Double occupancy as a universal probe for antiferromagnetic correlations and entropy in cold fermions on optical lattices

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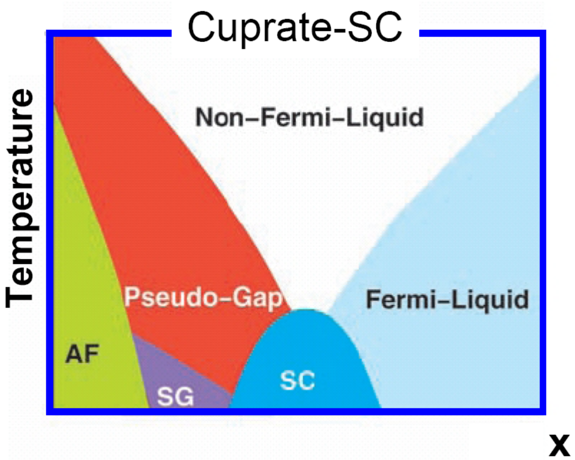
Transregional Collaborative Research Centre SFB / TRR 49

Condensed matter systems with variable many-body interactions

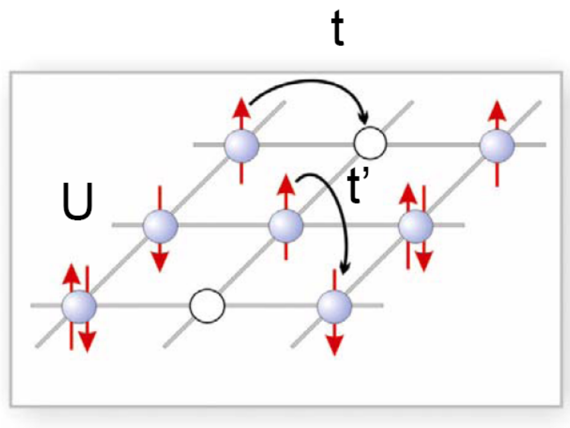
Frankfurt / Kaiserslautern / Mainz

Motivation: Ultracold lattice fermions as quantum simulators?

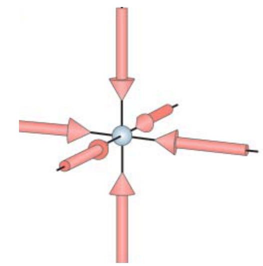
Correlated materials

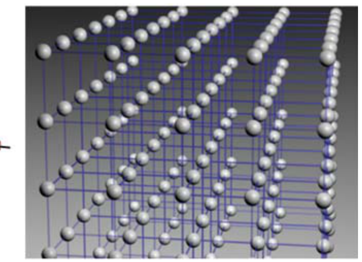


Fermionic Hubbard model



Ultracold fermions on optical lattices





Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures
[Schneider et al, Science **322**, 1520 (2008), Jördens et al., Nature **455**, 204 (2008)]

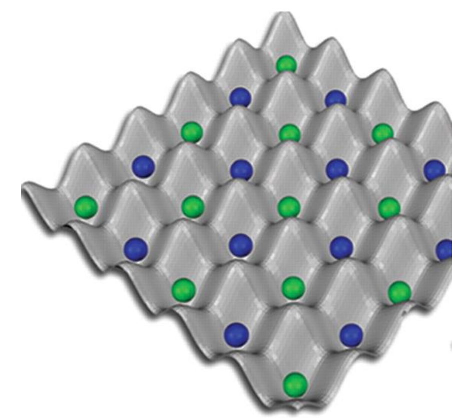
Remaining challenge: antiferromagnetism (staggered order)

Problems:

(i) difficult to reach sufficiently low temperatures/entropies

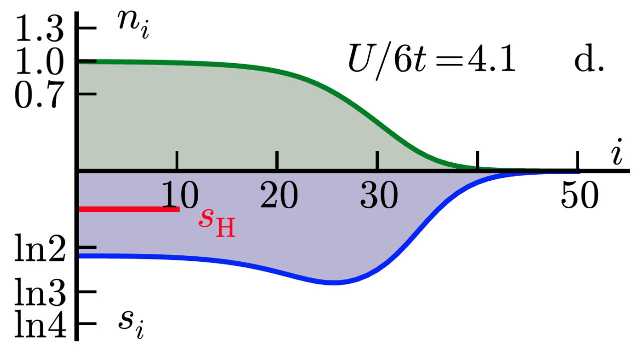
(ii) detection of AF order is not straightforward

(iii) inhomogeneity, time scale for global (spin) equilibrium



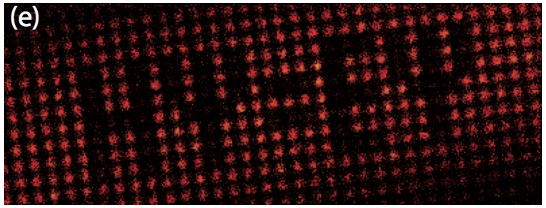
Questions for this talk

- How to detect AF order/correlations?
- Which entropy range is needed?
- How reliable are DMFT and LDA?
- General impact of dimensionality?

