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

Nils Blümer and Elena Gorelik, Univ. Mainz

Outline

Introduction: cold atoms on lattices, DMFT+QMC

Paramagnetic Mott transitions in 3-flavor mixtures

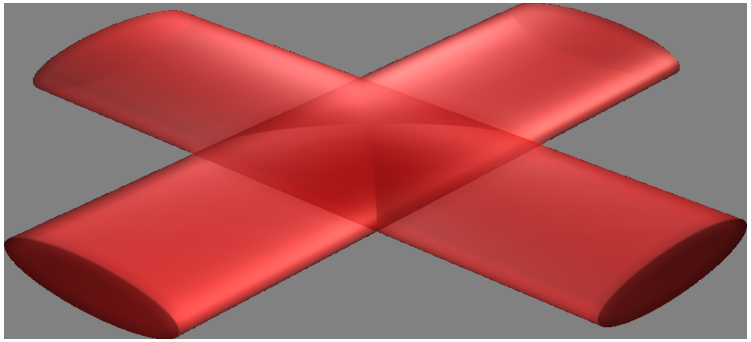
AF order at finite T in an optical trap: 2D results

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

Introduction

Correlated ultracold quantum gases on optical lattices: basics

Optical dipole trap (2 beams)



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

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

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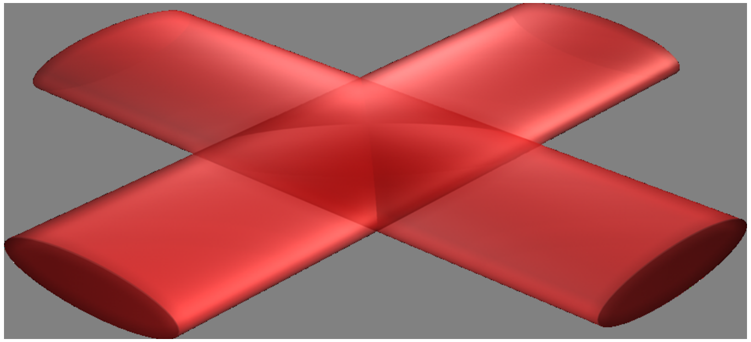

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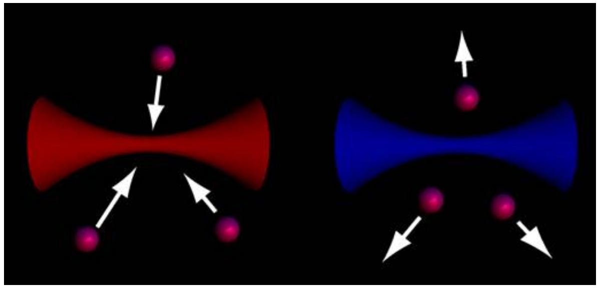
polarizability $\alpha(\omega_L)$ changes sign at ω_0



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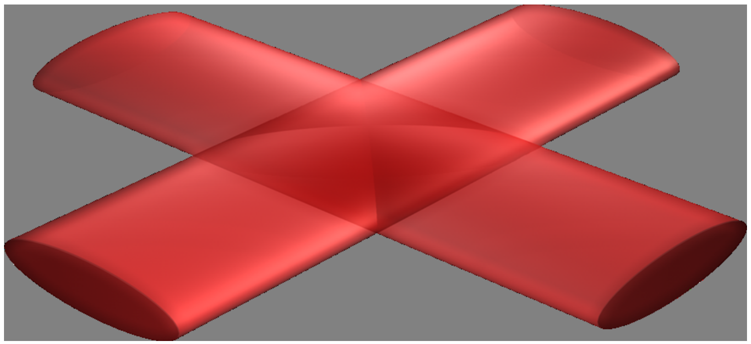

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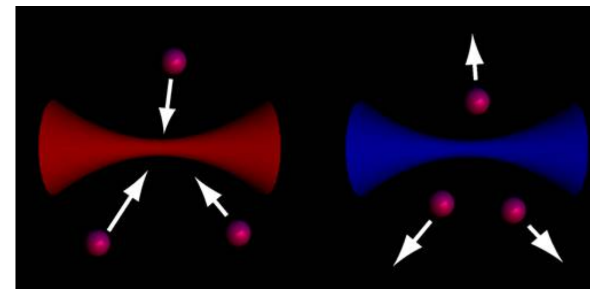
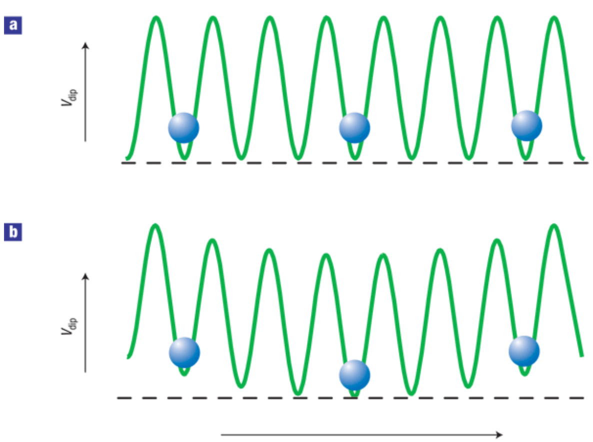


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



Beam profile: (anti) trapping

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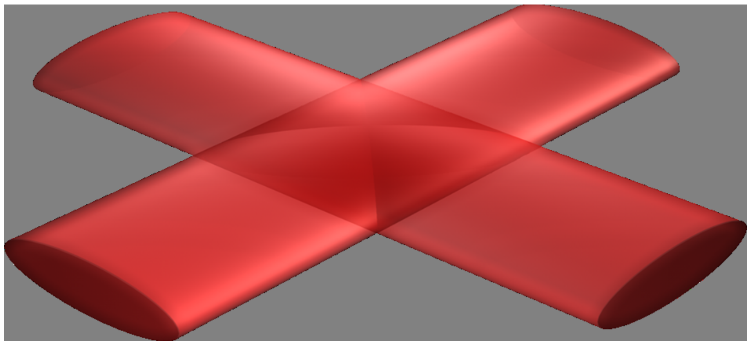

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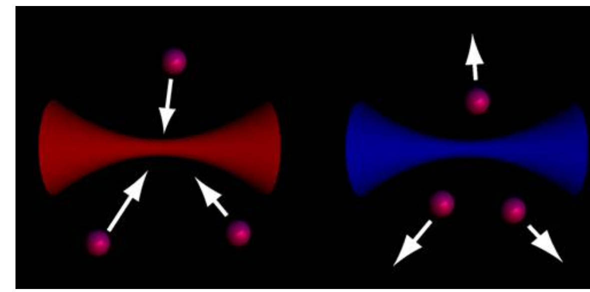

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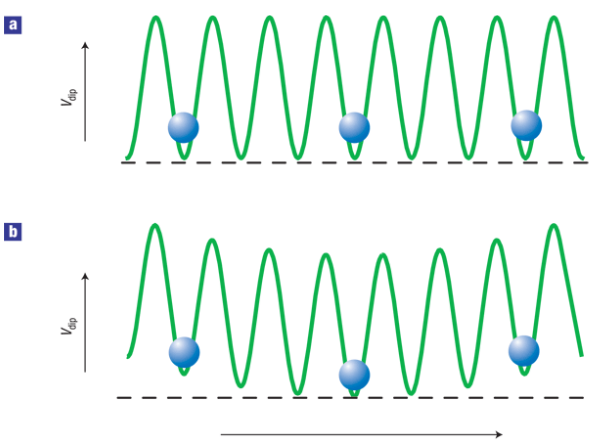
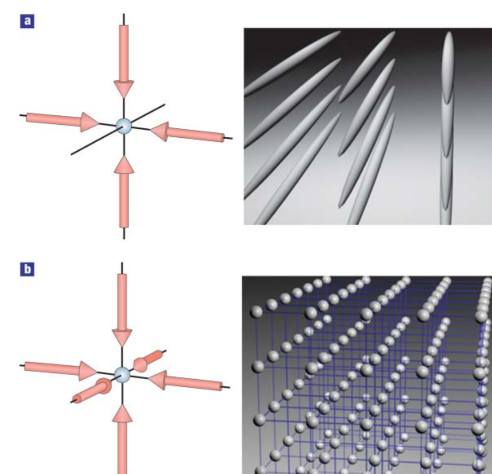


Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

2 pairs of lasers $\rightsquigarrow$ tubes

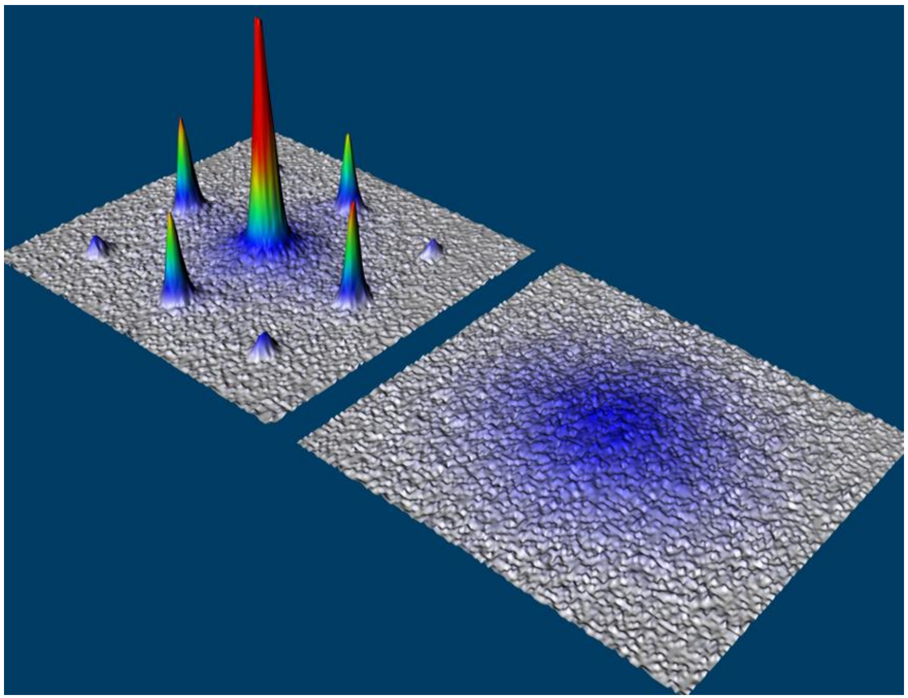
3 pairs of lasers $\rightsquigarrow$ lattice



Correlated ultracold quantum gases on optical lattices: bosons

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

TOF image – momentum distribution



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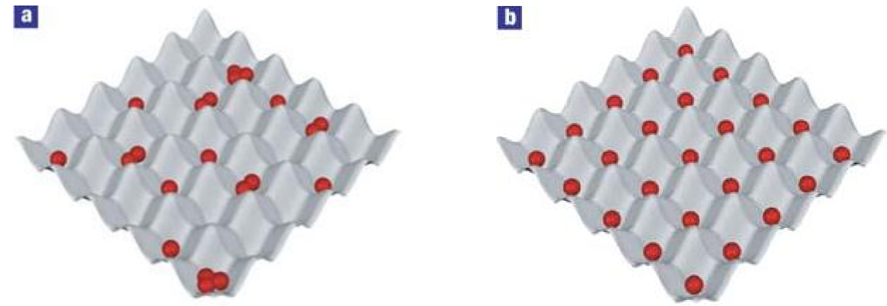

superfluidity destroyed at large U

[Bloch group, 2002]

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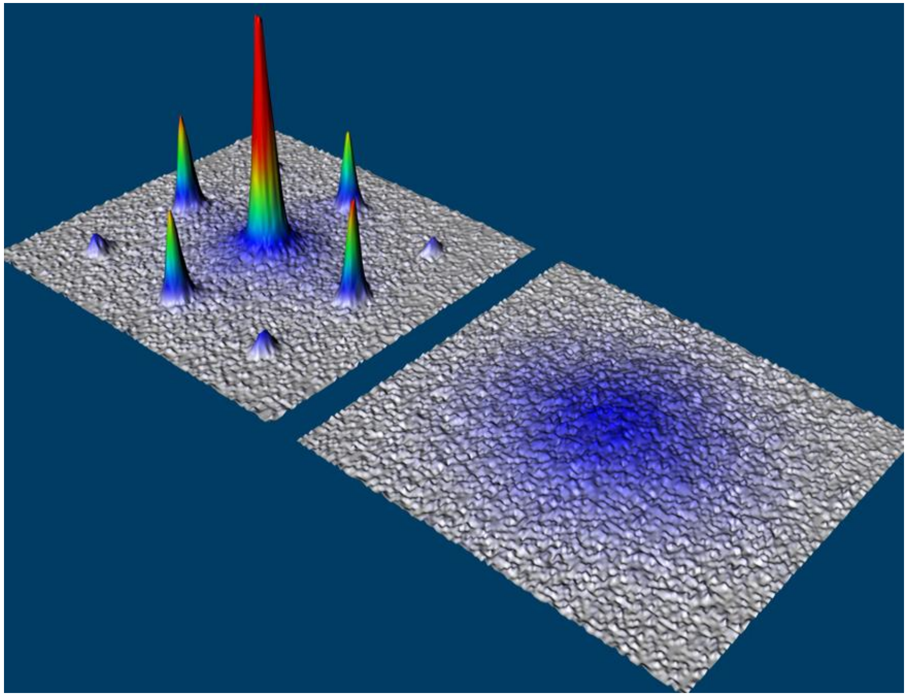

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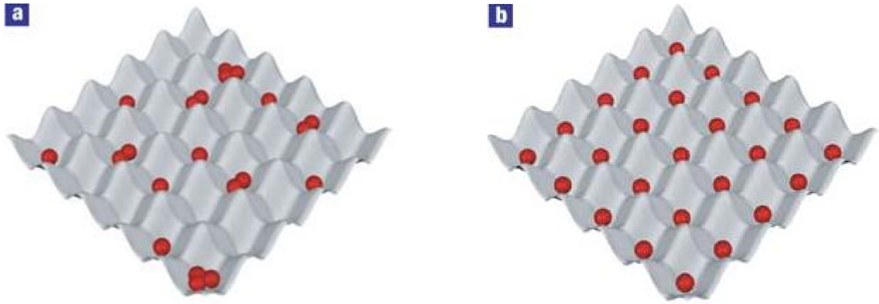
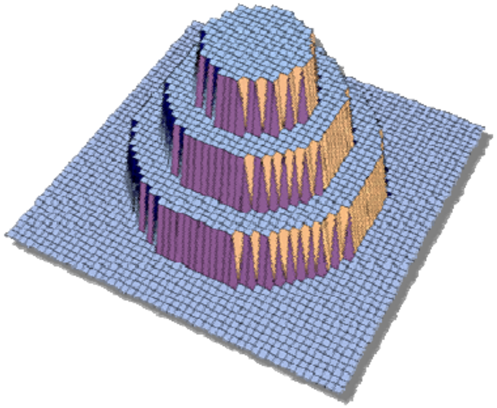
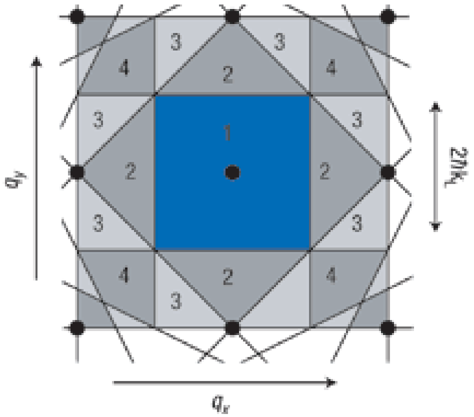


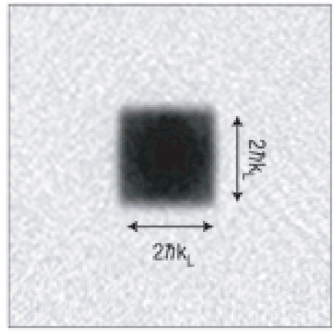
superfluidity destroyed at large U

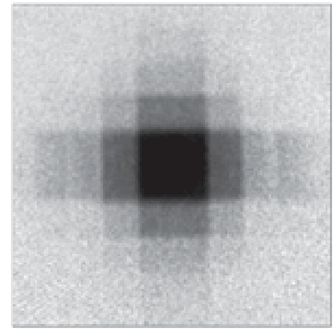
trapping potential $\rightsquigarrow$ "wedding cake"



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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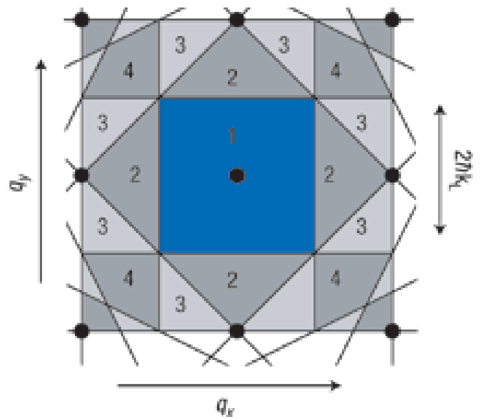

