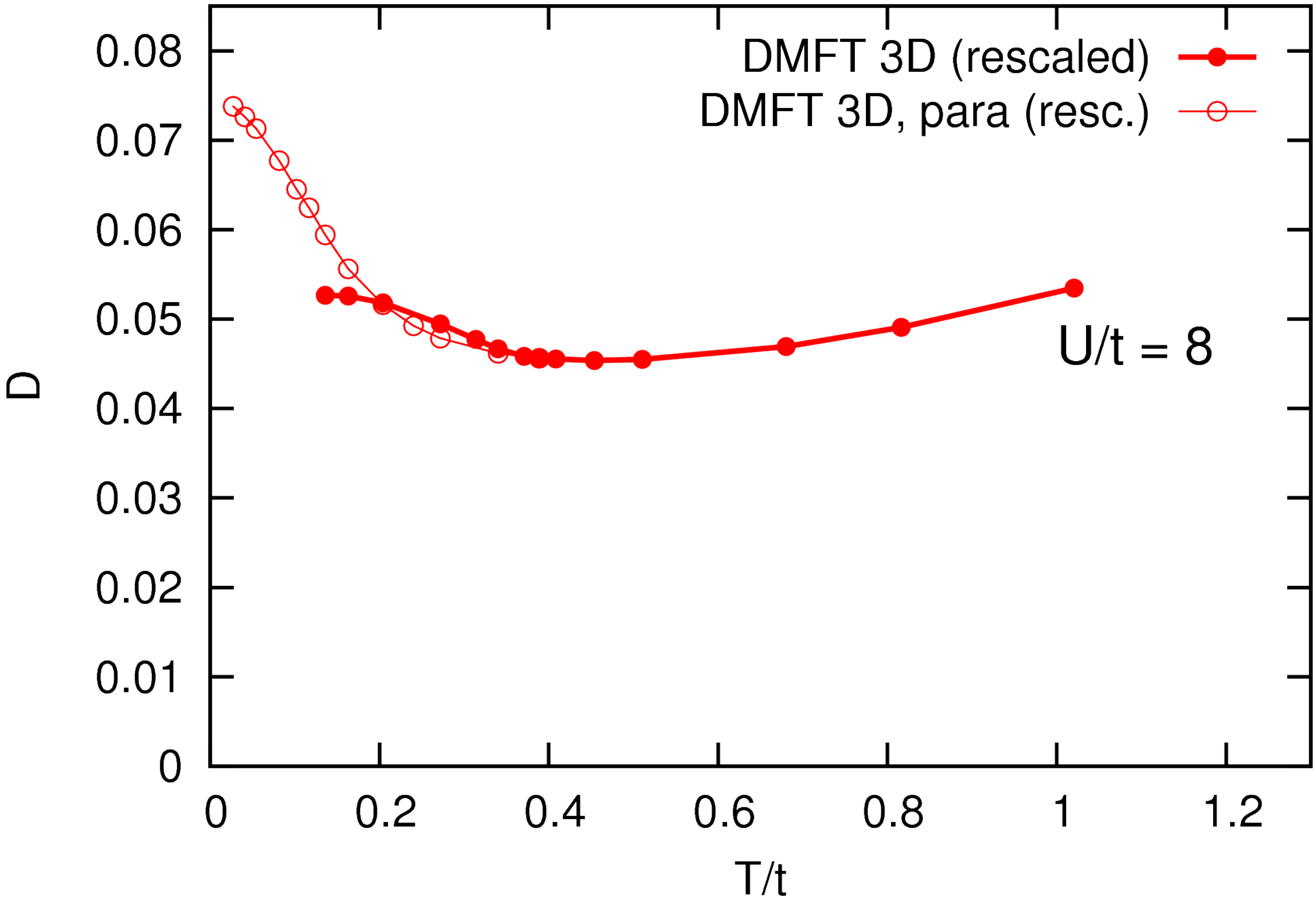
Strong proximity effects beyond LDA (thin lines)