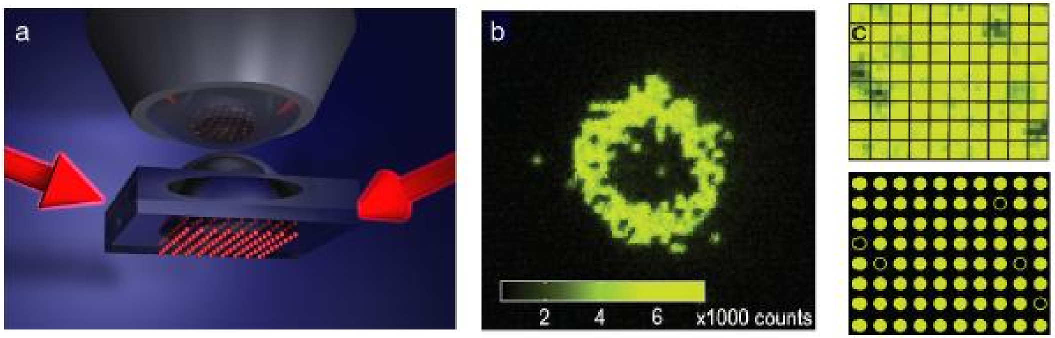


[Jördens et al., PRL **104**, 180401 (2010)]

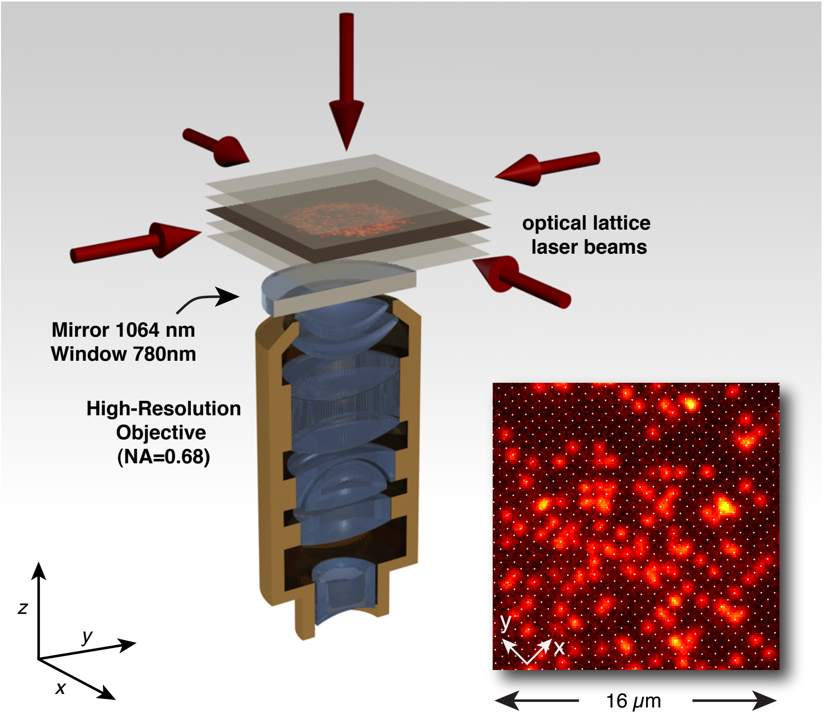
Experimental advantage of 2 dimensions:
single-site resolution (for bosons)



[Würtz et al., PRL **103**, 080404 (2009)]



[Bakr et al., Science **329**, 547 (2010)]



[Sherson et al., Nature **467**, 68 (2010)]

Outline

Motivation: Ultracold lattice fermions as quantum simulators?

Methods: (Real-space) DMFT, slab approximation, QMC

[N. Blümer and E. V. Gorelik, Computer Physics Communications **118**, 115 (2011)]

Results: Néel transition of lattice fermions in a harmonic trap

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

Effect of nonlocal correlations? Comparisons with direct QMC + BA

[E. V. Gorelik, T. Paiva, R. Scalettar, A. Klümper, N. Blümer, arXiv:1105.3356]

Summary and outlook

Collaborators

Postdoc

Elena Gorelik
Univ. Mainz

Real-space DMFT collaboration

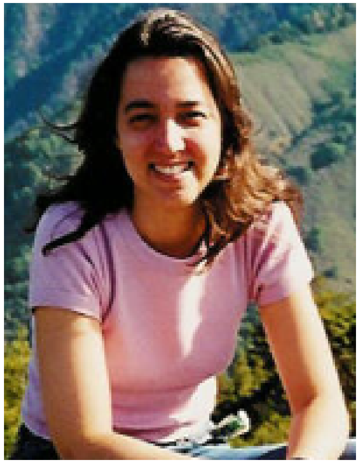
[Gorelik et al., PRL **105**, 065301 (2010)]

Walter Hofstetter
Univ. Frankfurt

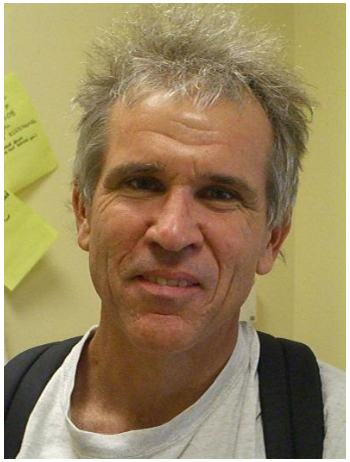
Irakli Titvinidze
Univ. Hamburg

Michiel Snoek
Univ. Amsterdam

Andreas Klümper
Univ. Wuppertal



Thereza Paiva
Rio de Janeiro



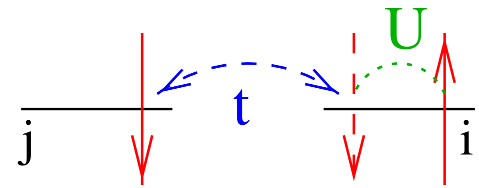
Richard Scalettar
UC Davis

AF in finite dimensions

[Gorelik et al., arXiv:1105.3356]