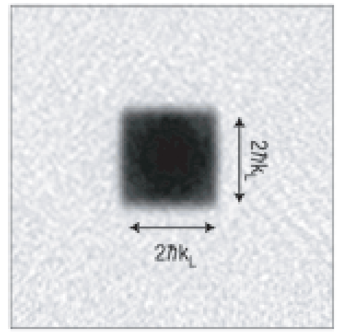

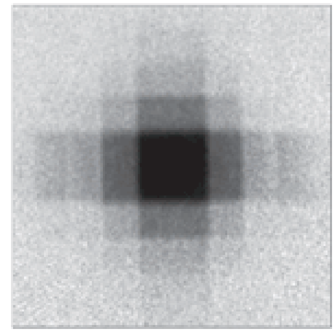

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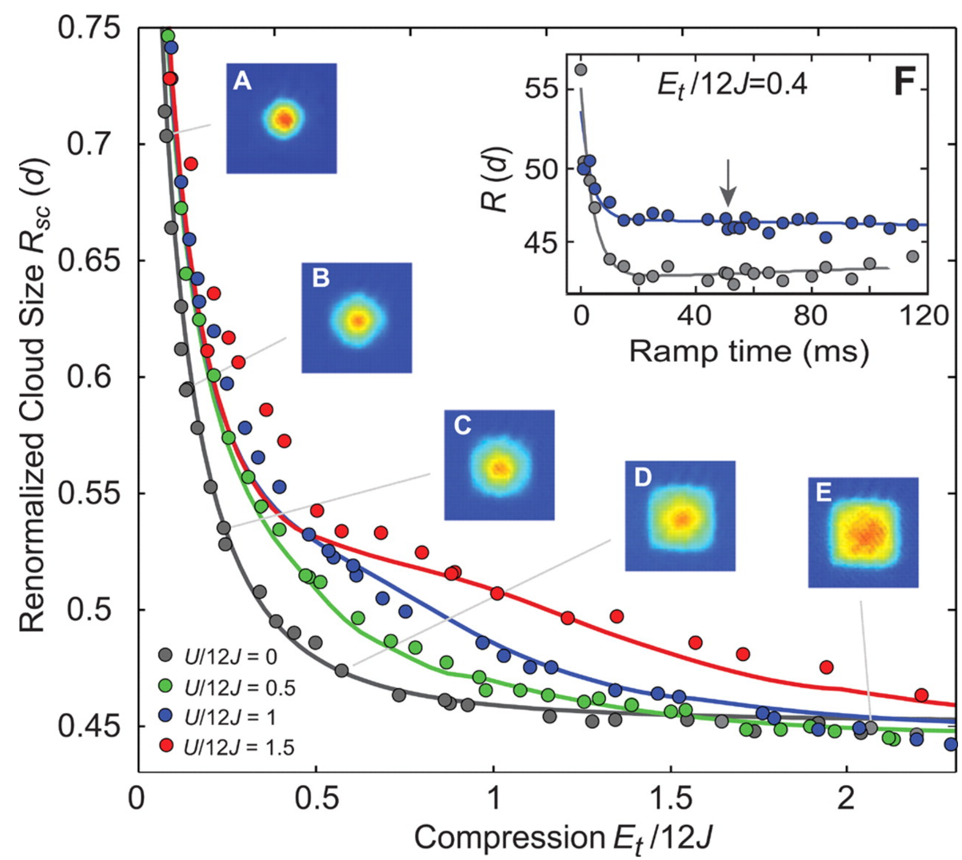
Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

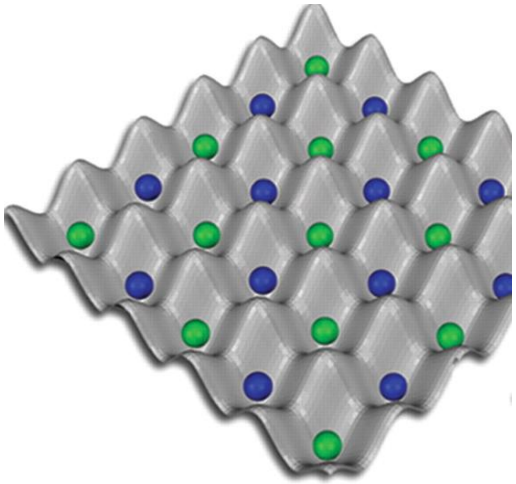
Detection method: measure cloud diameter vs. trap strength

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

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



Urgent todo items:



Antiferromagnetism (staggered order) in ultracold fermions

Problems:

(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of order parameter is not straightforward

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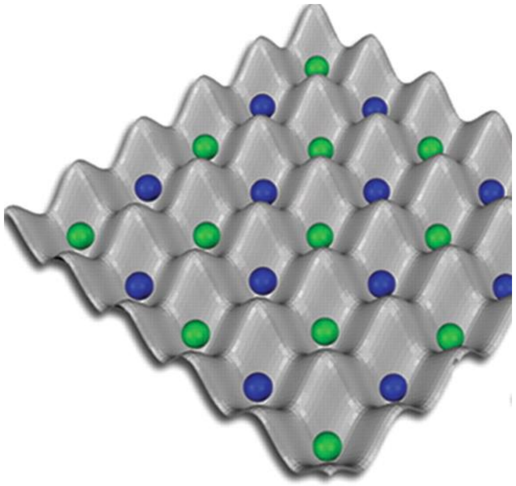

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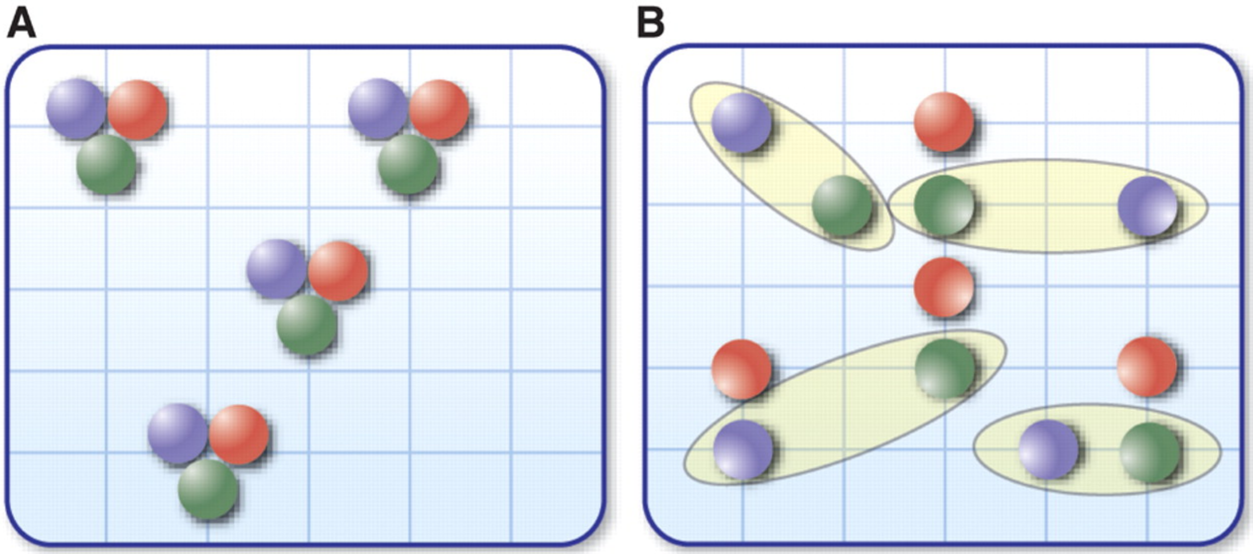
Multiflavor phenomena, e.g. trions versus color superconductivity for 3 flavors



Paramagnetic Mott transitions in 3-flavor mixtures

Calculations for homogeneous system (no trapping potential)

Signatures of Mott transitions persist to high T $\rightsquigarrow$ experimentally accessible

$1 < n < 2$: "semi-compressible" phase: compressibility κ independent of μ, U, T

RAPID COMMUNICATIONS

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

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

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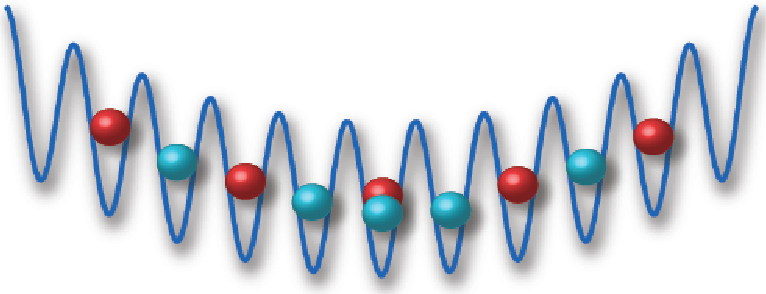
Ternary flavor mixtures of ultracold fermionic atoms in an optical lattice are studied in the case of equal repulsive on-site interactions $U > 0$. The corresponding SU(3) invariant Hubbard model is solved numerically exactly within dynamical mean-field theory using multigrid Hirsch-Fye quantum Monte Carlo simulations. We establish Mott transitions close to integer filling at low temperatures and show that the associated signatures in the compressibility and pair occupancy persist to high temperatures, i.e., they should be accessible to experiments. In addition, we present spectral functions and discuss the properties of a "semicompressible" state observed for large U near half filling.