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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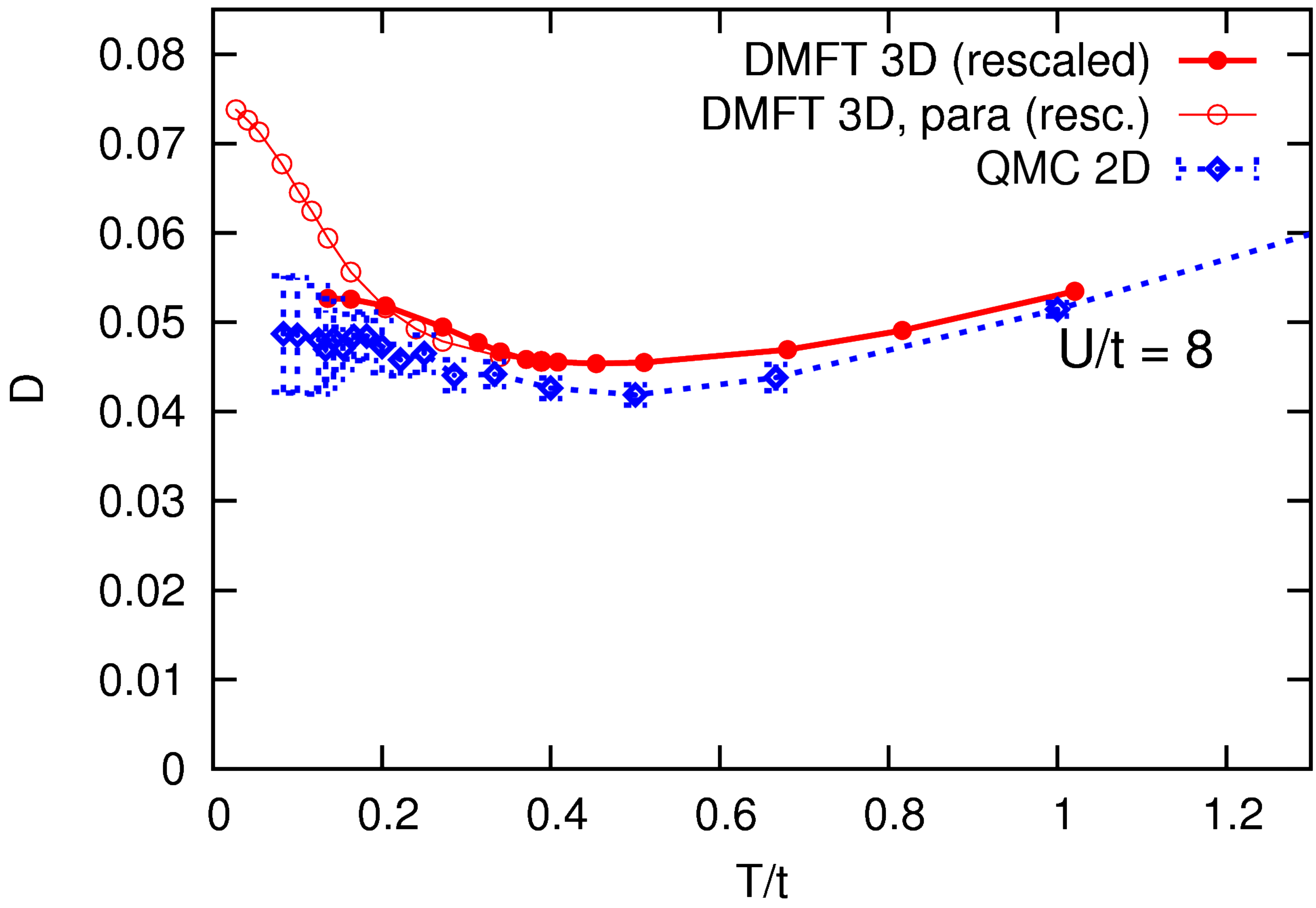