Methods: Approaches for Hubbard-type models

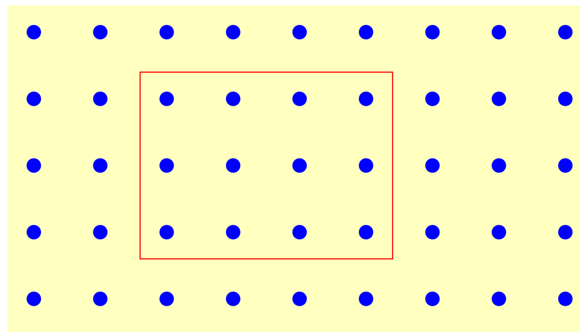
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



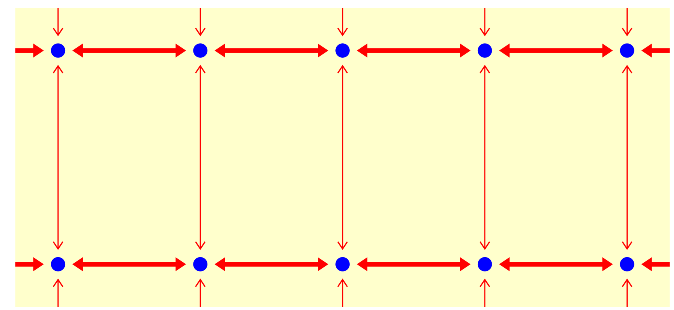
Perturbation theory

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

finite clusters: ED, QMC



$d \to 1$: Bethe ansatz, DMRG

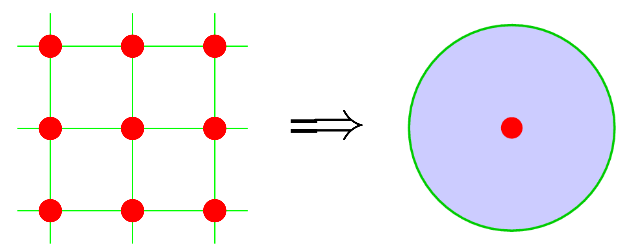


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

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

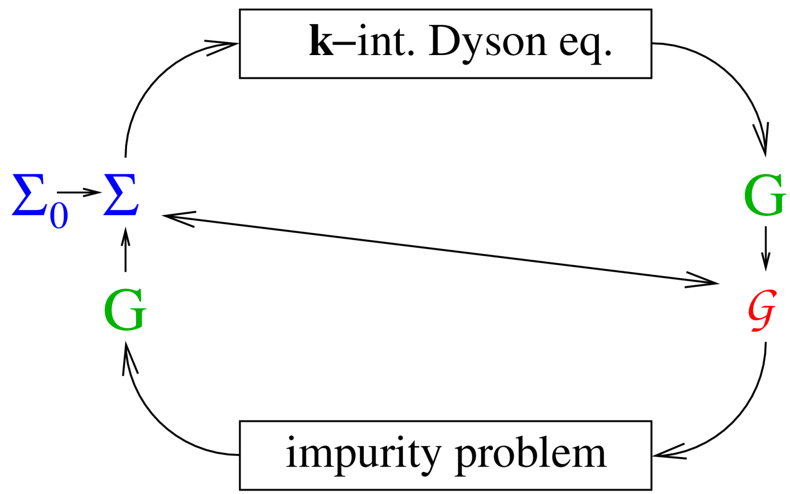
+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit

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



Iterative solution of DMFT equations

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

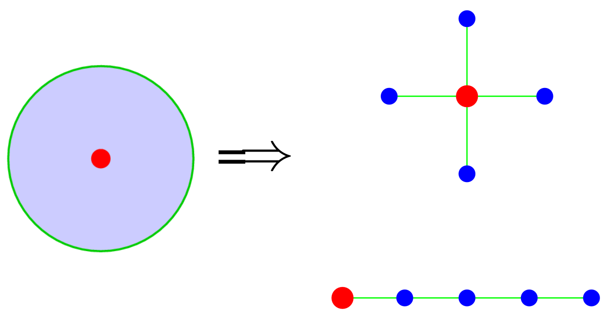


$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu\boldsymbol{k}}$

$\longleftarrow$ local interactions

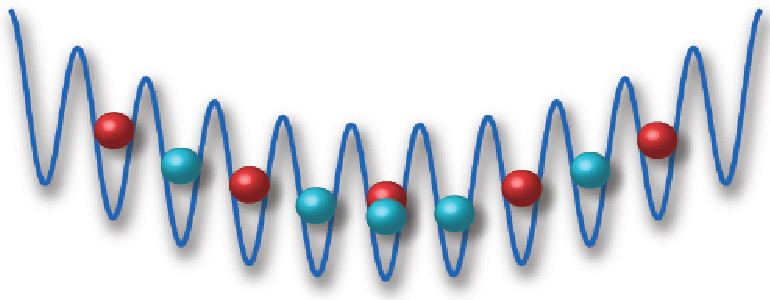
Impurity solver:

