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

Nils Blümer and Elena Gorelik, Univ. Mainz

Outline

Introduction: SCES, cold atoms on lattices

Methods: Dynamical mean-field theory, QMC, RDMFT

Results: signature of AF order in cubic optical lattice

Summary

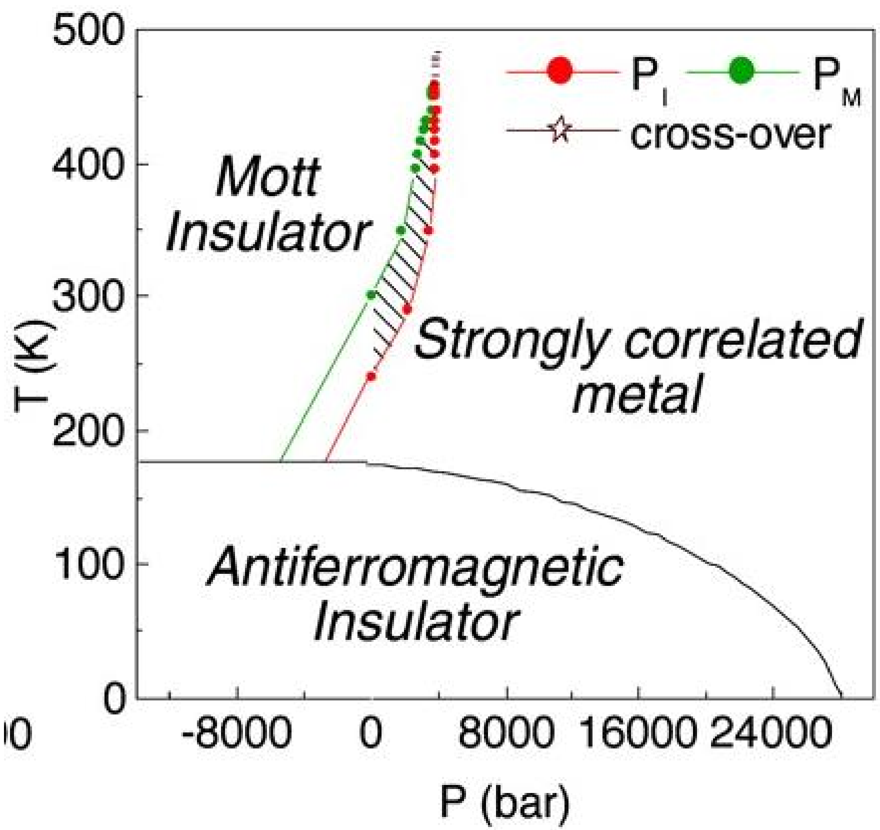
[E. V. Gorelik, N. Blümer, arXiv:1006.2716]

[E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, N. Blümer, arXiv:1004.4857]

Introduction: Systems with strong electronic/fermionic correlations

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

Phase diagram



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

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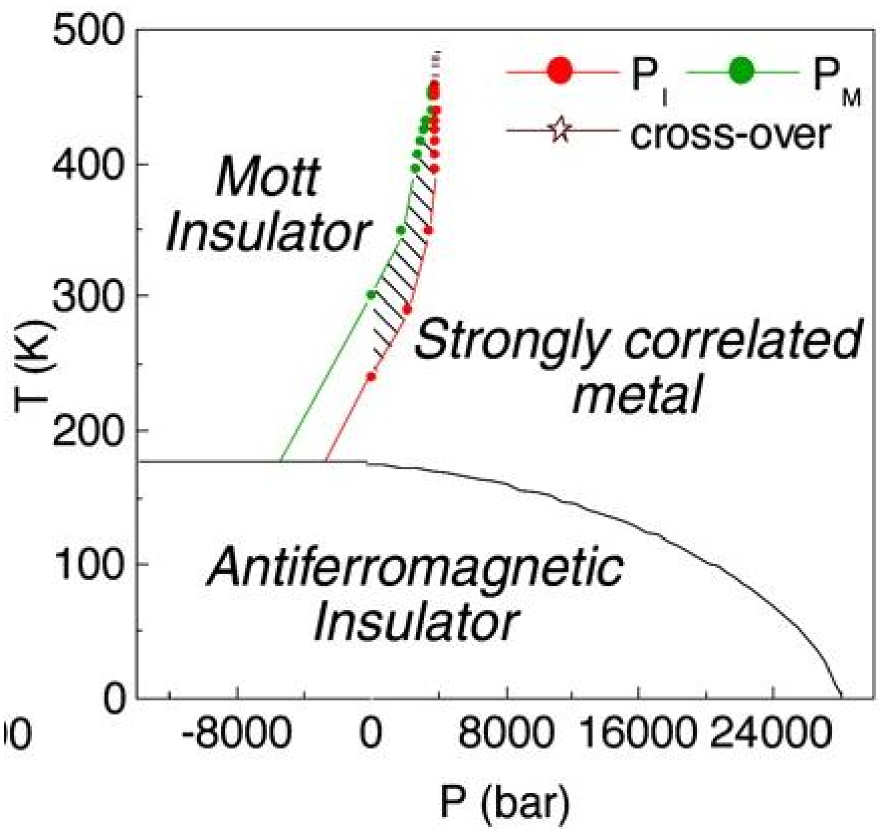

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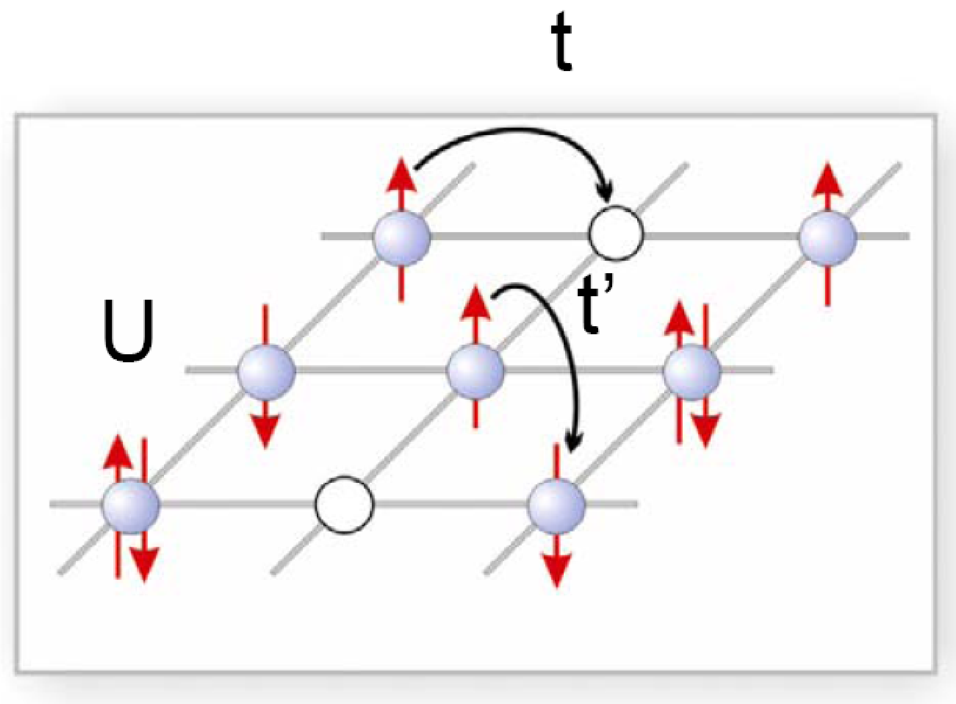

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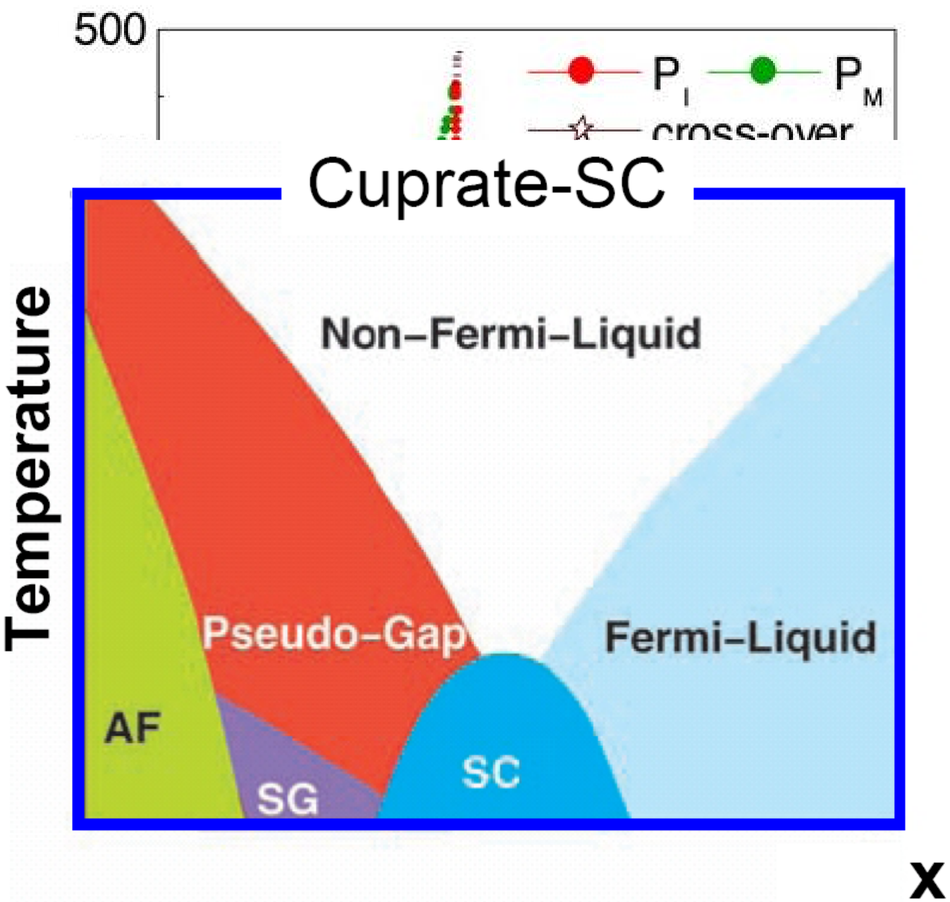
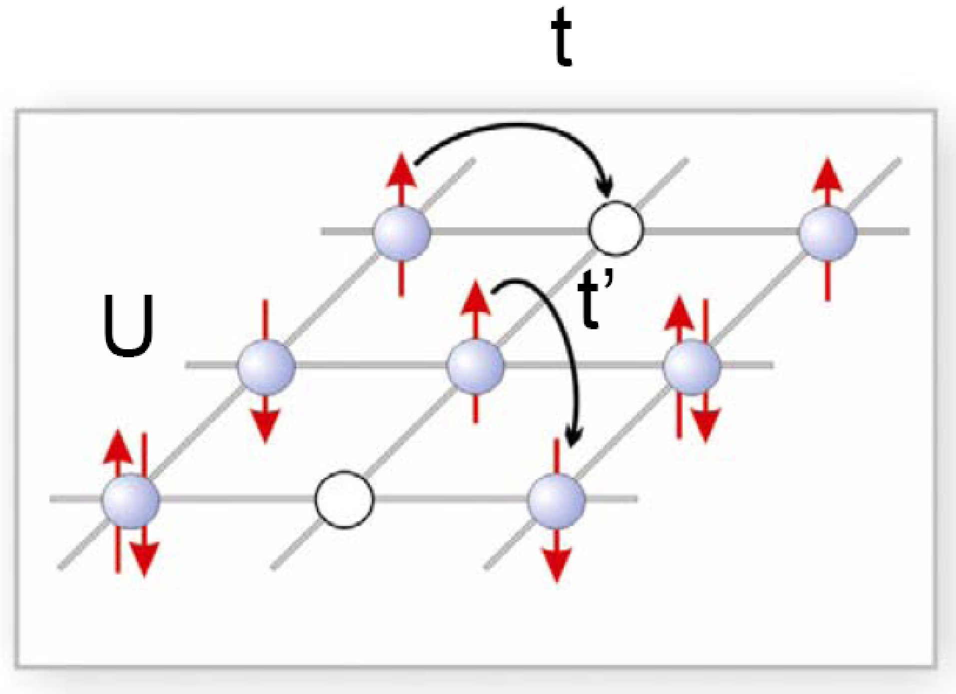


Mott metal-insulator transition and AF: generic physics of 1-band Hubbard model



Are AF and Mott phases essential for superconductivity?