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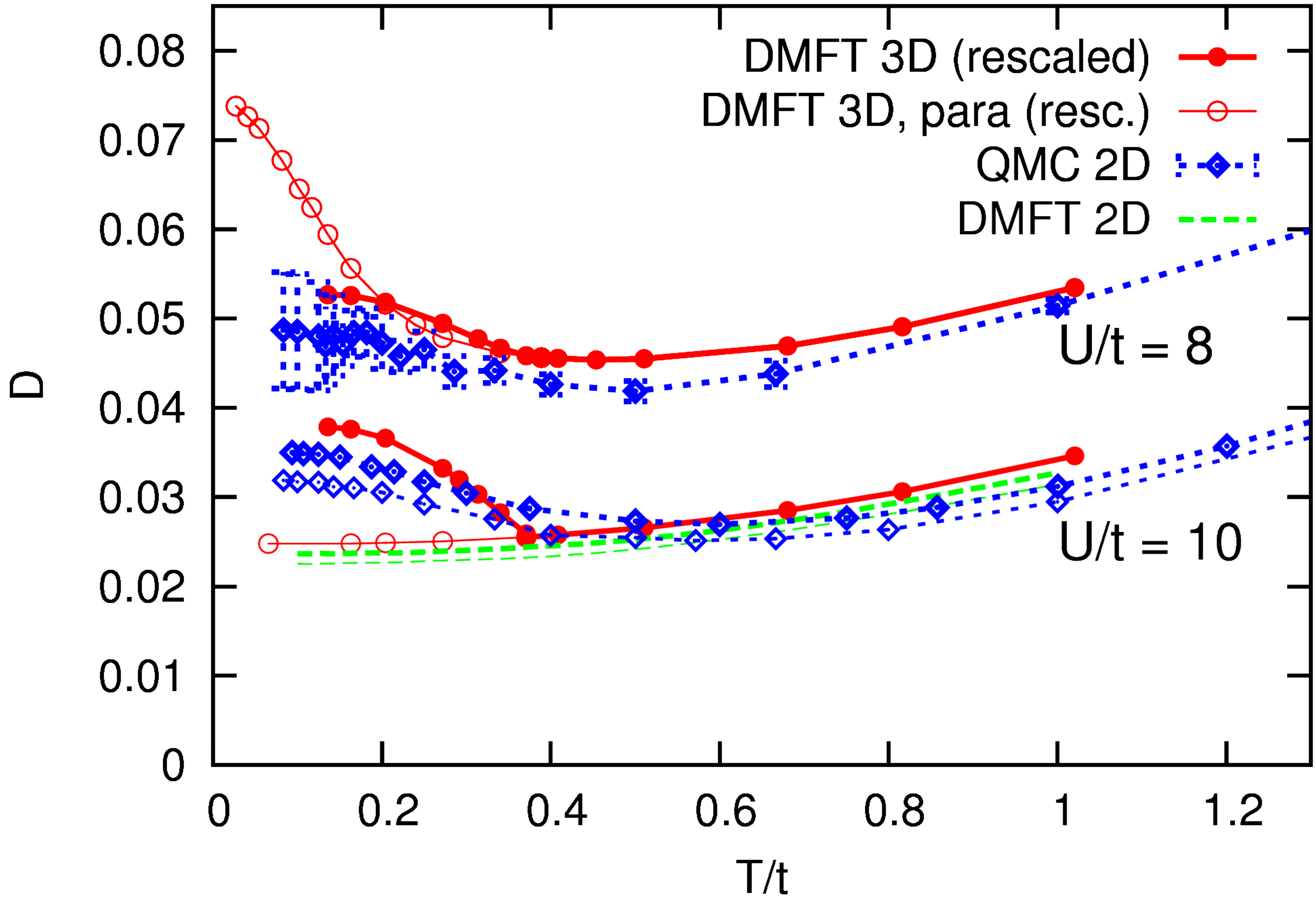

Summary

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, PRL **105**, 065301 (2010)]