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



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

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



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

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

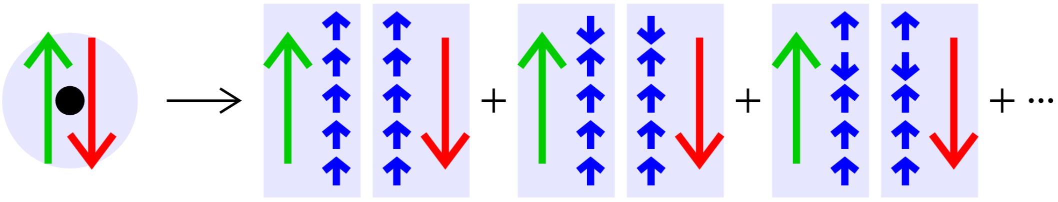
$$\left[G_\sigma(i\omega_n)\right]^{-1}_{ij} = \left(\mu_\sigma + i\omega_n\right)\delta_{ij} - t_{ij} - \left(V_i + \Sigma_{i\sigma}(i\omega_n)\right)\delta_{ij}$$

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

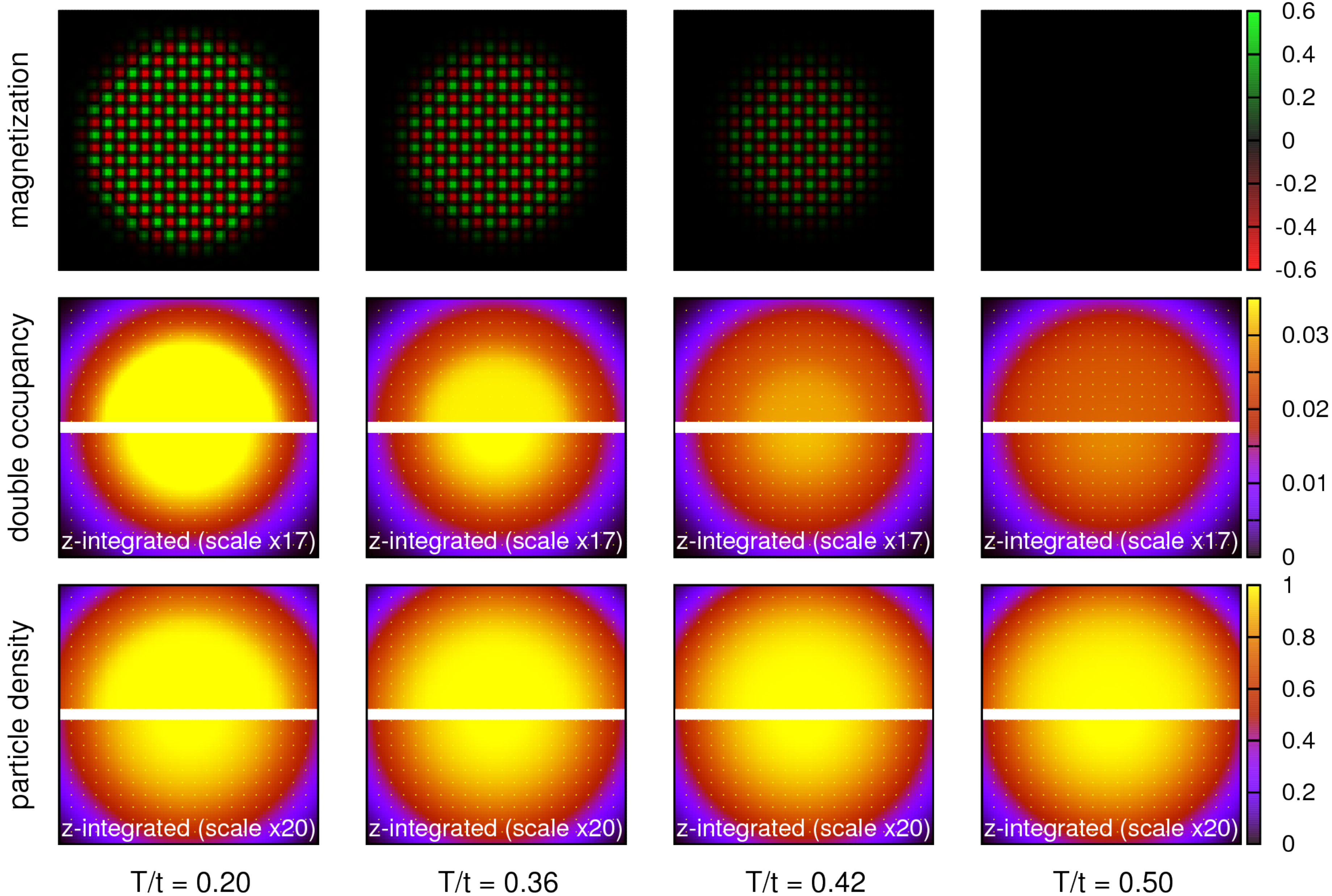
Note: impurity problems are site-parallel,
lattice Dyson equation is frequency-parallel