DOI: 10.1103/PhysRevA.80.051602 PACS number(s): 67.85.−d, 03.75.Ss, 71.10.Fd, 71.30.+h

Melting of an antiferromagnet 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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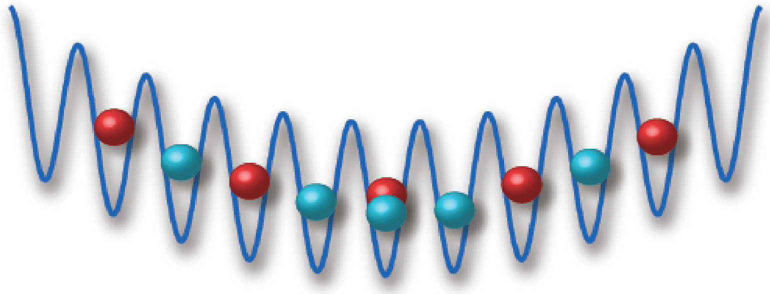

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Real-space DMFT: use local self-energy in inhomogeneous system

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

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

[Snoek et al., NJP (2008), Helmes et al., PRL (2008)]

Also: inhomogeneous DMFT [Freericks], layered DMFT [Potthoff]

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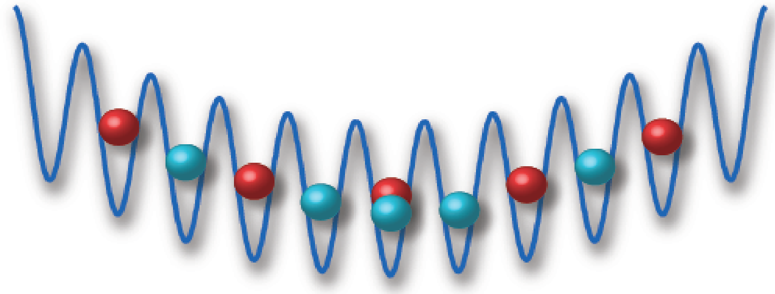

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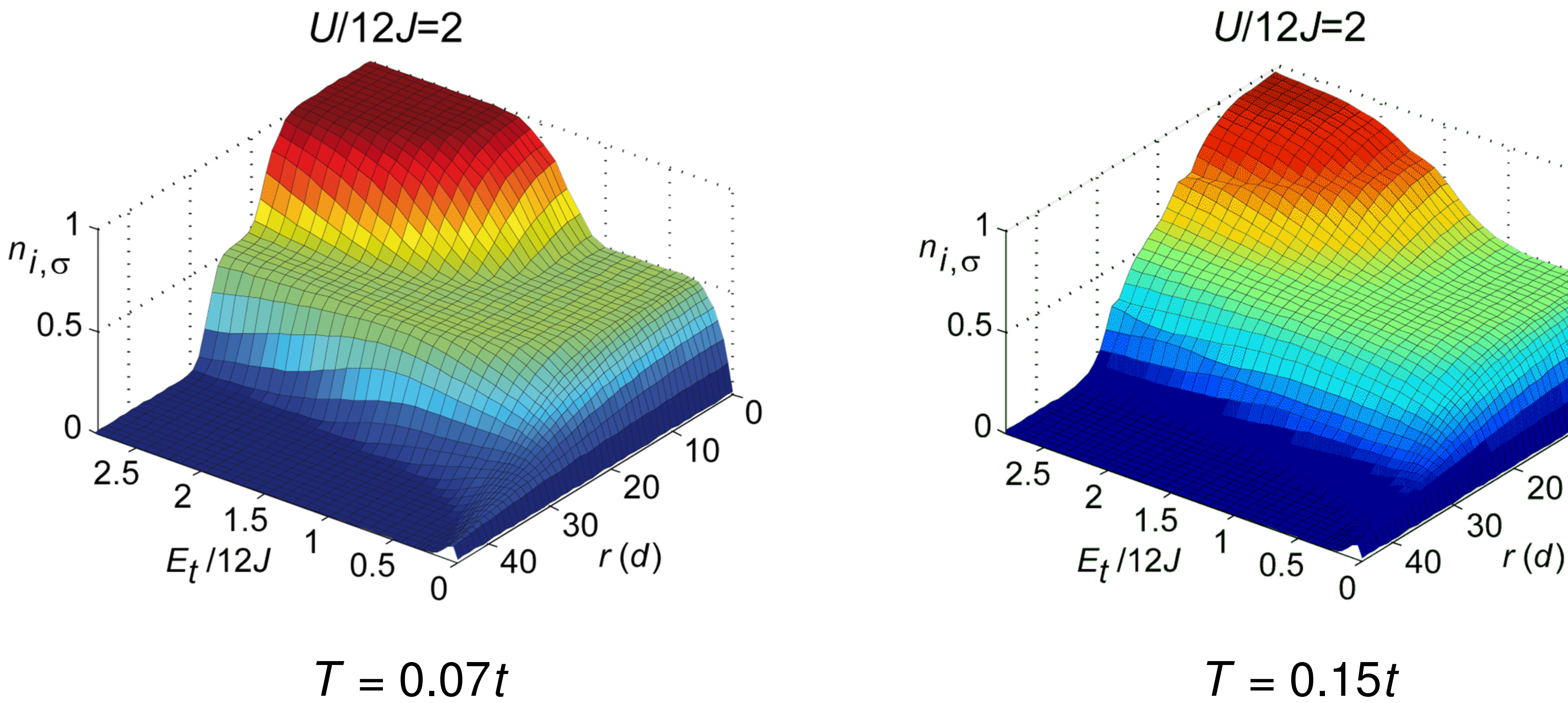
Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

All previous implementations: RDMFT+NRG

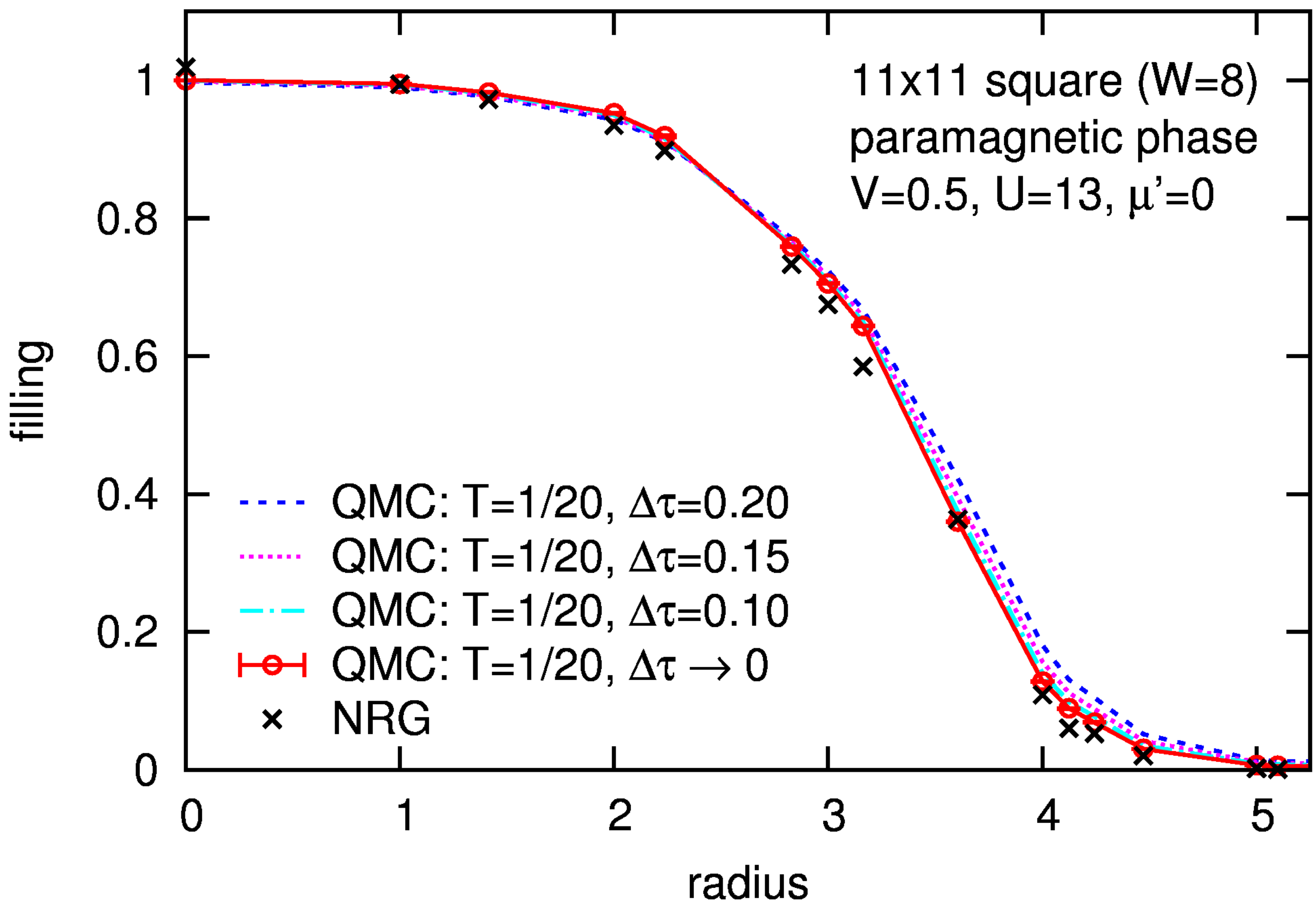
NRG: problematic at elevated temperatures



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!