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

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

Direct computation of F and S using full enumeration

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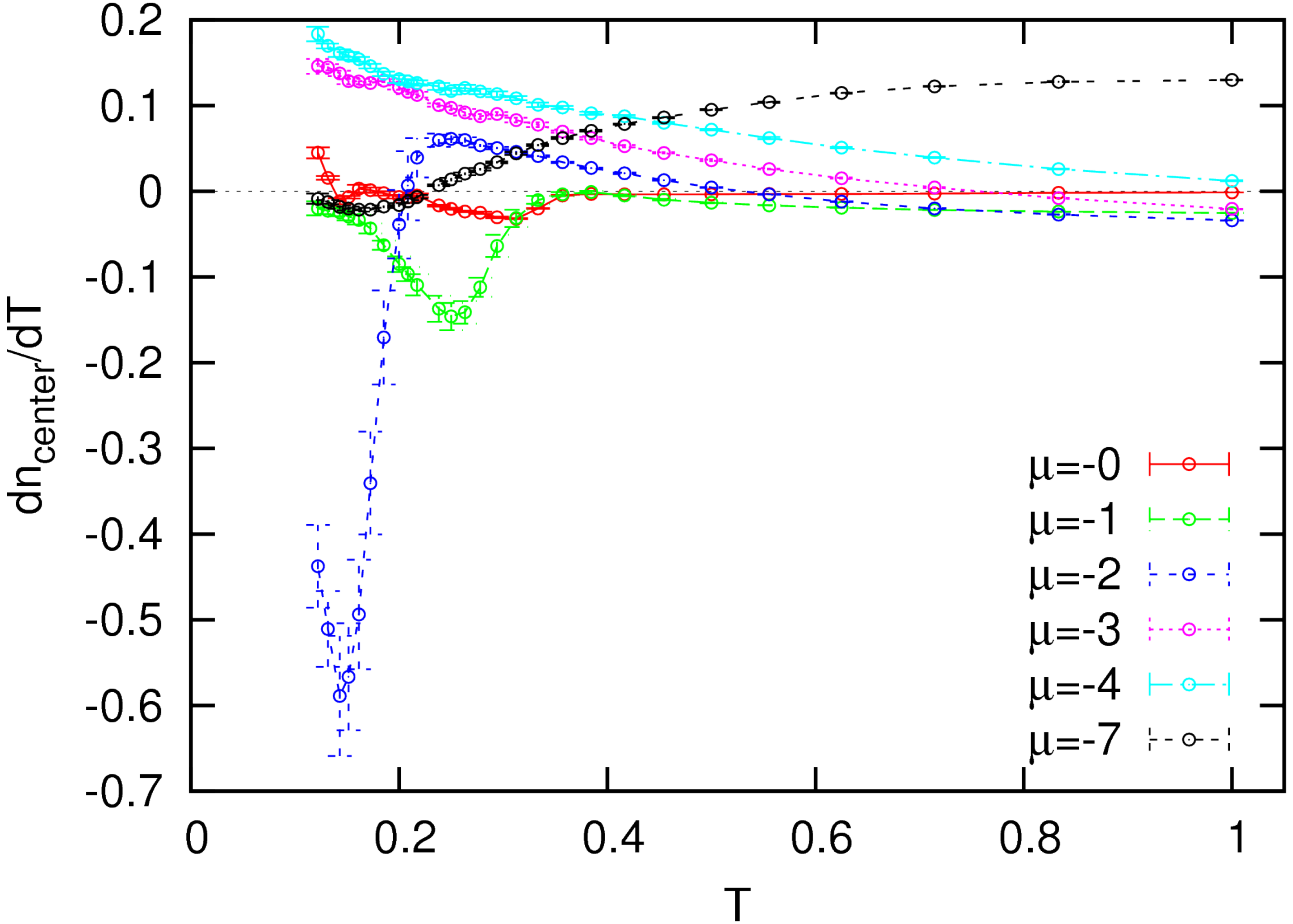
Spin-off: solids with large unit cells (distortions, surfaces, impurities, . . .)