Previous implementations: RDMFT+NRG (problematic at elevated T)

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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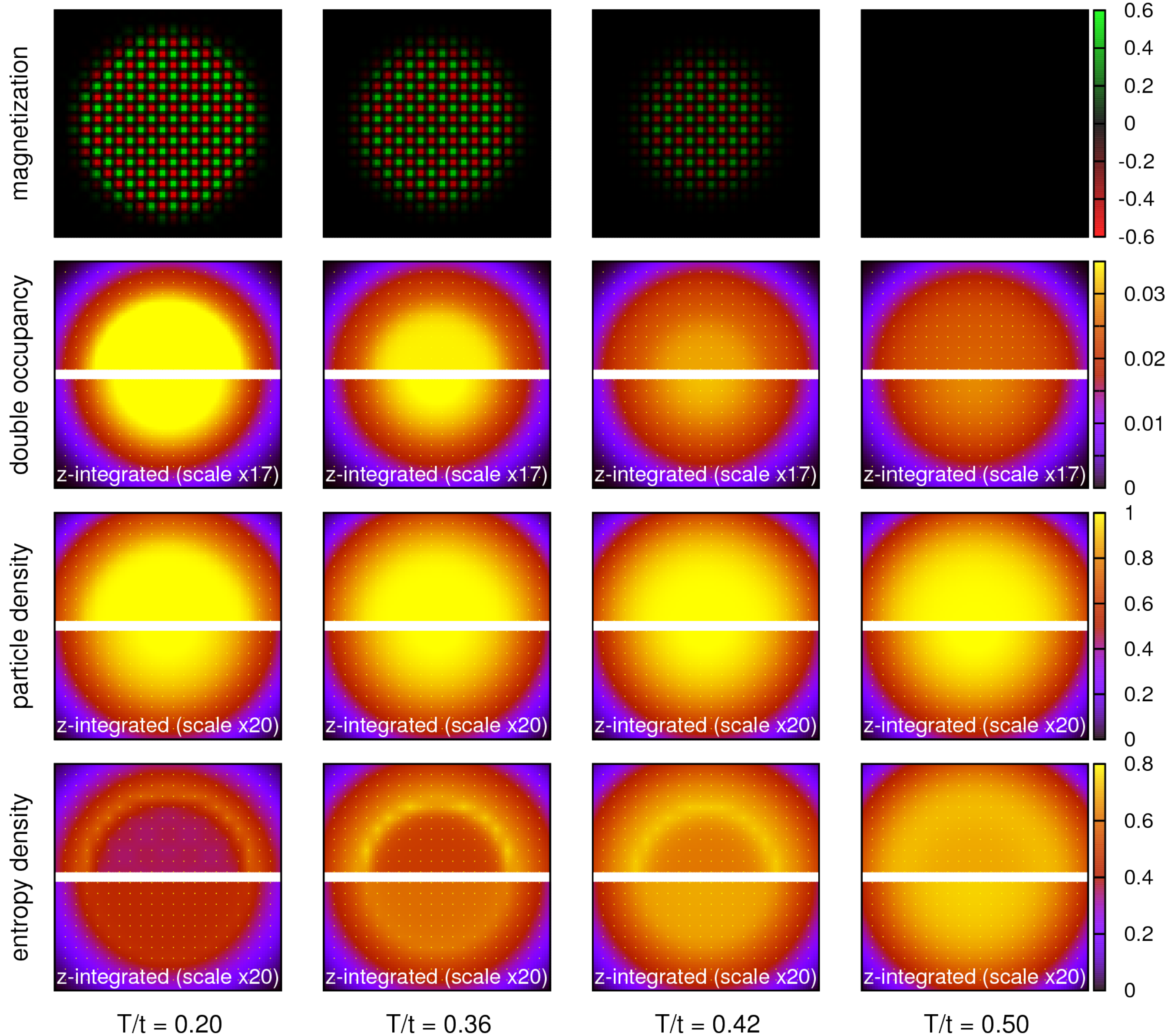