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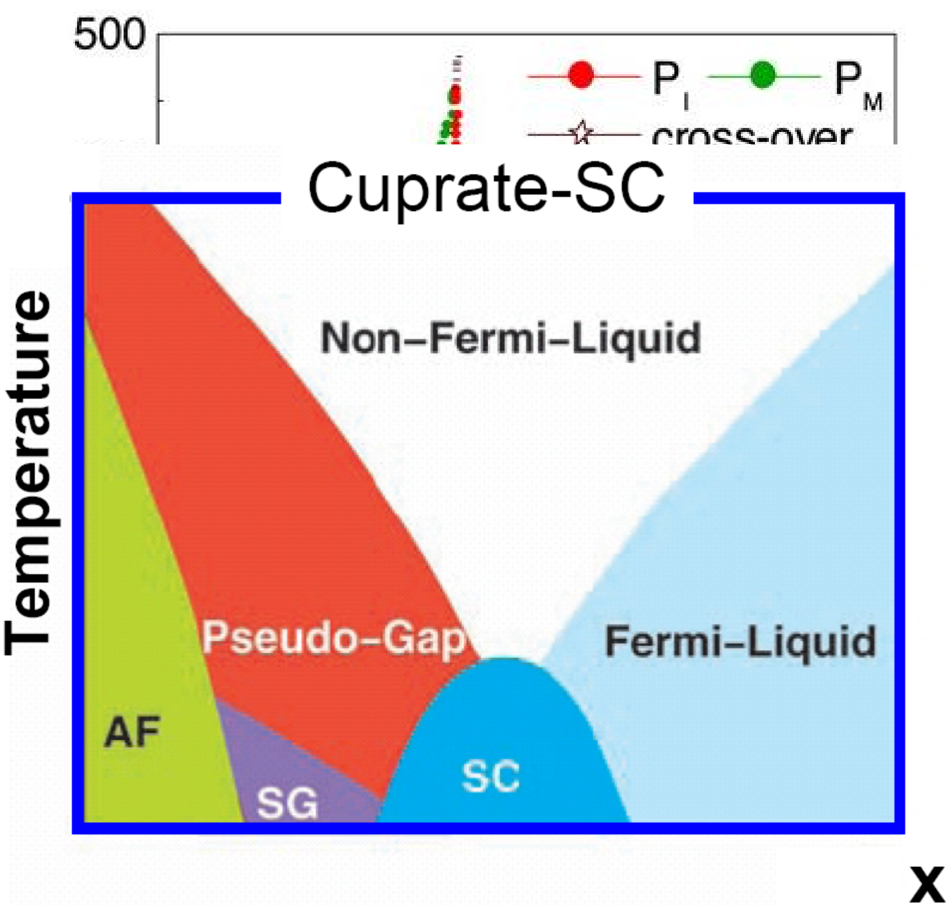
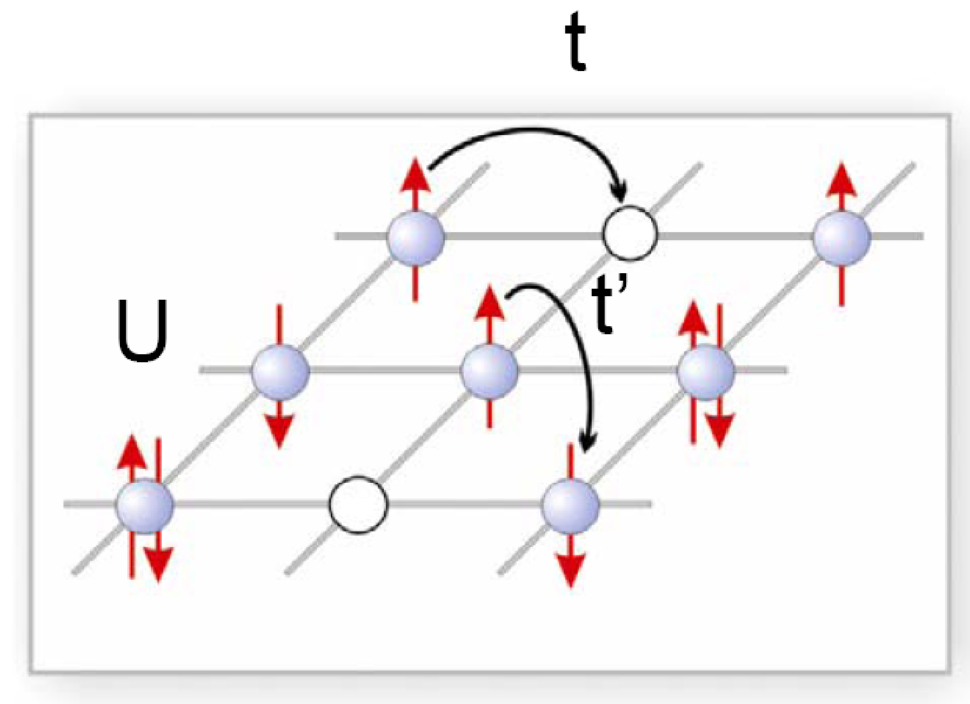


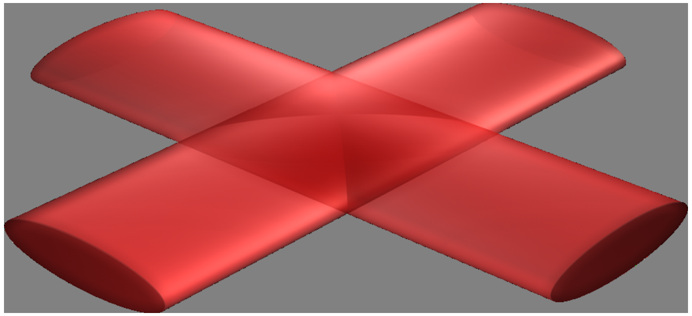


Are AF and Mott phases essential for superconductivity?

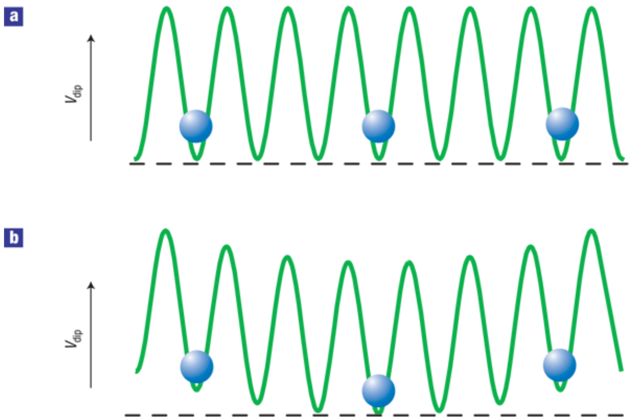
Claim: cold atoms $\rightsquigarrow$ quantum simulators

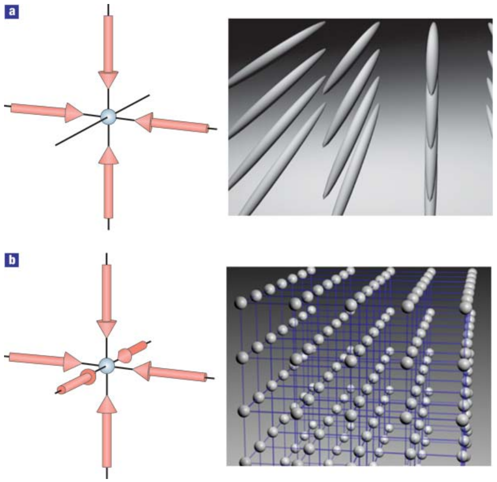
Correlated ultracold quantum gases: traps and optical lattices

Optical dipole trap (2 beams)



Interference ⇝ modulation





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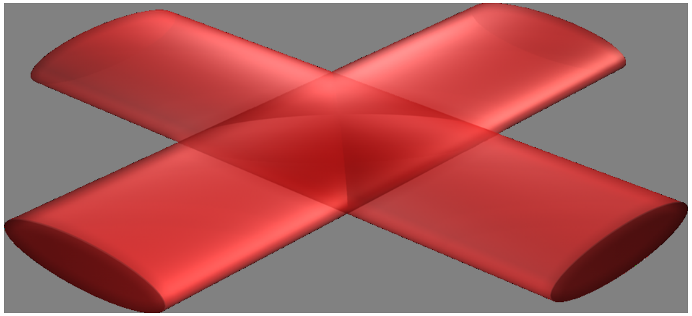

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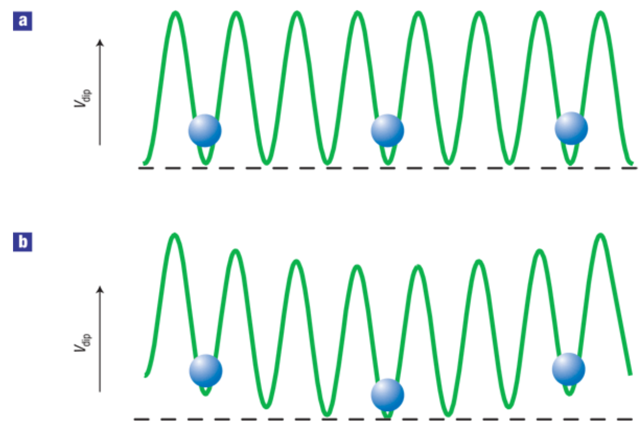
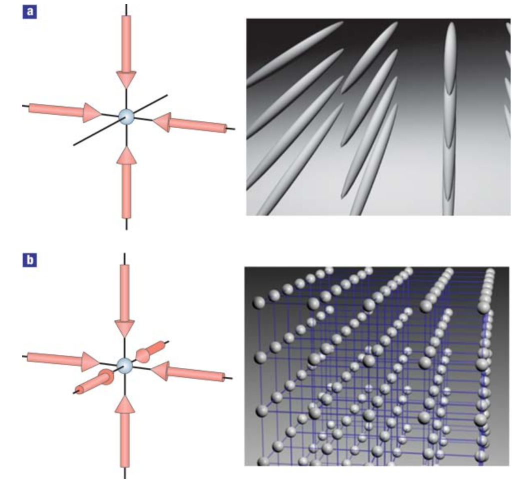
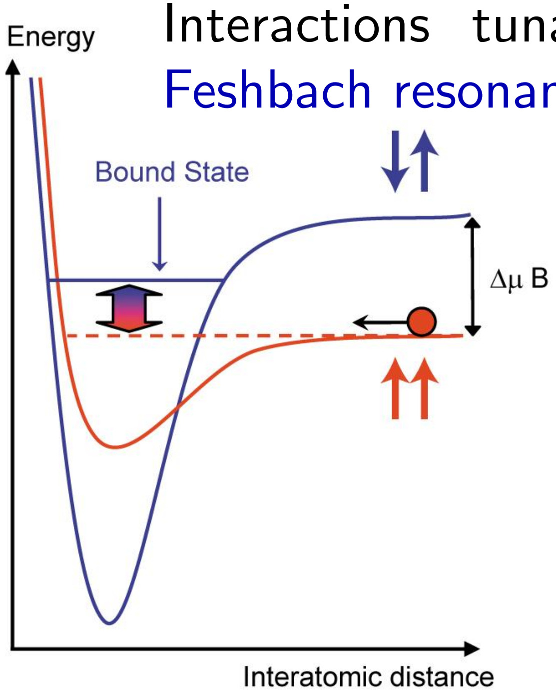