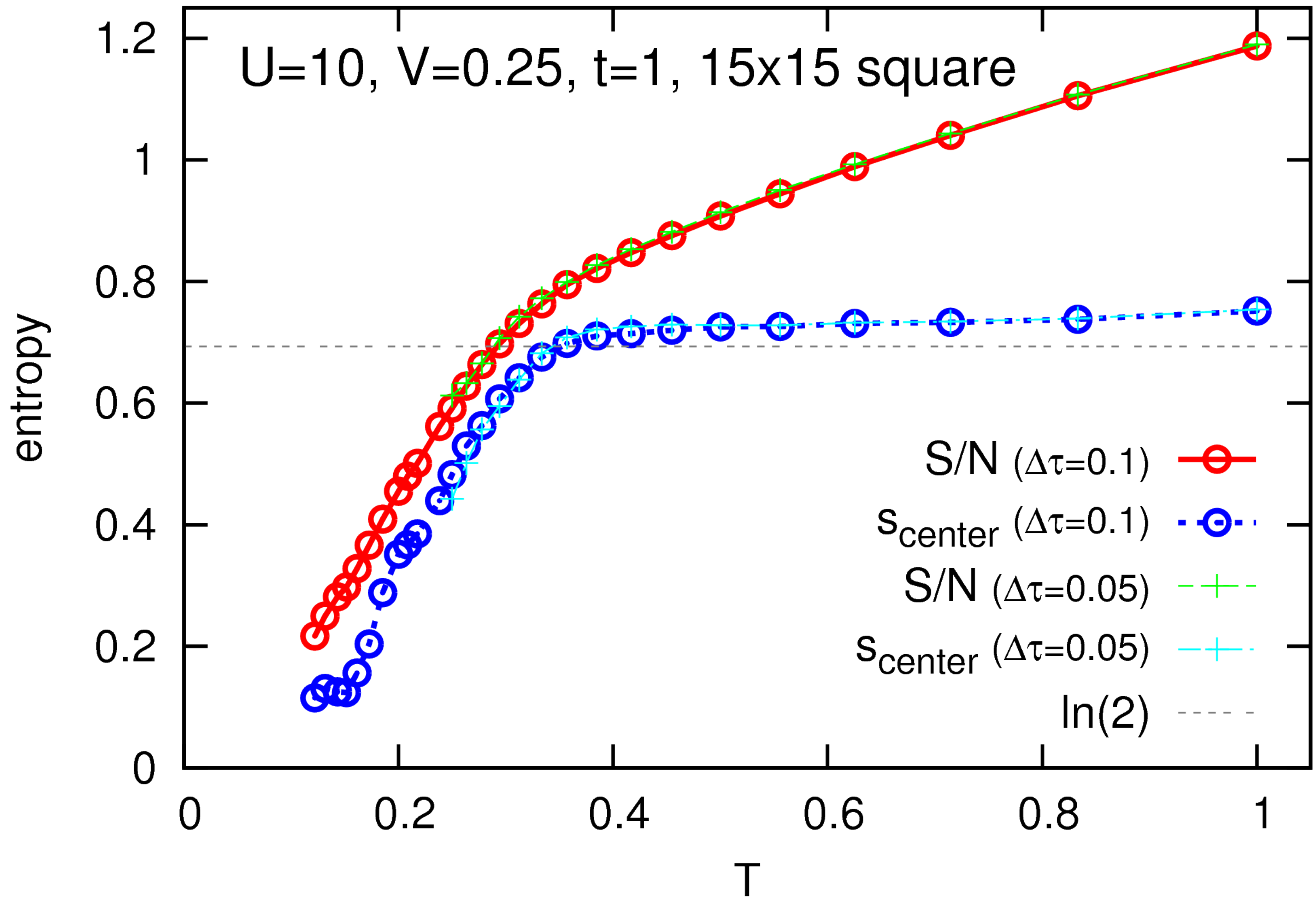
Thanks to: U. Schneider, I. Bloch and Hofstetter and DFG (TR49)

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 ($\leadsto$ need fine integration grid)



very small discretization dependence

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