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

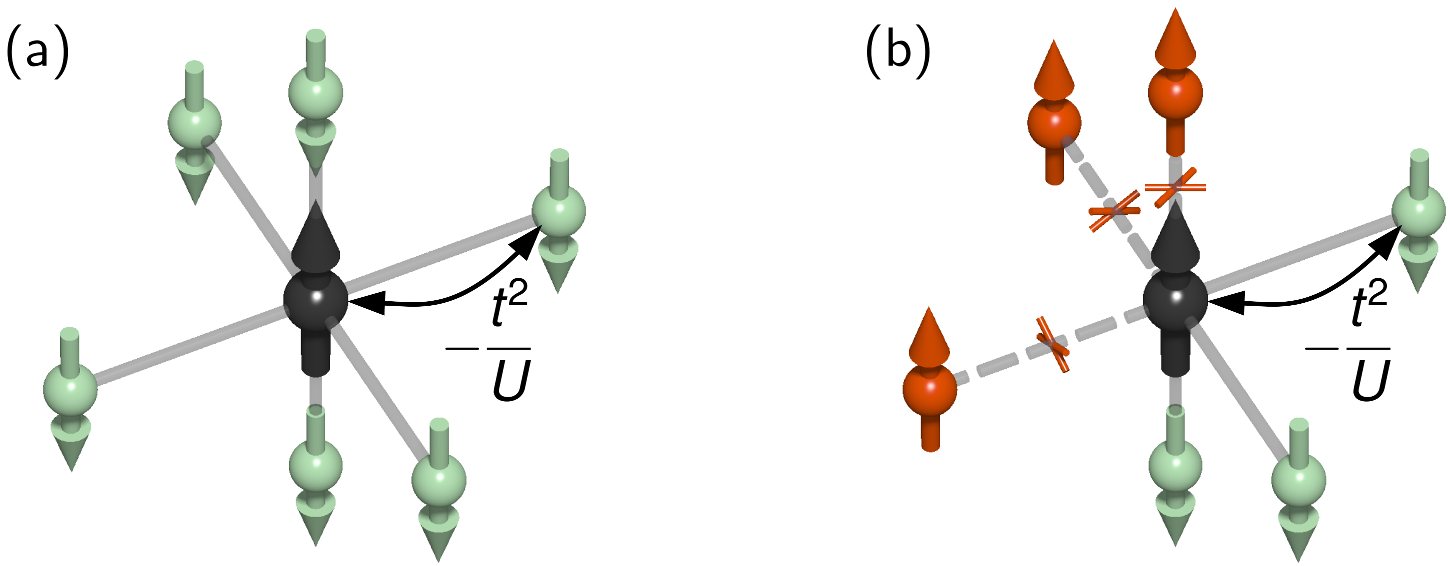
$\sim$ 6000 atoms
(naively $\sim 30^3 = 27000$ sites needed)

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):



AF state: hopping
to all $Z = 6$ neighbors

$$E_{\mathrm{AF}} = -\frac{Zt^2}{U}$$

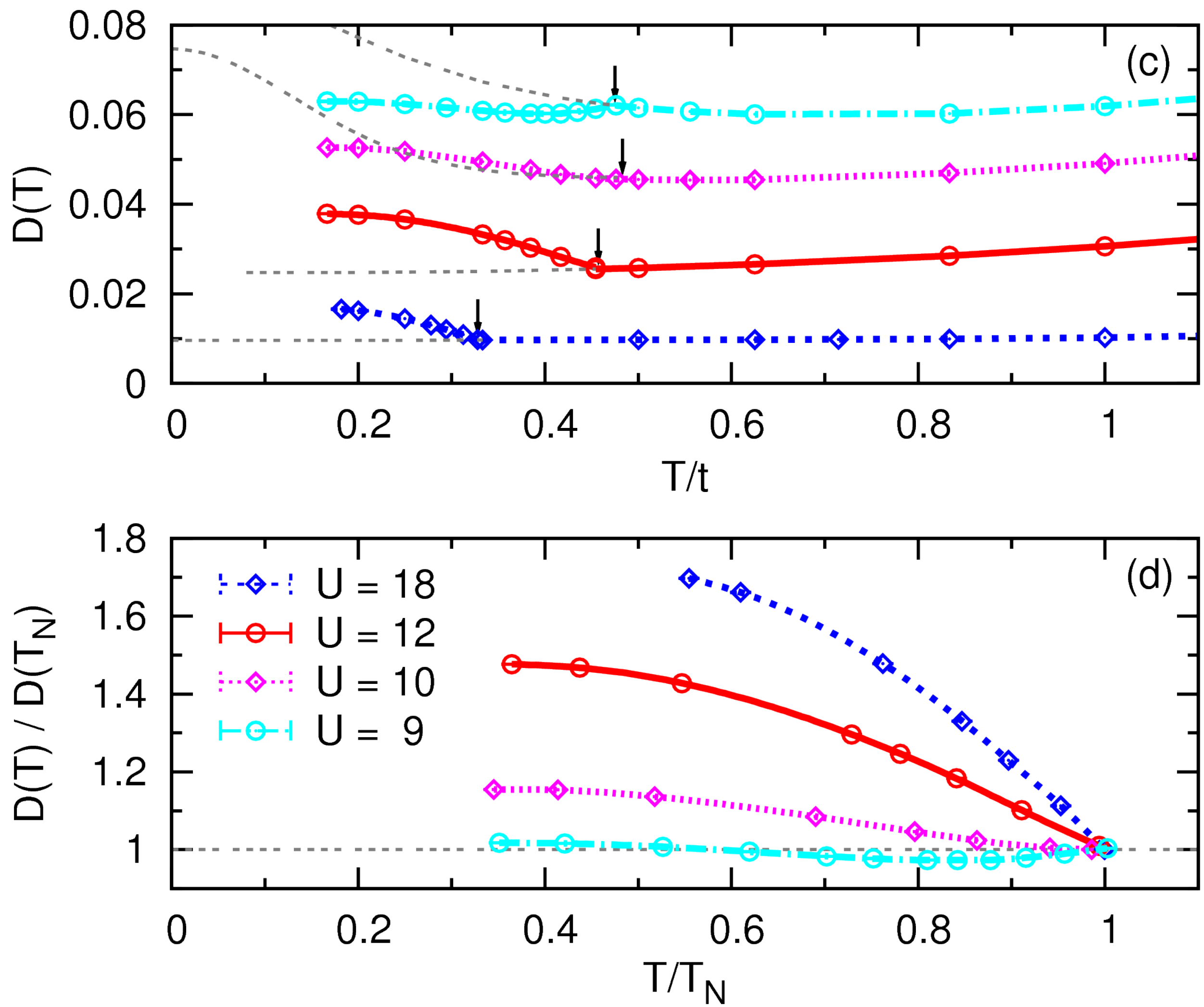
Para/nonmagnetic state:
1/2 of neighbors Pauli forbidden

$$E_{\mathrm{p}} = -\frac{Zt^2}{2U}$$

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

Exact relation for all d [Takahashi, 1977]: $E_0 = -\frac{Zt^2}{2U}\left(1 - \langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle\right) + \mathcal{O}\left(\frac{t^4}{U^3}\right)$