Interactions tunable via Feshbach resonances



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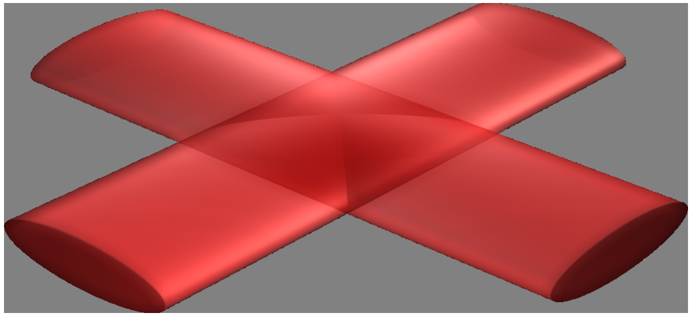

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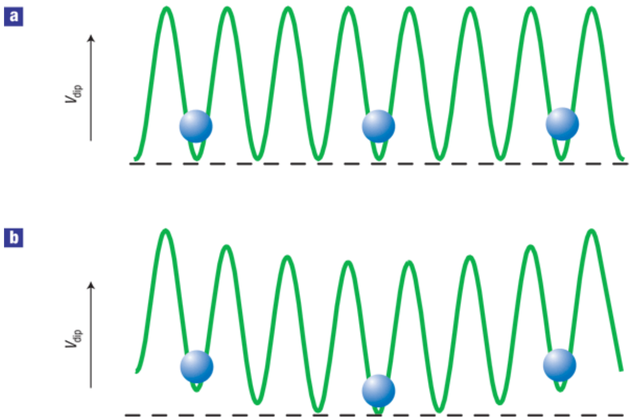

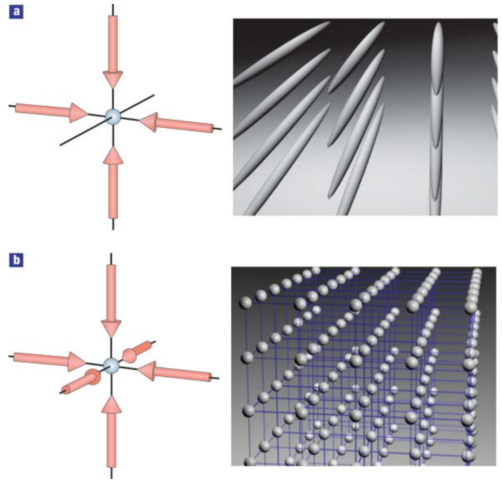

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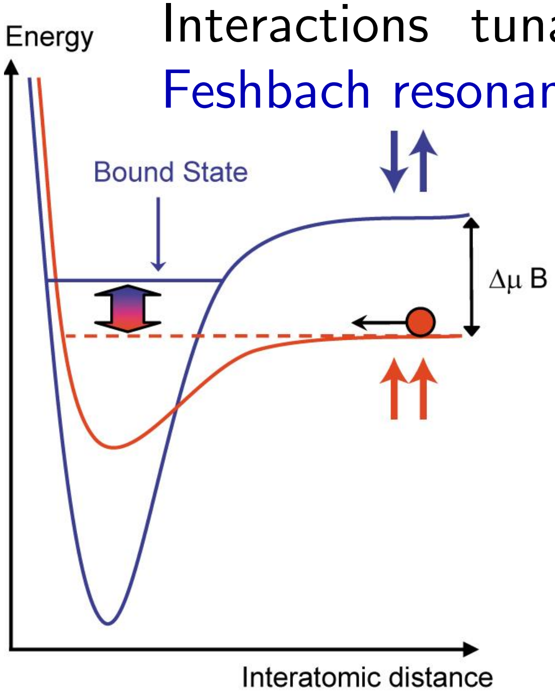
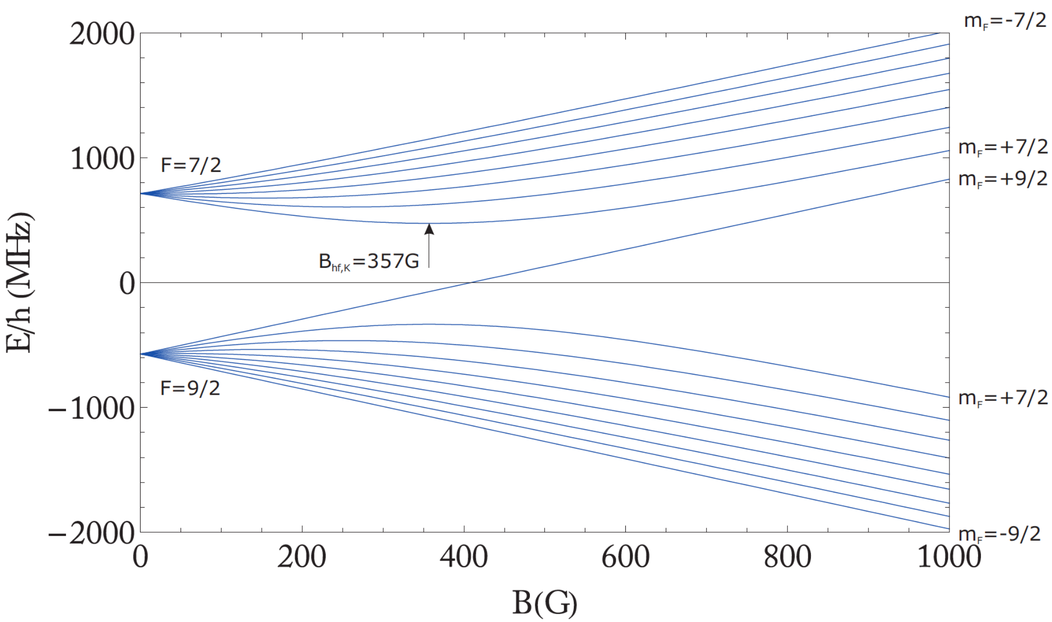


Large multiplets accessible (here ^{40}K)



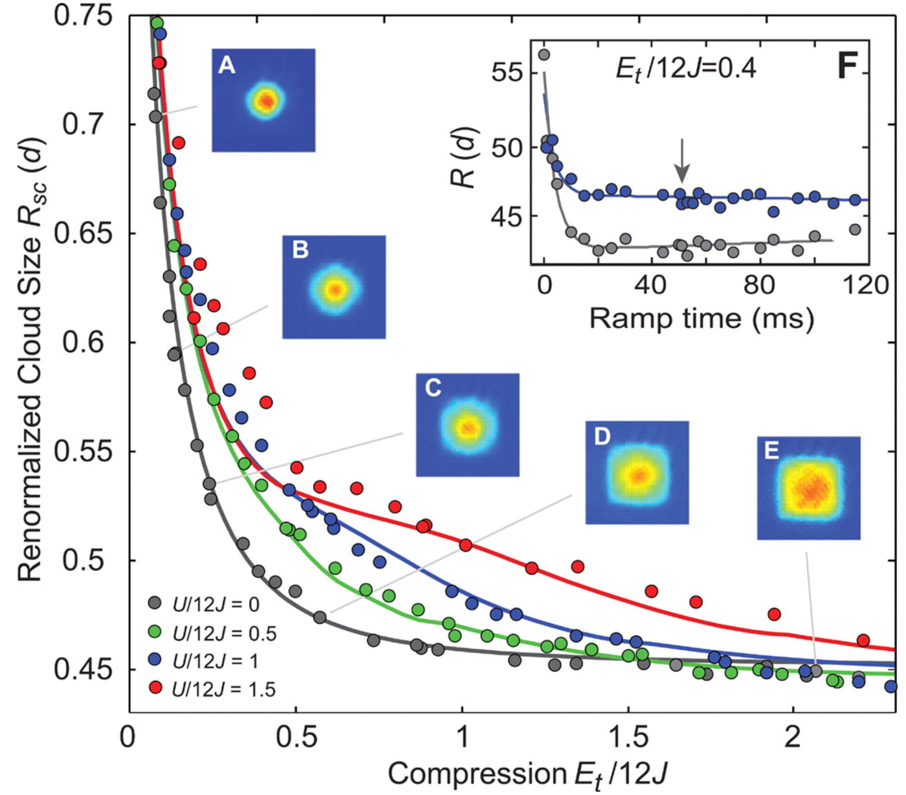
Correlations in ultracold fermions on optical lattices

Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

Detection: cloud diameter vs. trap strength ⇝ incompress. Mott phase

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

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



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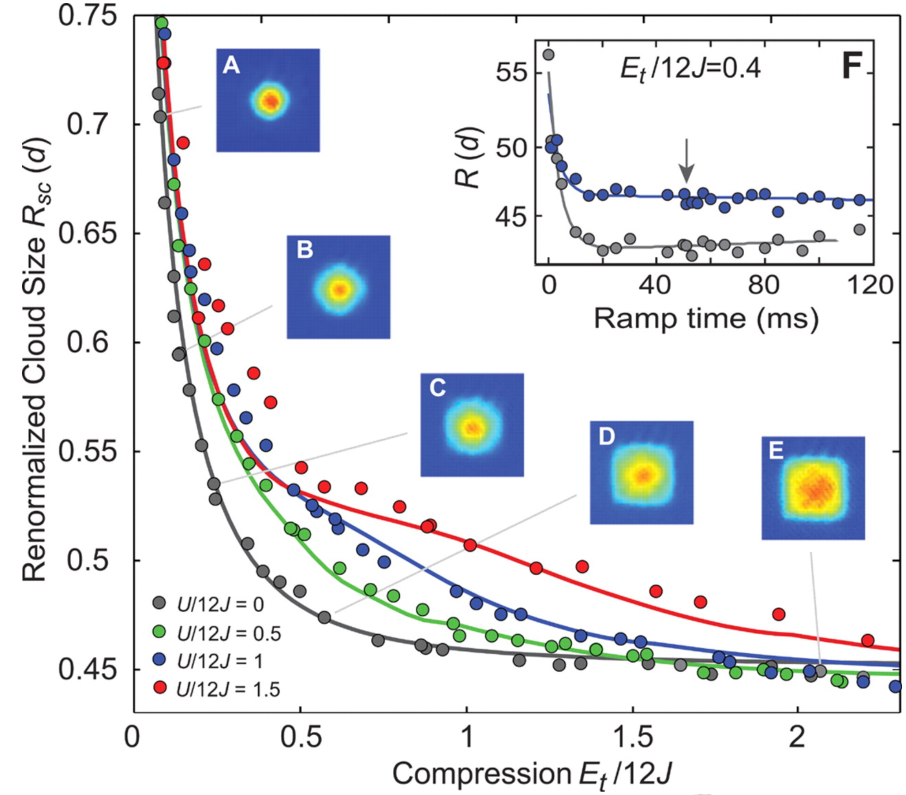
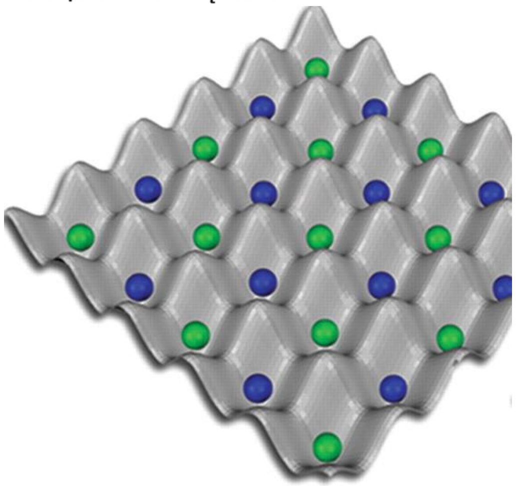