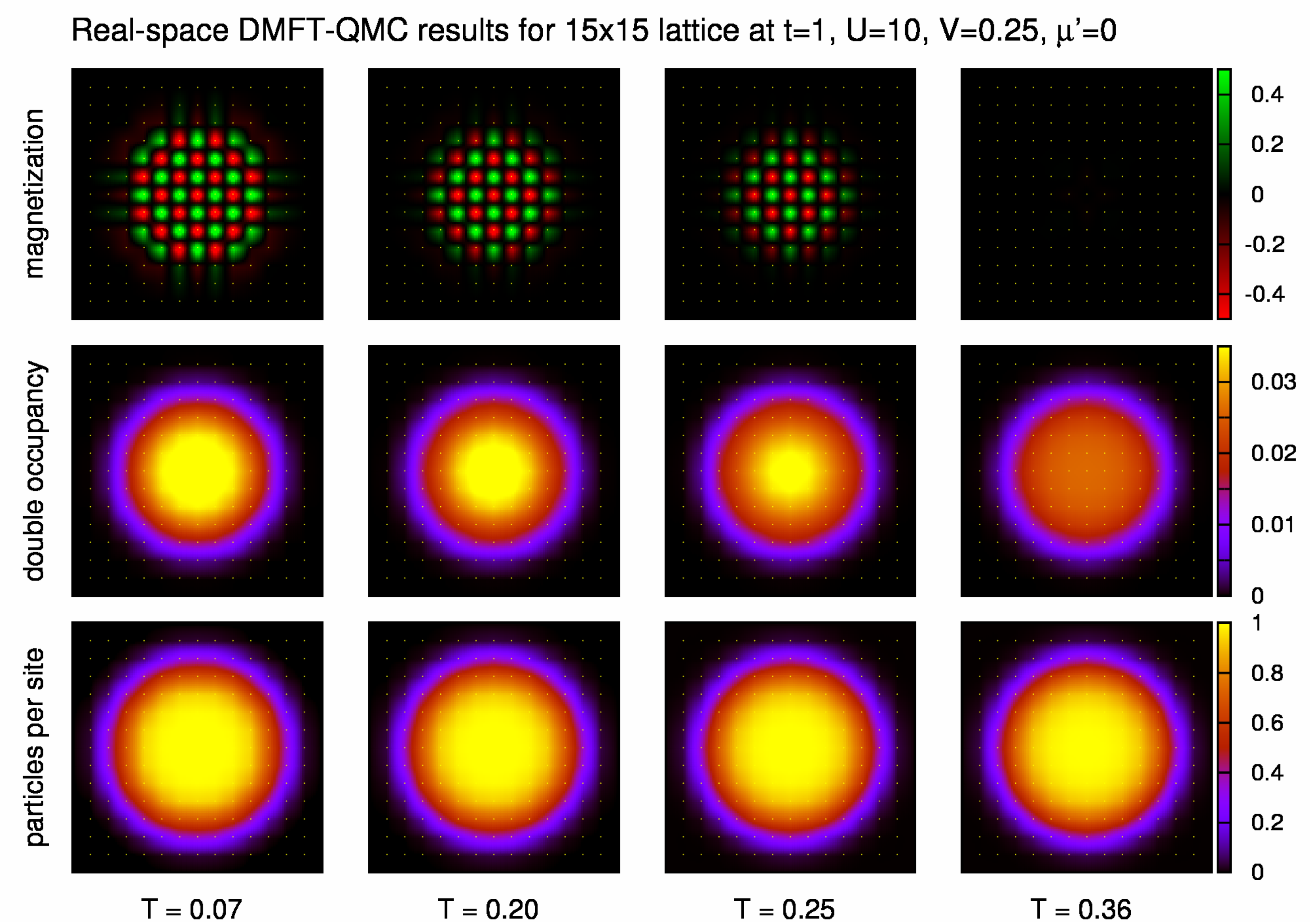
2D real-space DMFT results for paramagnetic phase: QMC vs. NRG



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

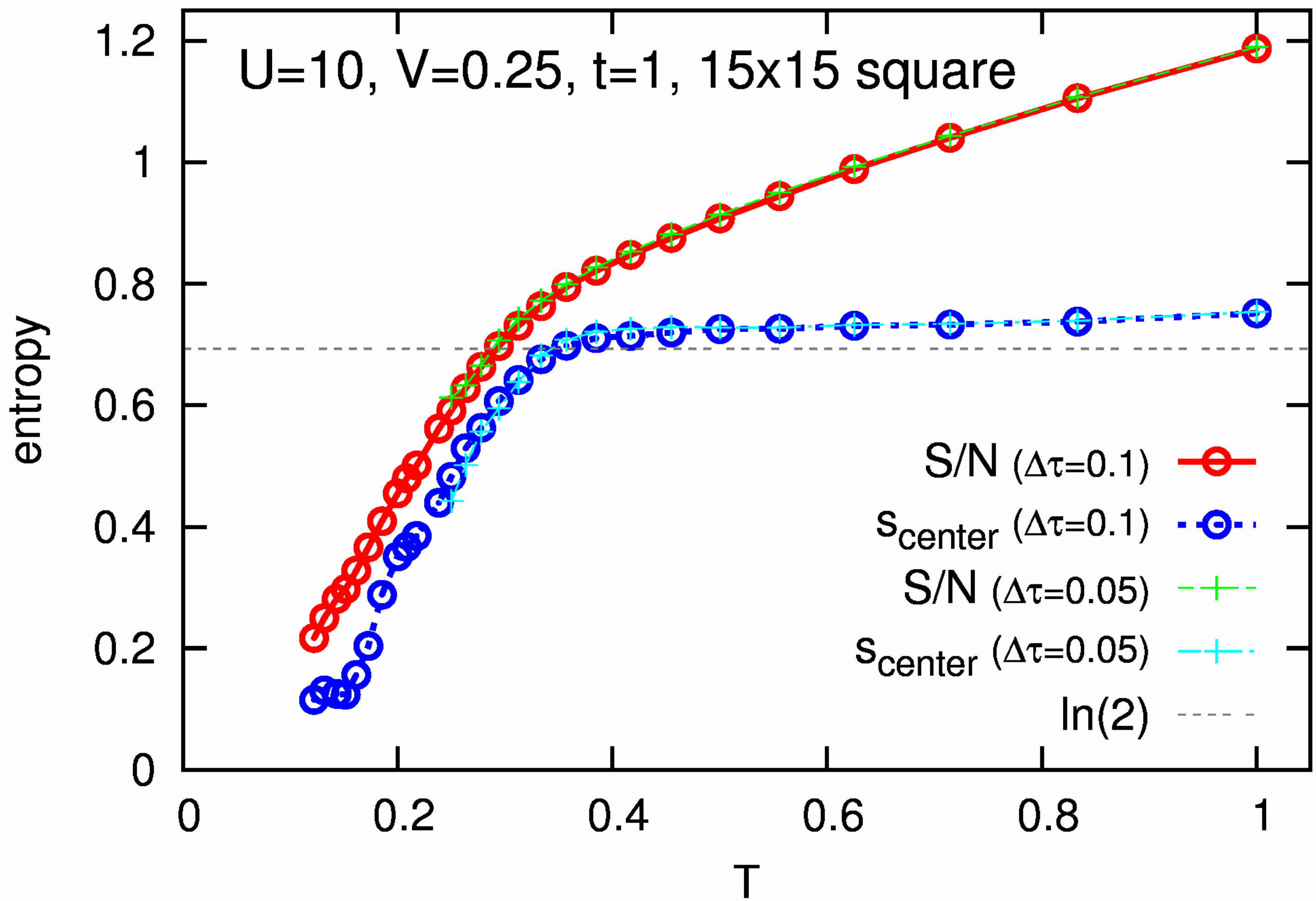
[NRG data by I. Titvinidze (collaboration within SFB/TR 49)]

Melting of a central antiferromagnetic phase



Antiferromagnetic order signaled by enhanced double occupancy - entropy?

Entropy: no direct computation, use $S = \int_{-\infty}^{0} d\mu' \, \frac{dN}{dT}$ (need fine T and μ grids)