DMFT-QMC estimates of D at half filling



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

arrows: Néel temperatures

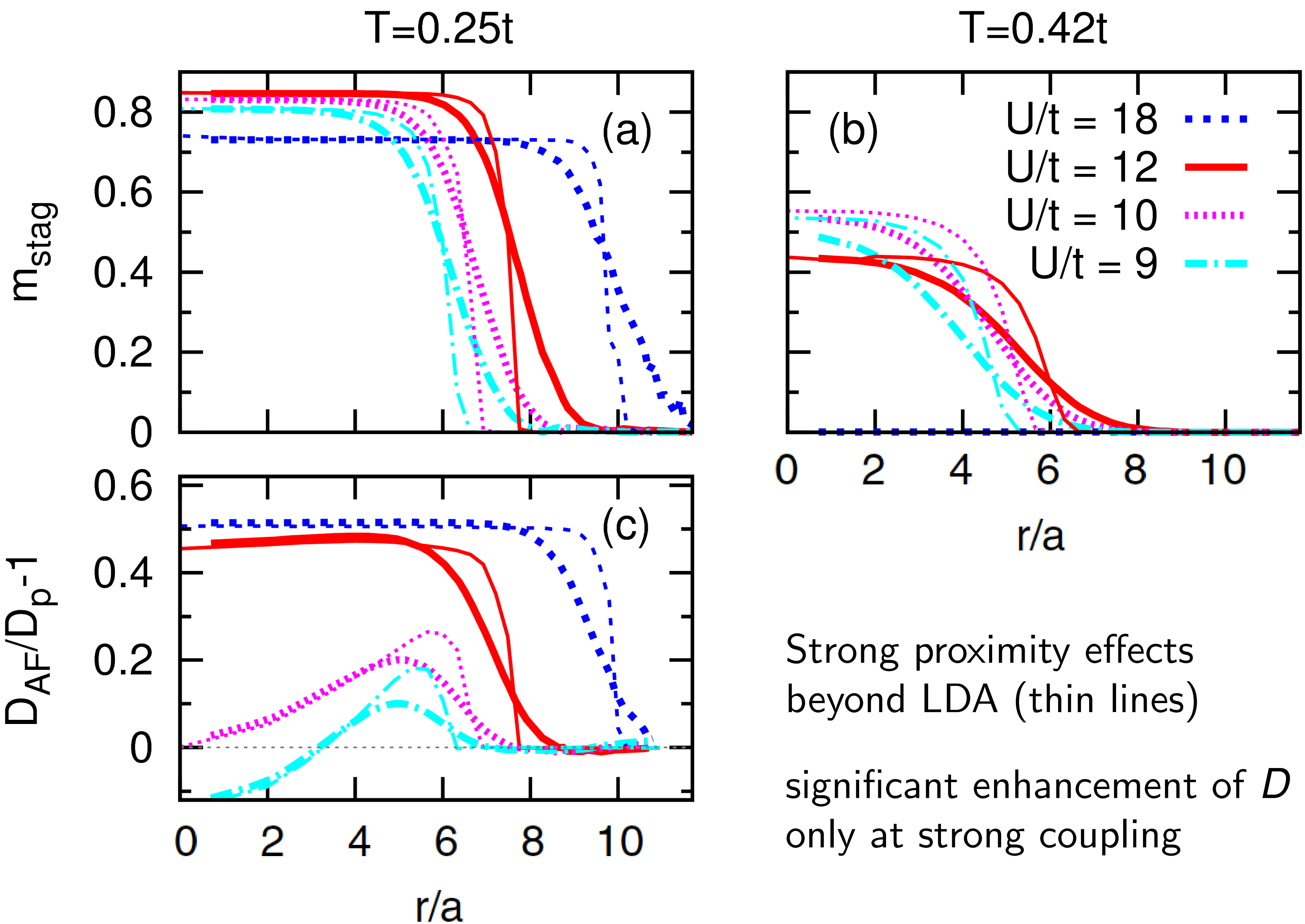
thin lines: metastable paramagnetic phase.