Next grand challenge: AF

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



Problems:

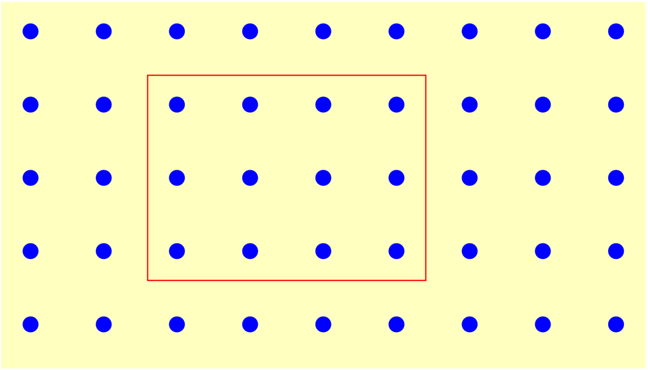
(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of order parameter is not straightforward

Methods: approaches for Hubbard model

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

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



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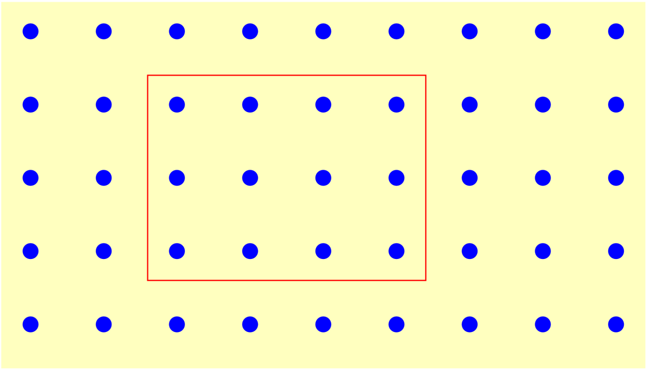
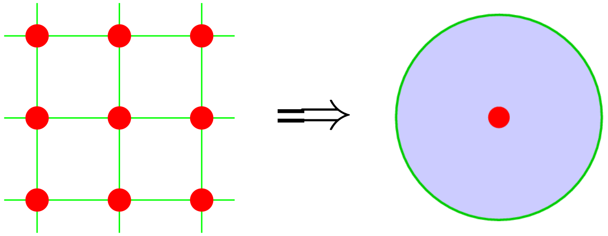


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

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

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

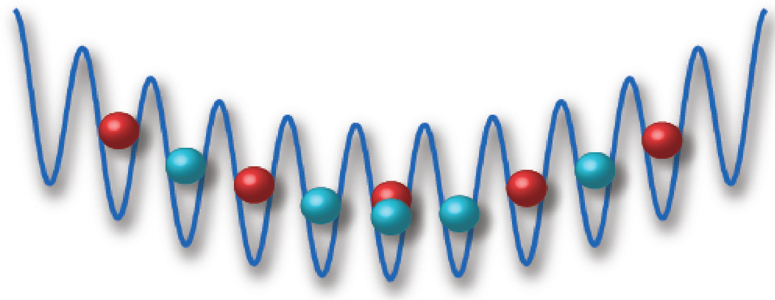
+/− exact for coordination $Z \to \infty$



DMFT impurity solver:
- QMC
- ED, DMRG, NRG ...

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

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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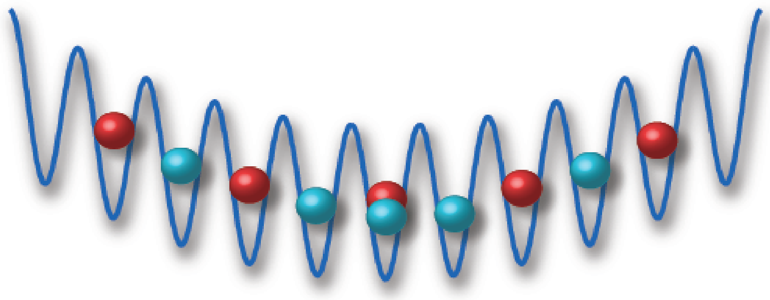

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⇝ N single-site impurities, coupled by real-space lattice Dyson equation:

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

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

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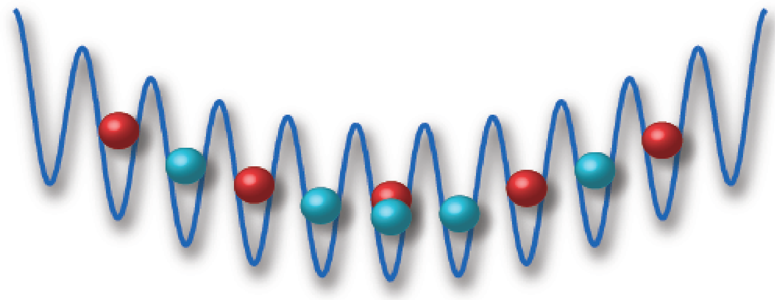

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Note: impurity problems are site-parallel,
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Previous implementations: RDMFT+NRG (problematic at elevated T)

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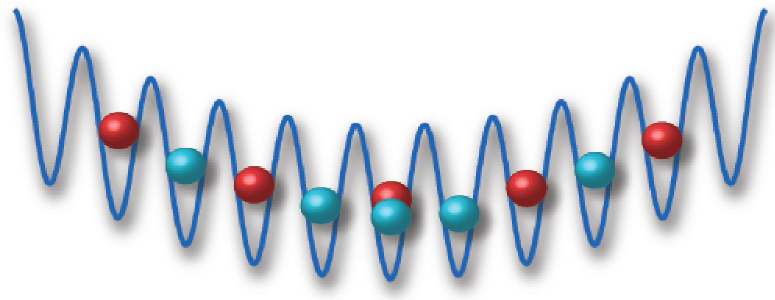

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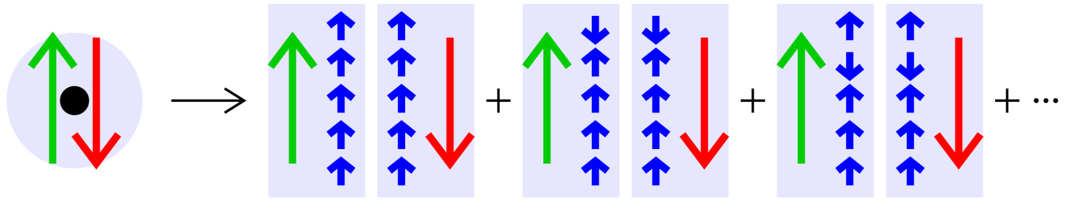
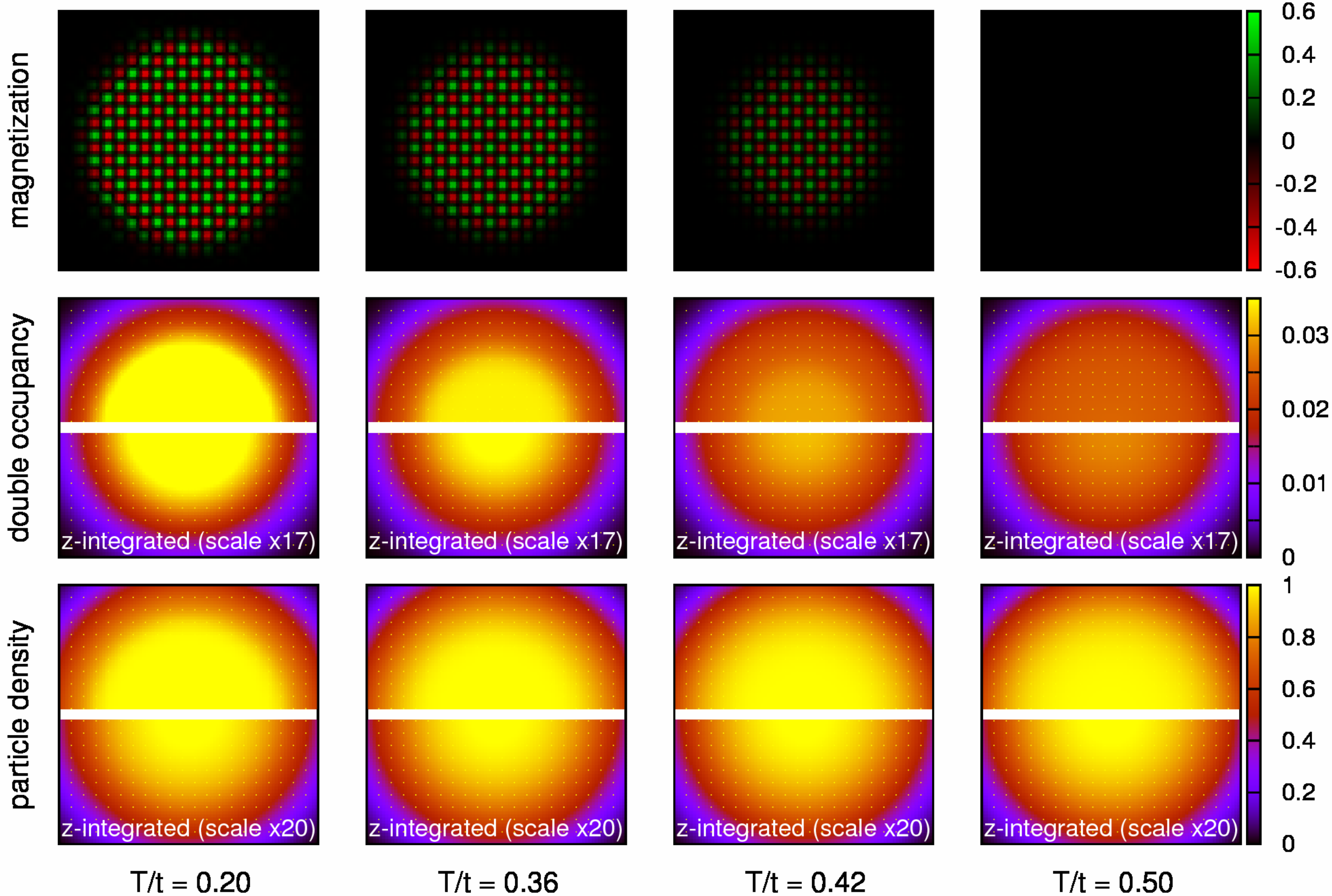
Here: QMC (cost $\propto T^{-3}$)
"slab method" + pbc
$\sim$ exact for $\mathcal{O}(10^5)$ atoms