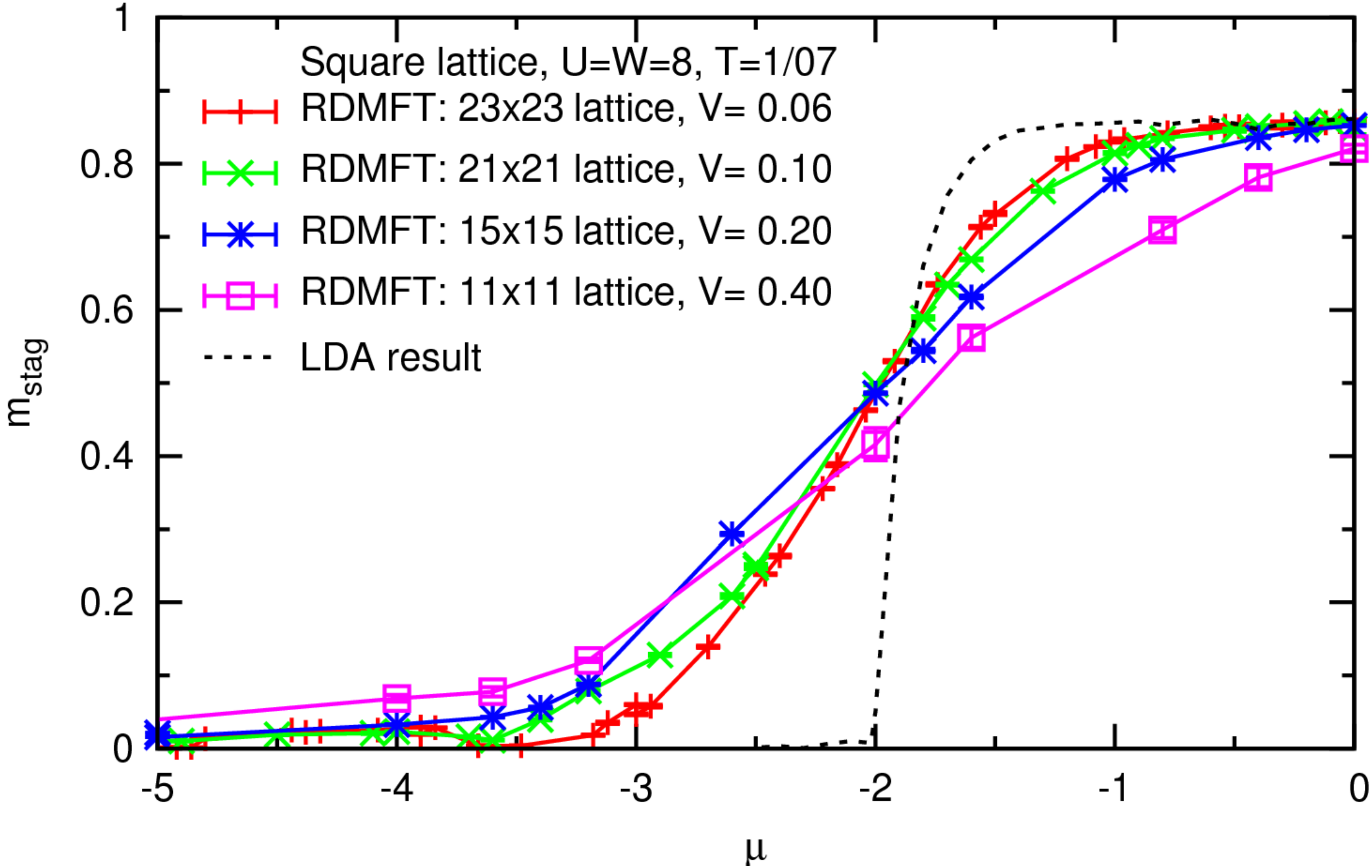
central entropy: plateau $s \approx \ln(2)$ in paramagnetic insulator

(mean field)

average entropy is higher

very small discretization dependence

RDMFT: strong proximity effects (not in "LDA" approximation)



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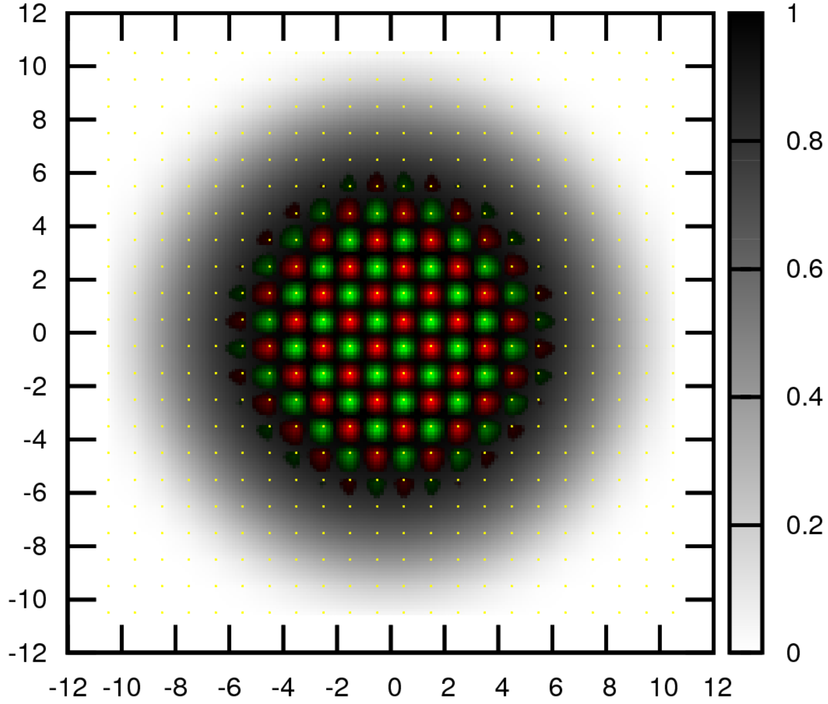
Practical (dense inversion, fully parallel): $\lesssim$ 10000 sites $\rightsquigarrow$ need smart strategies



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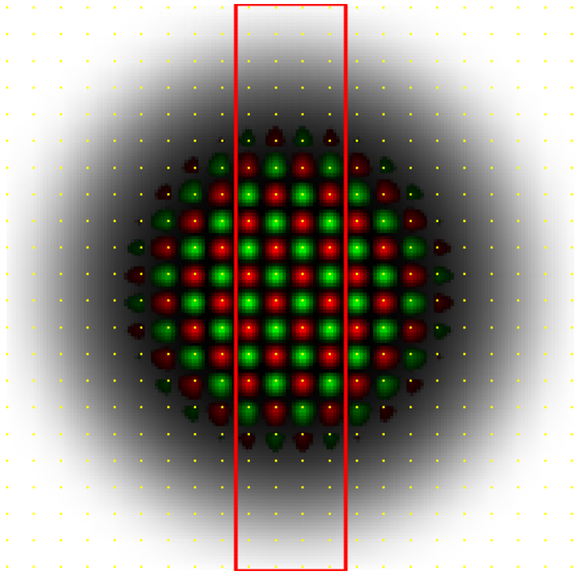