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



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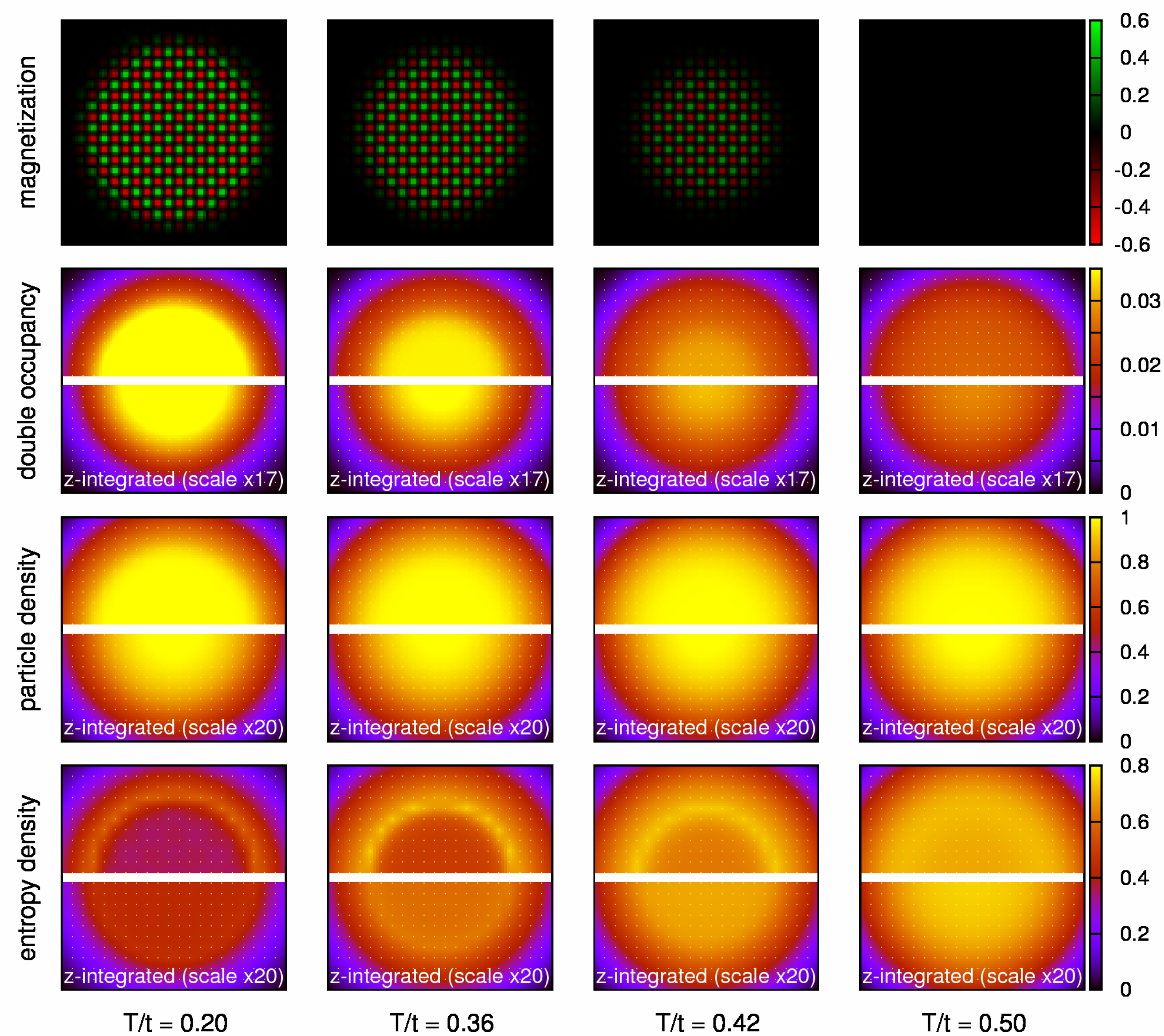


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

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

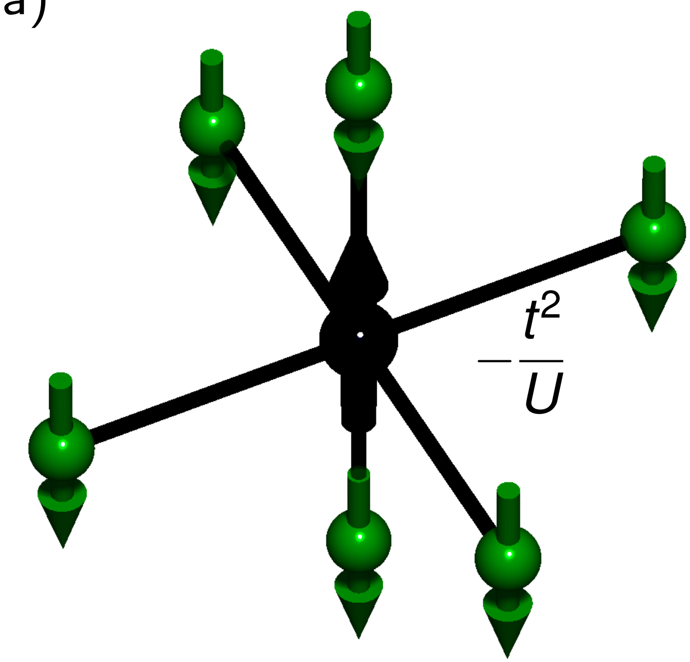
Entropy

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

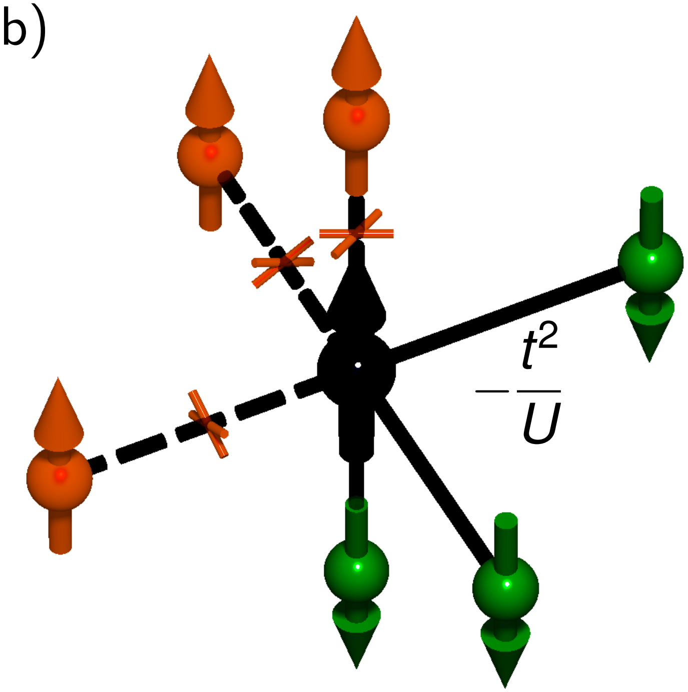
Enhanced double occupancy: a signature of AF order

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

(a)



(b)



AF state:

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

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

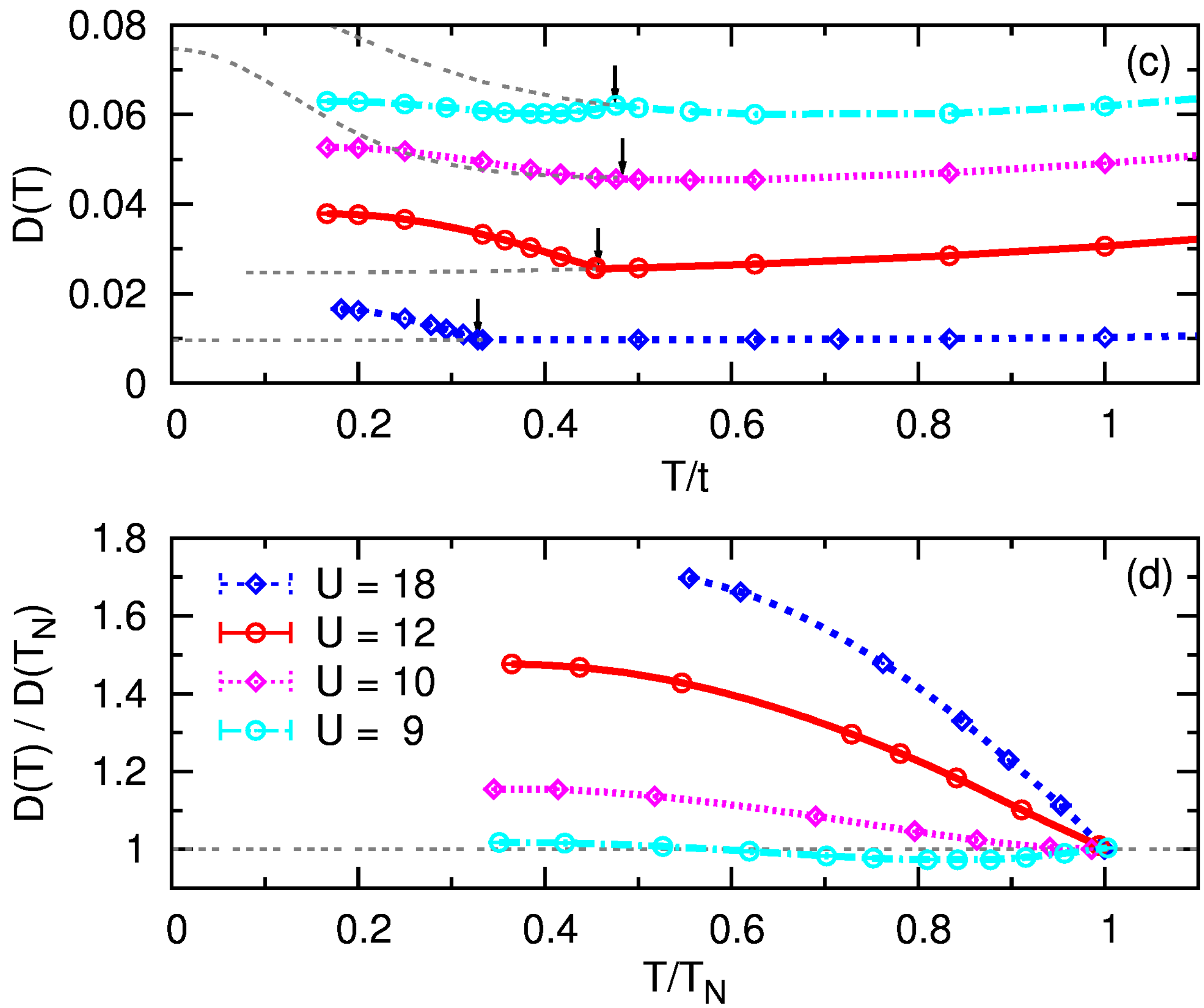
Paramagnetic state:

1/2 of the neighboring sites
are forbidden for hopping

$$E_p = -\frac{Z\,t^2}{2U}$$

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

DMFT-QMC estimates of D at half filling



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

arrows: Néel temperatures

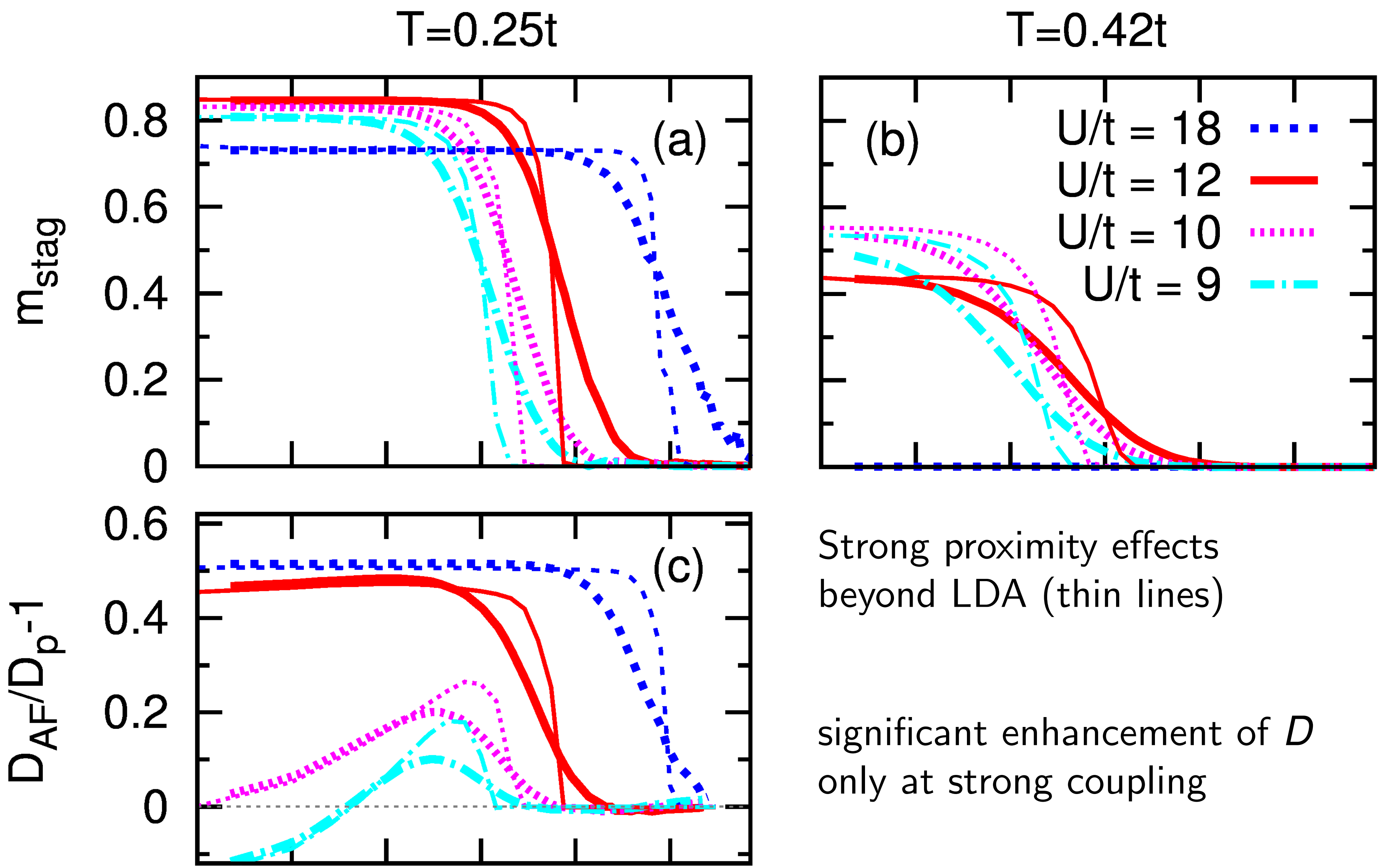
thin lines: metastable paramagnetic phase.

Data scaled to values of critical point:

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

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

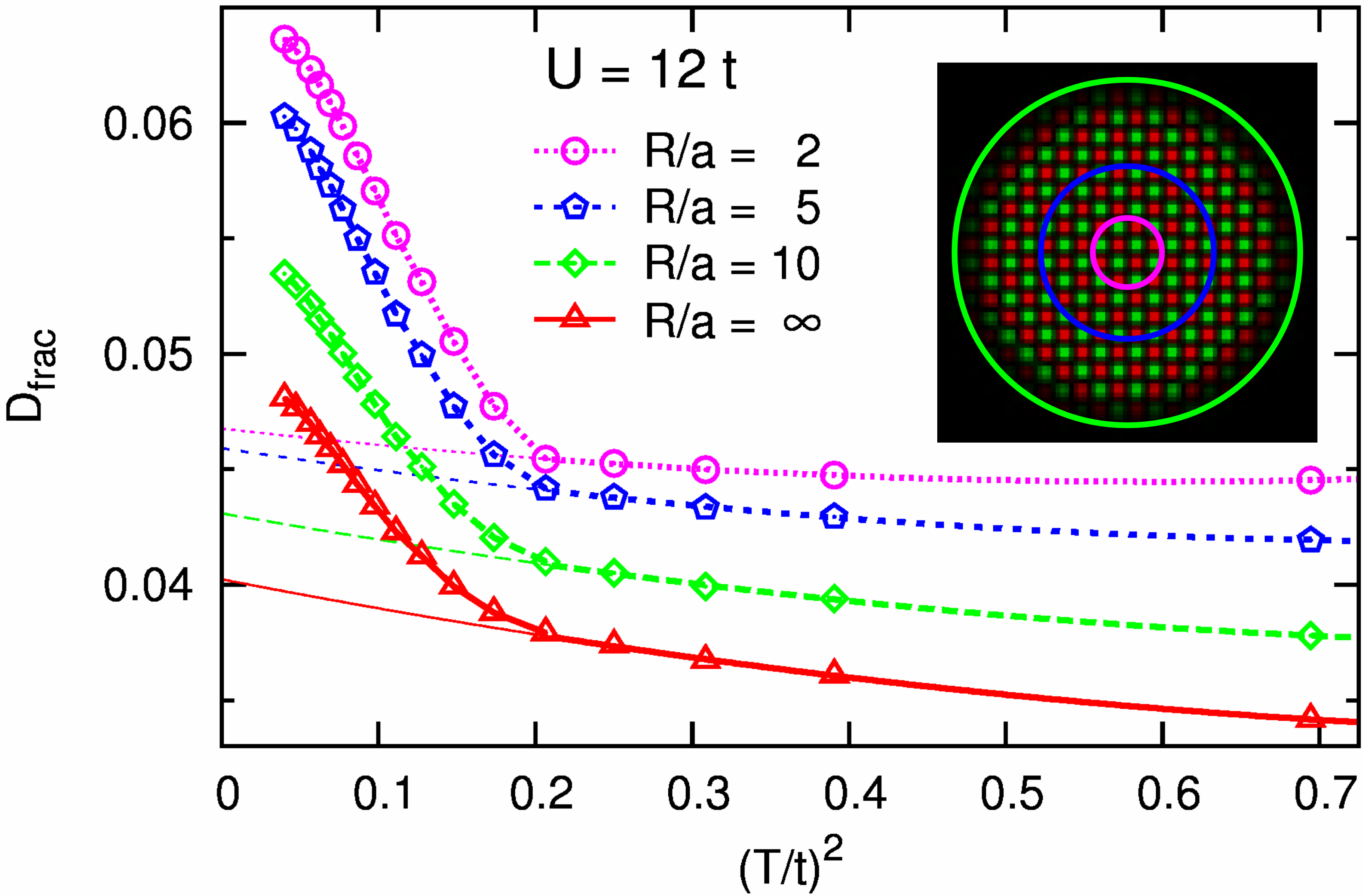
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



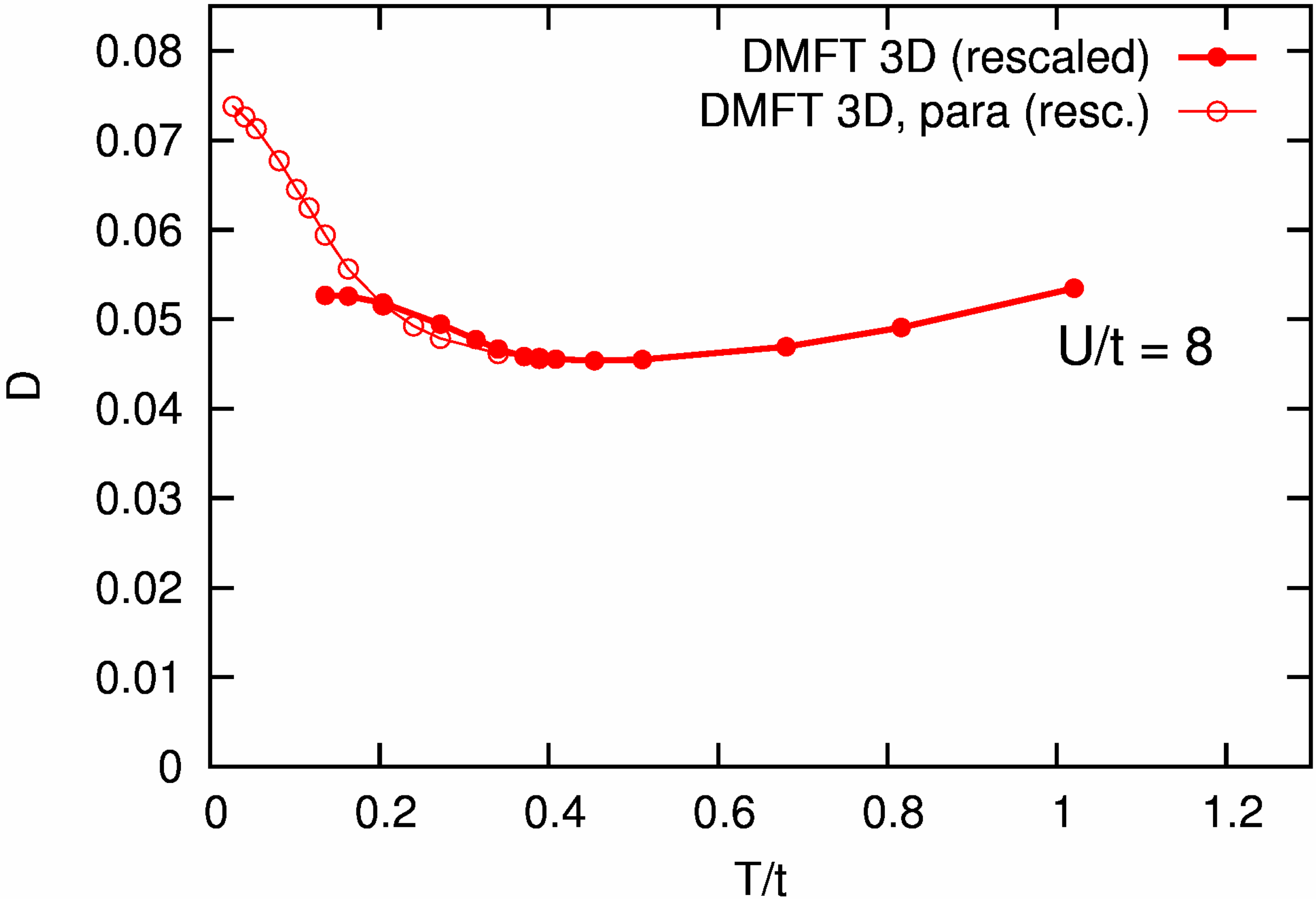
Strong proximity effects beyond LDA (thin lines)

significant enhancement of D only at strong coupling

Néel transition visible in integrated quantities? Yes!