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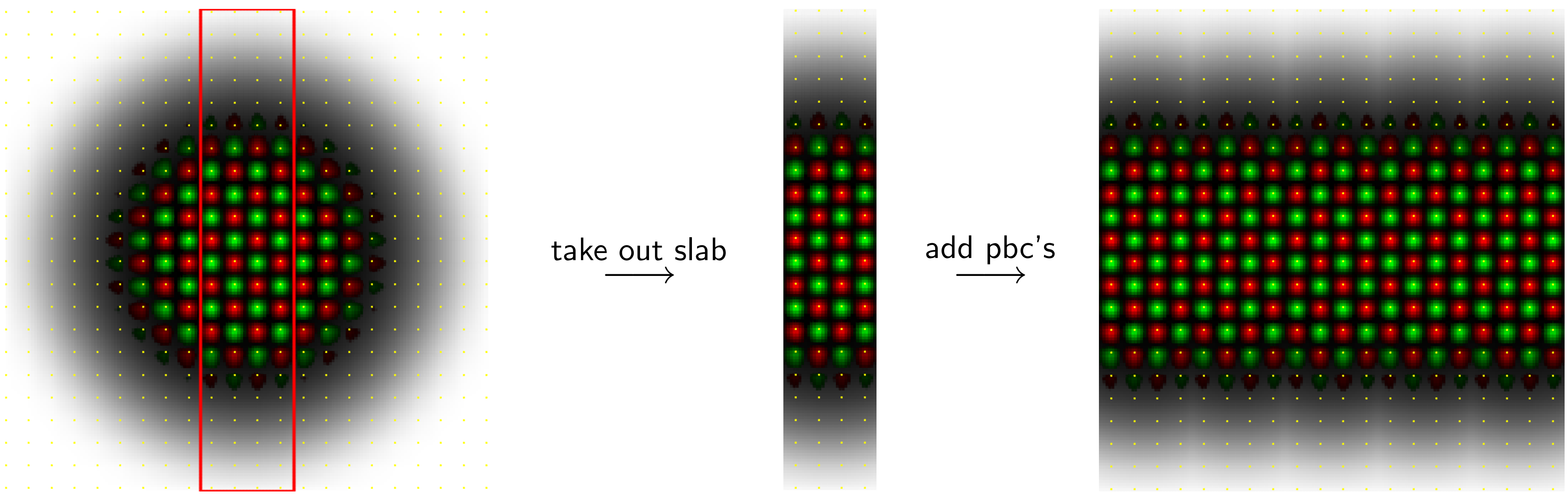
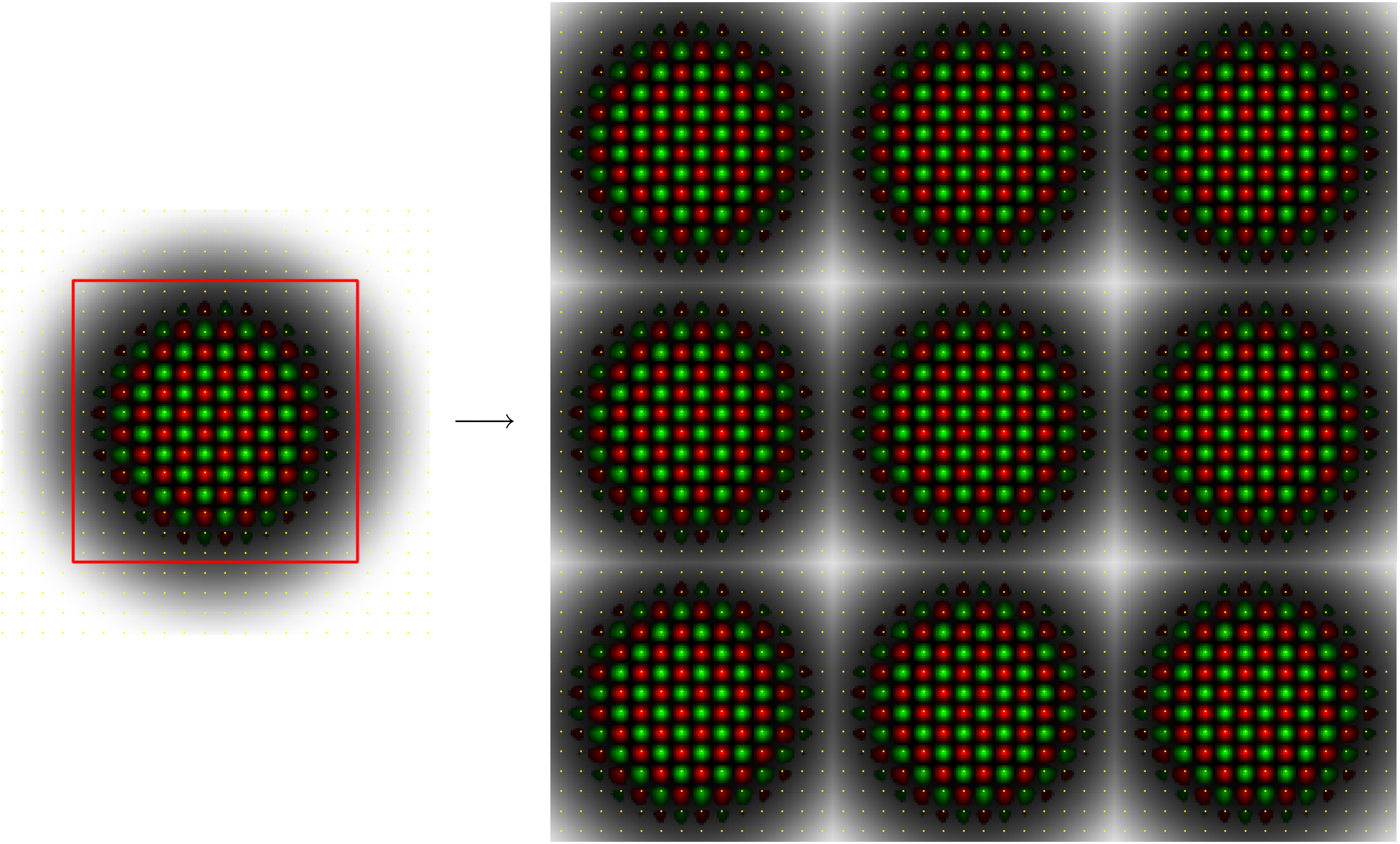
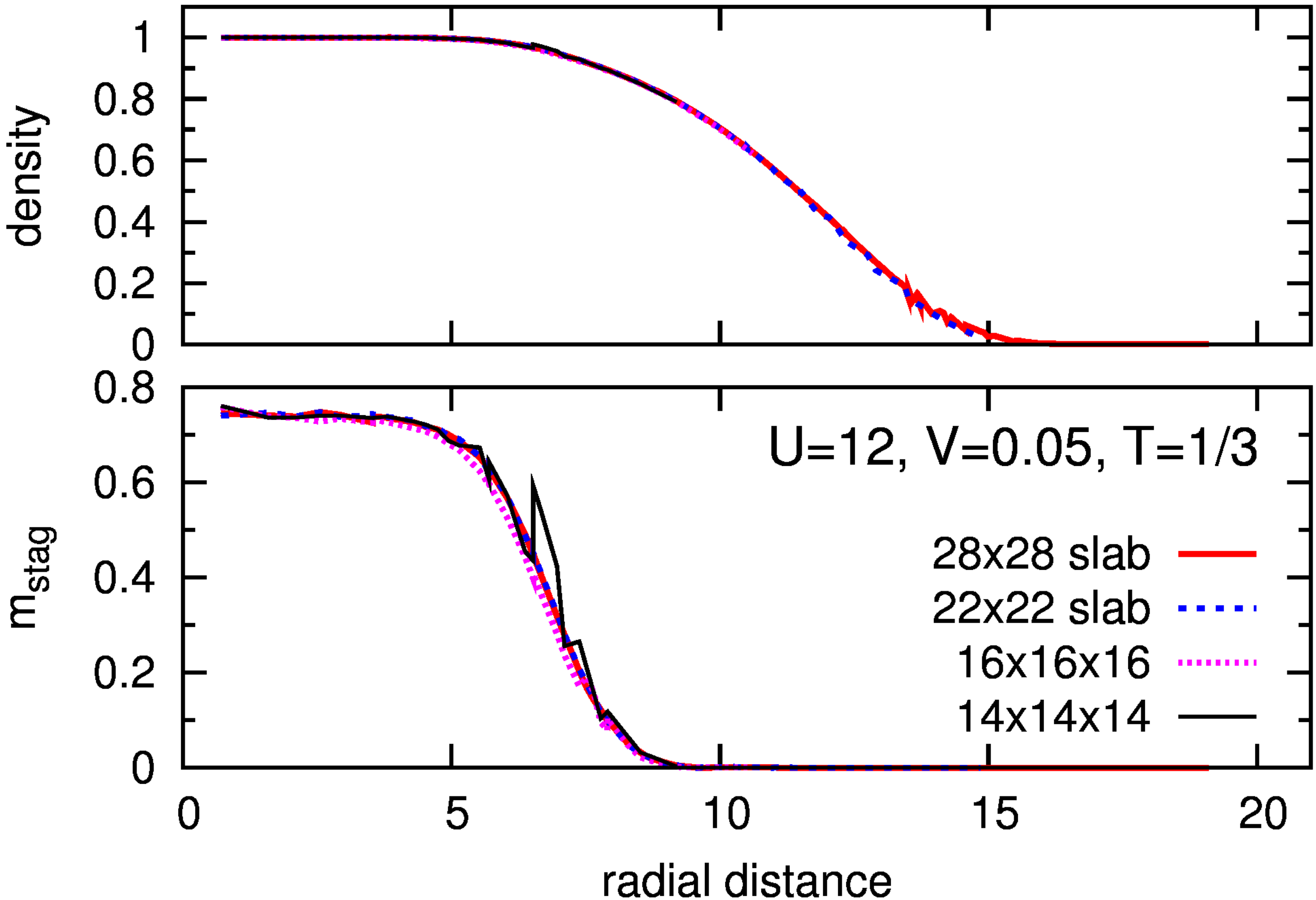


In practice: cylindrical potential (equivalent layers)

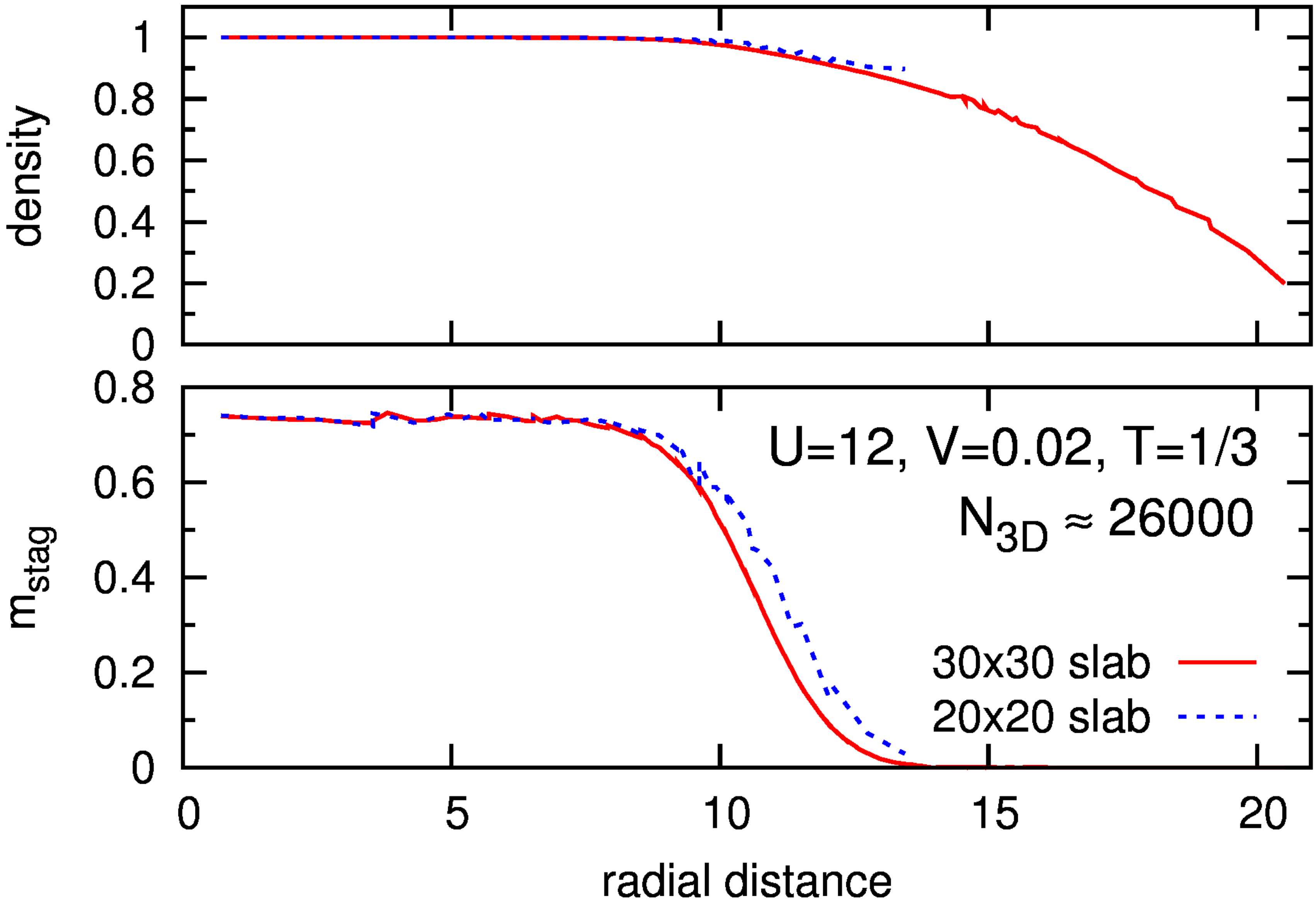
Alternative: 3D calculation, but focus on AF core (pbc's in all 3 directions):