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



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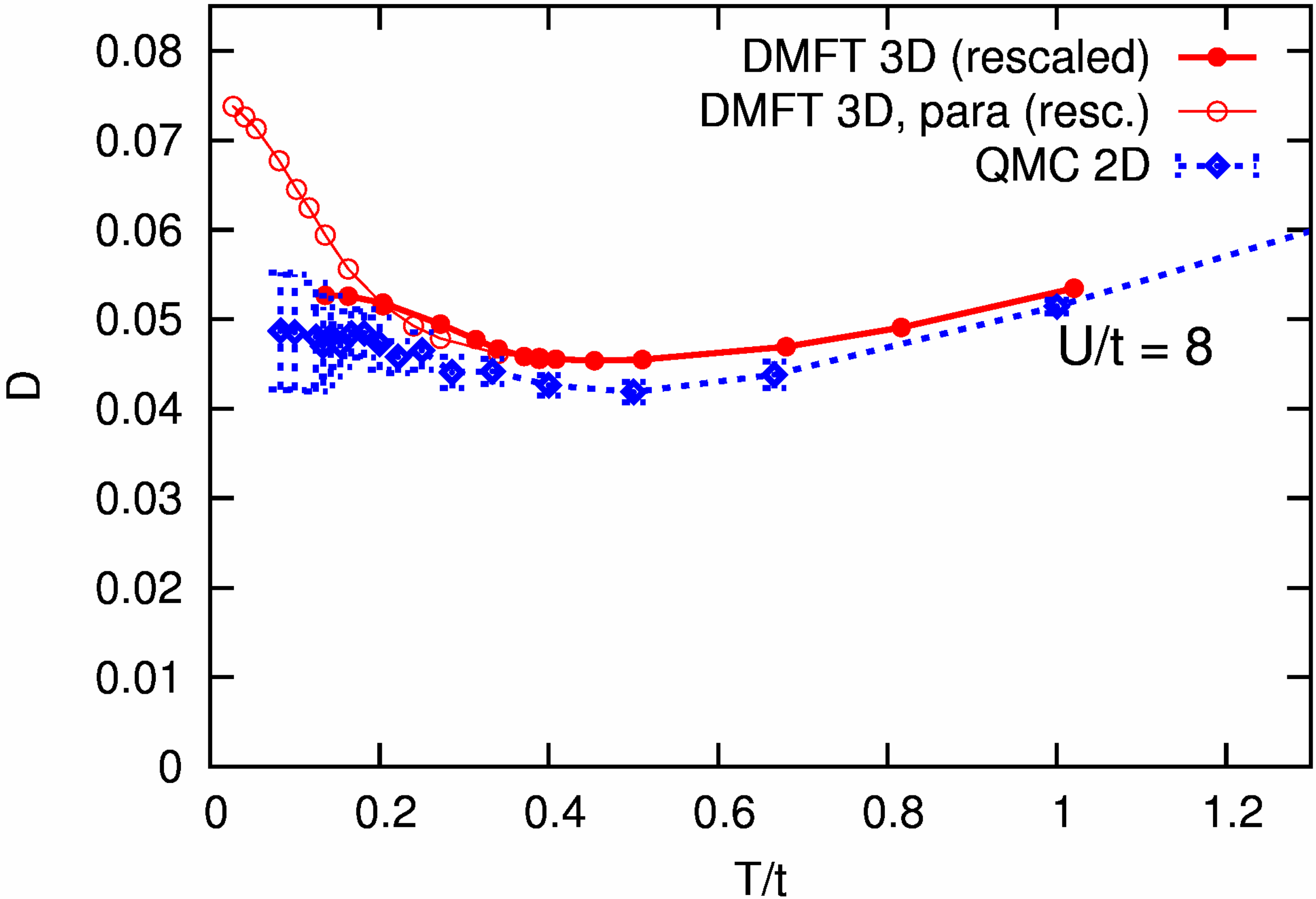

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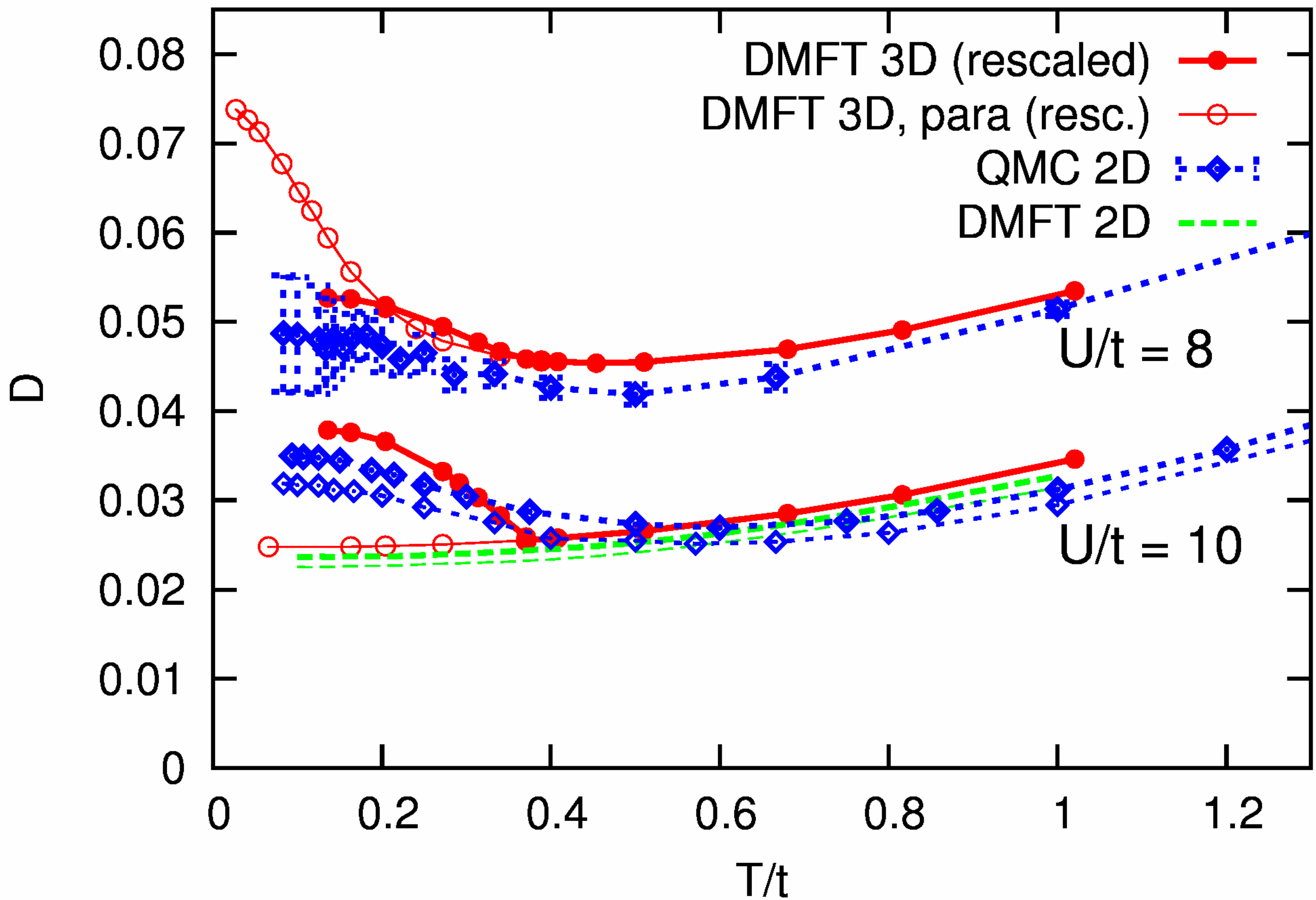

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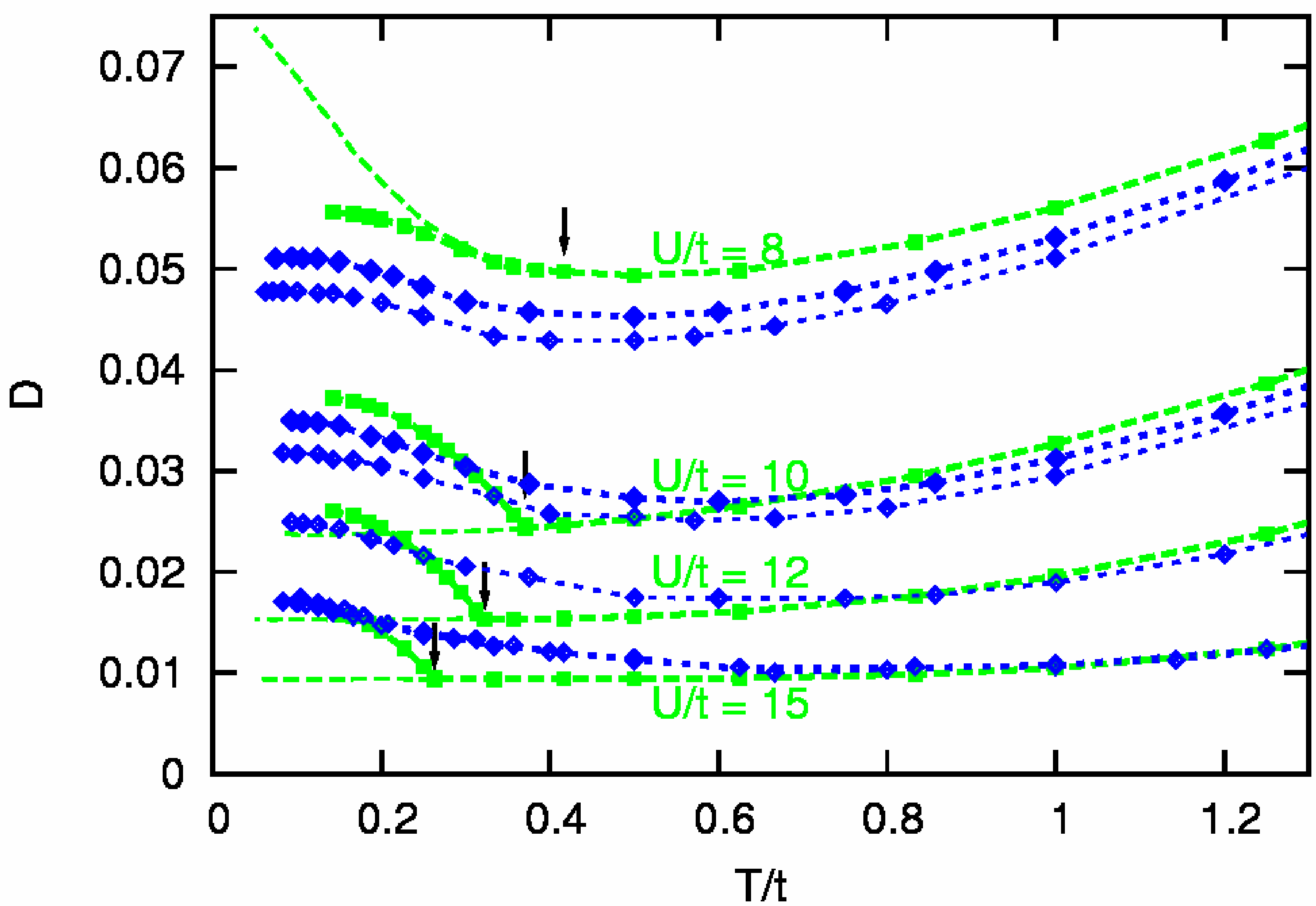

QMC data by Scalettar and Paiva

Summary

Real-space DMFT study of antiferromagnetism

Efficient and flexible RDMFT-QMC code, slab approximation

[E. V. Gorelik, N. Blümer, arXiv:1006.2716]

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]

Thanks to: DFG (TR49)

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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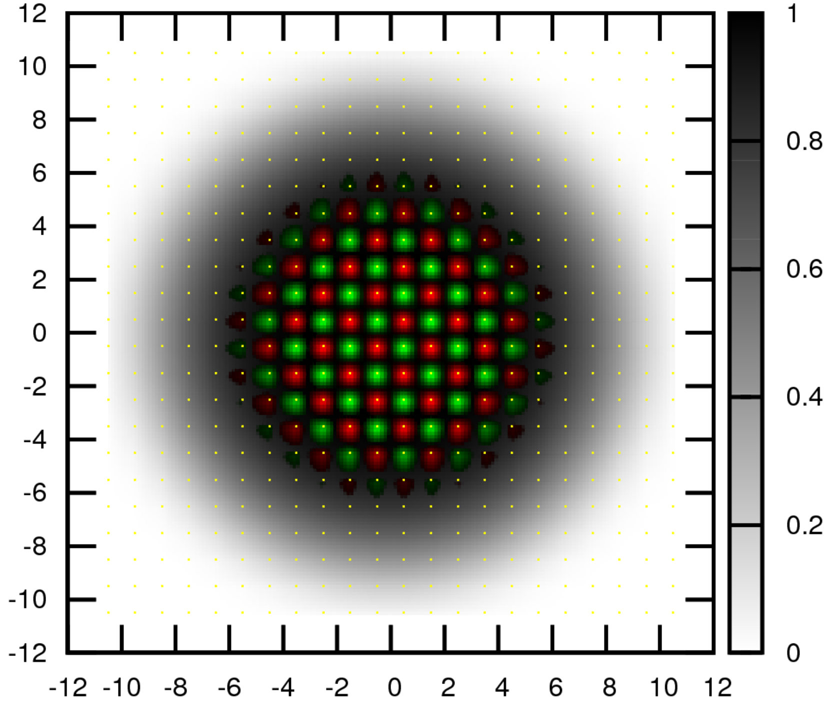

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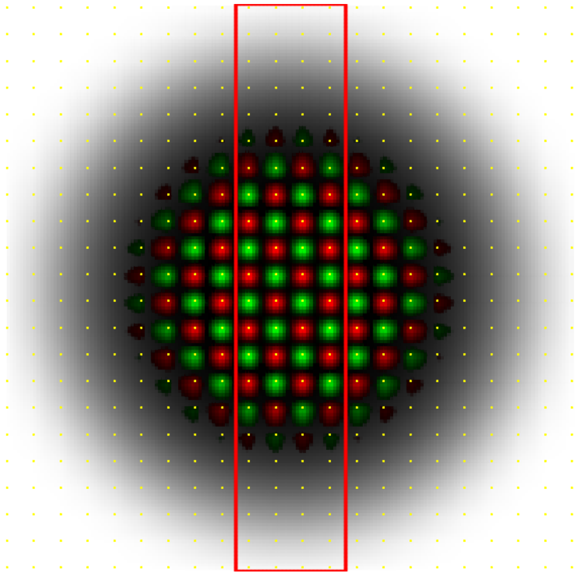

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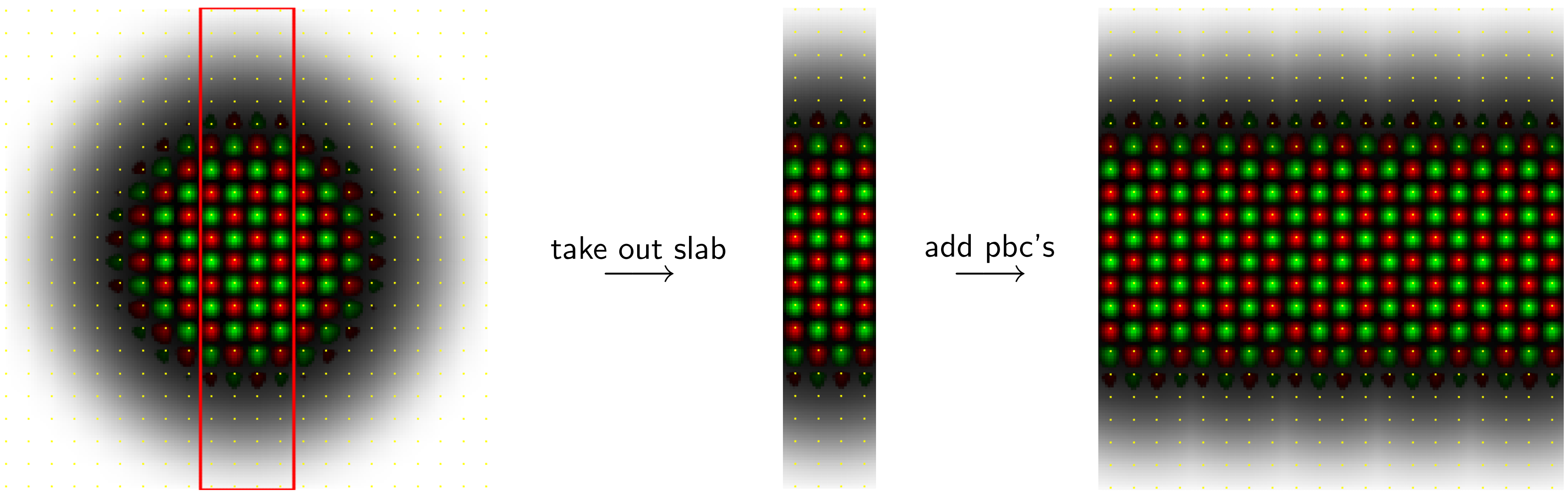
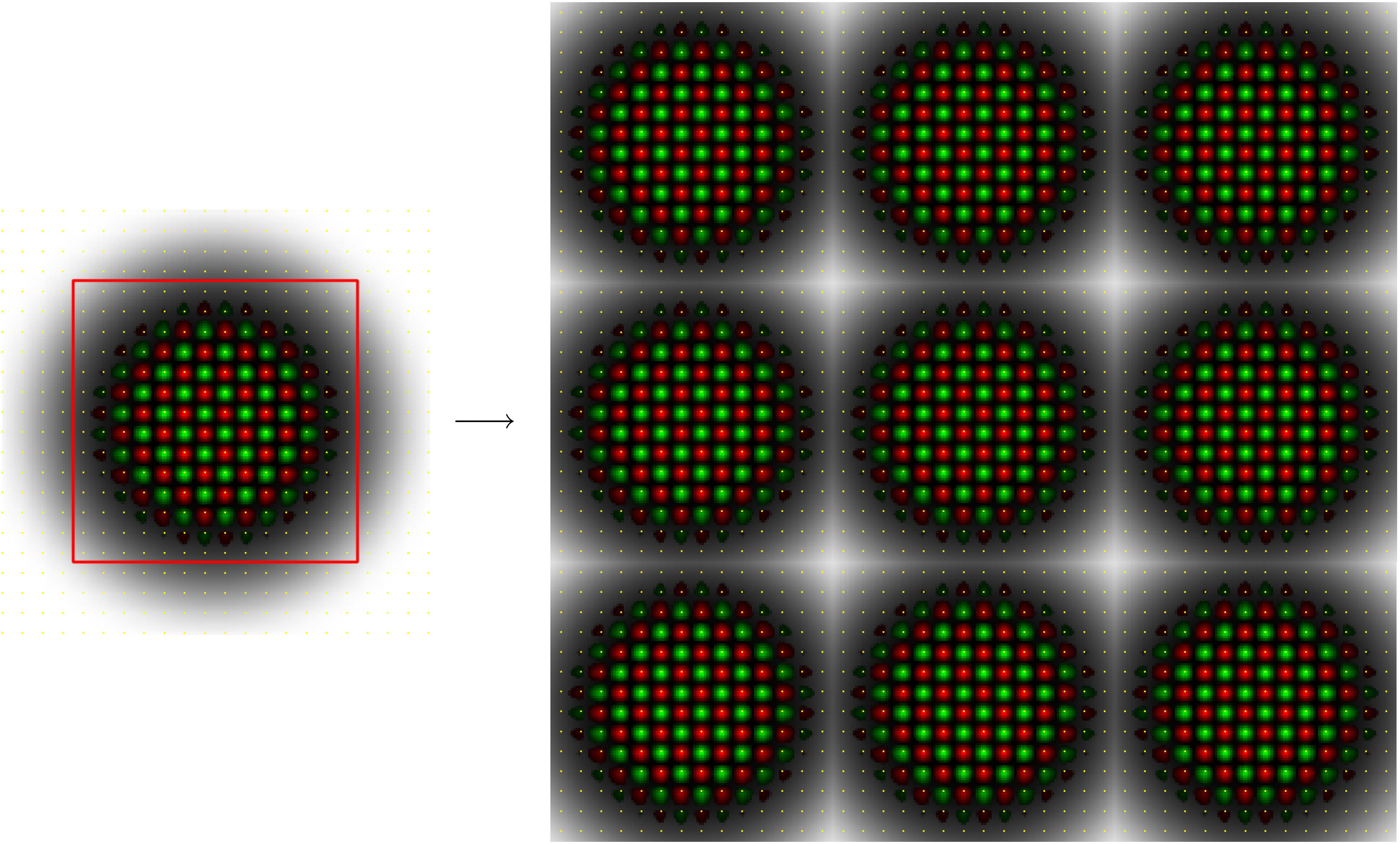


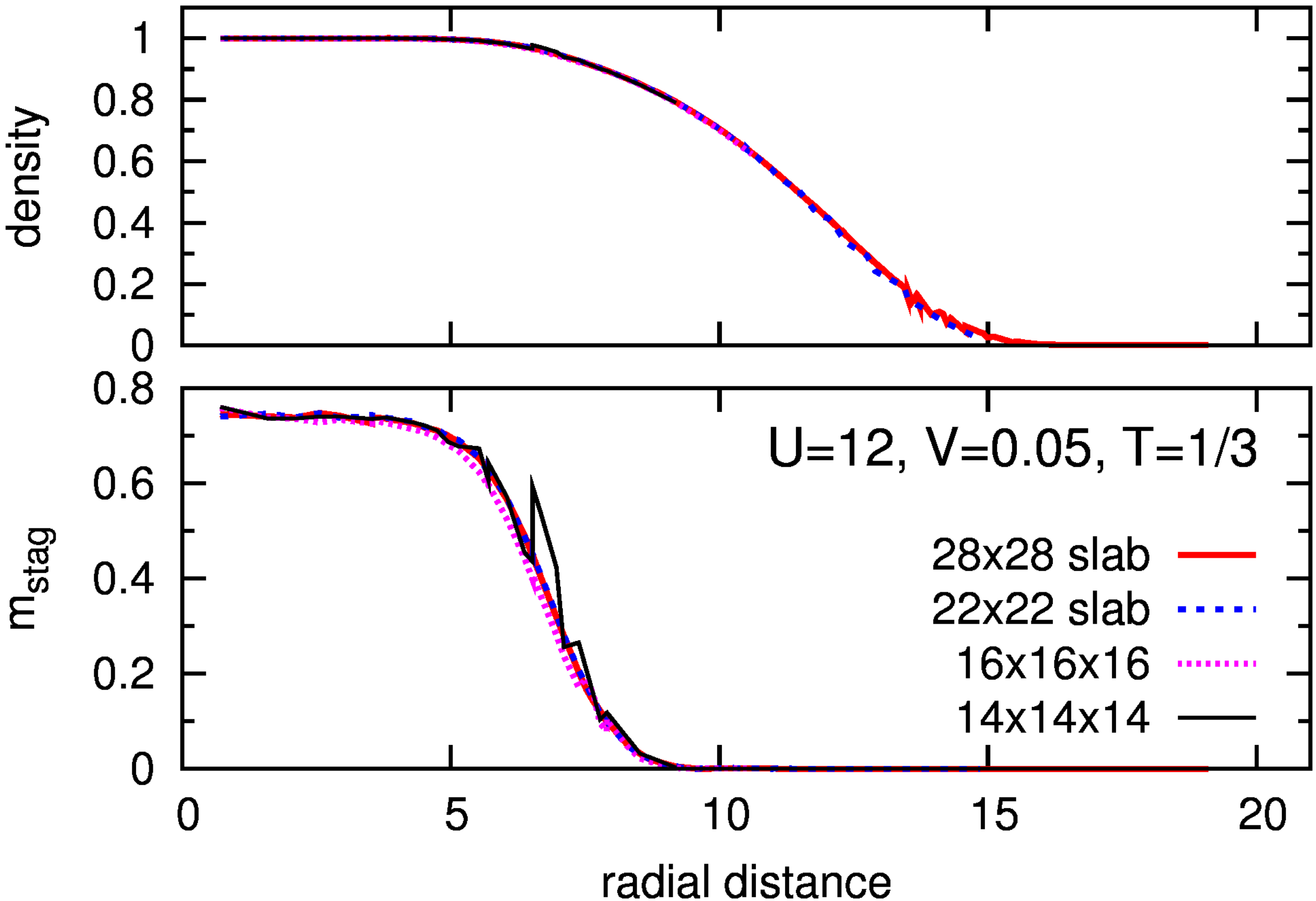
In practice: cylindrical potential (equivalent layers)

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!