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



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



Summary

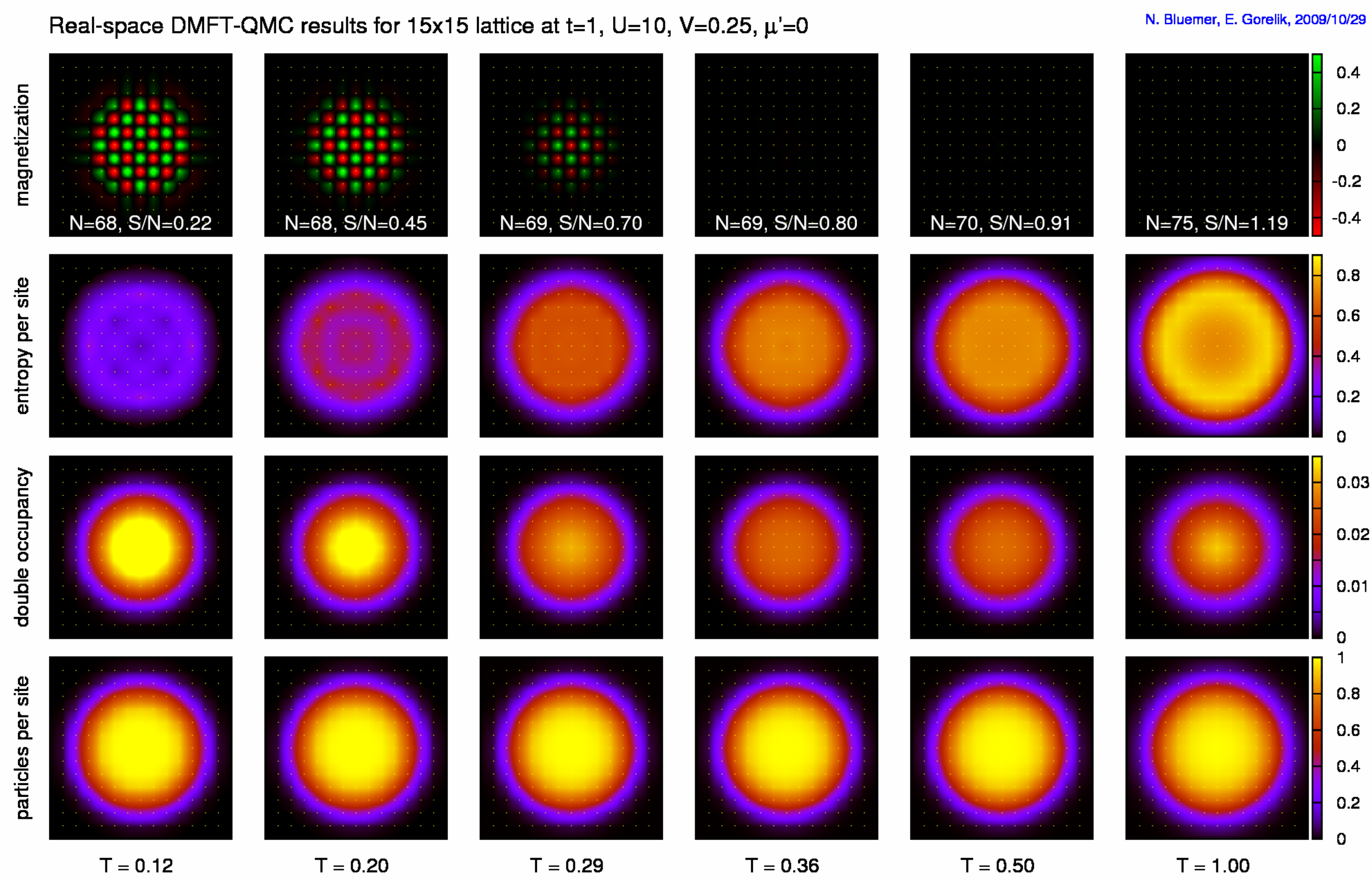
1) Antiferromagnetic phases signaled by enhanced double occupancy

2) LDA fails for ordered phases: misses proximity effects

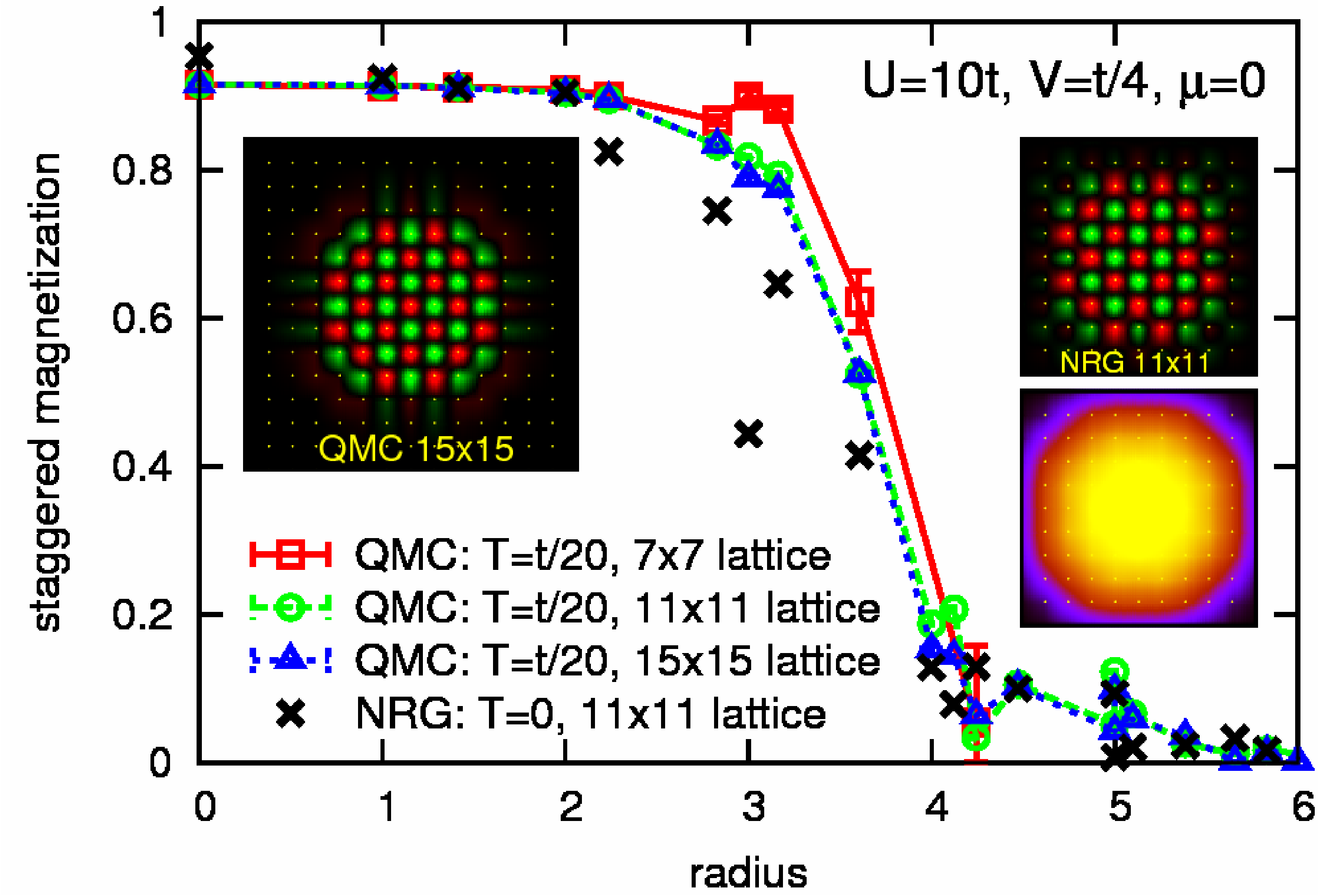
3) We can treat systems with $\mathcal{O}(100000)$ particles at full DMFT level

Thanks to: Hofstetter and Bloch groups, DFG (in SFB/TR 49)

Entropy distribution



2D real-space DMFT results for AF phase: QMC vs. NRG



Finite-size effects surprisingly small; QMC apparently more accurate (even at low T)