Data scaled to values of critical point:

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

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

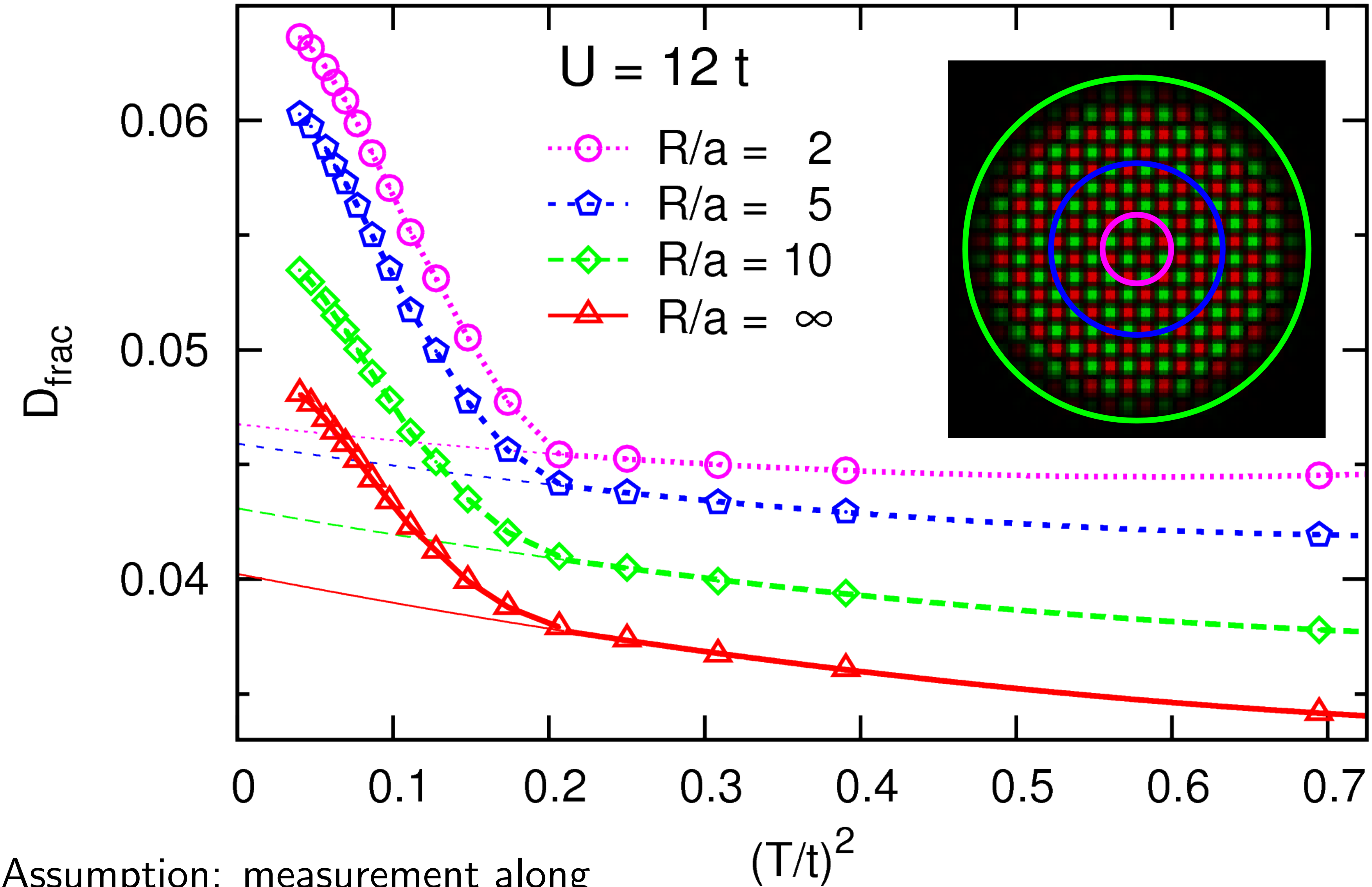
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



Strong proximity effects beyond LDA (thin lines)

significant enhancement of D only at strong coupling

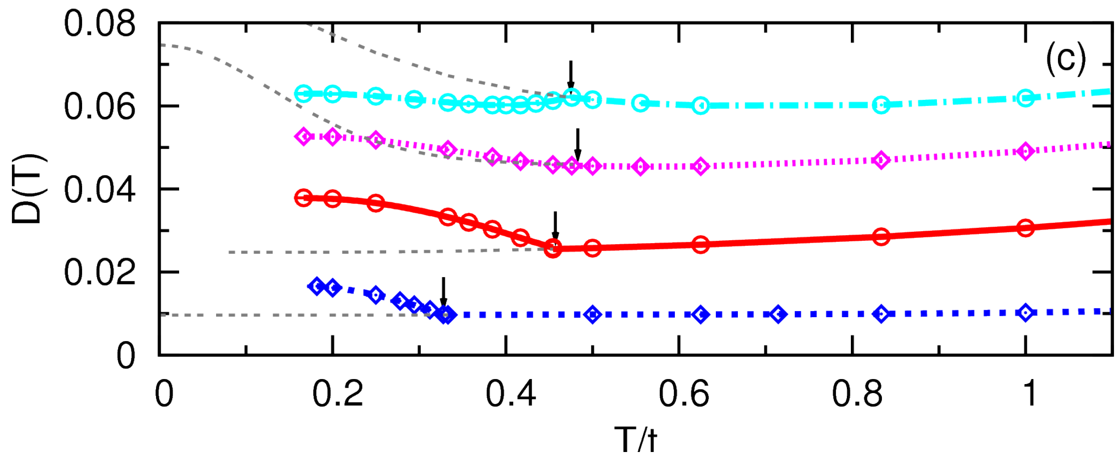
Néel transition visible in integrated quantities? Yes!

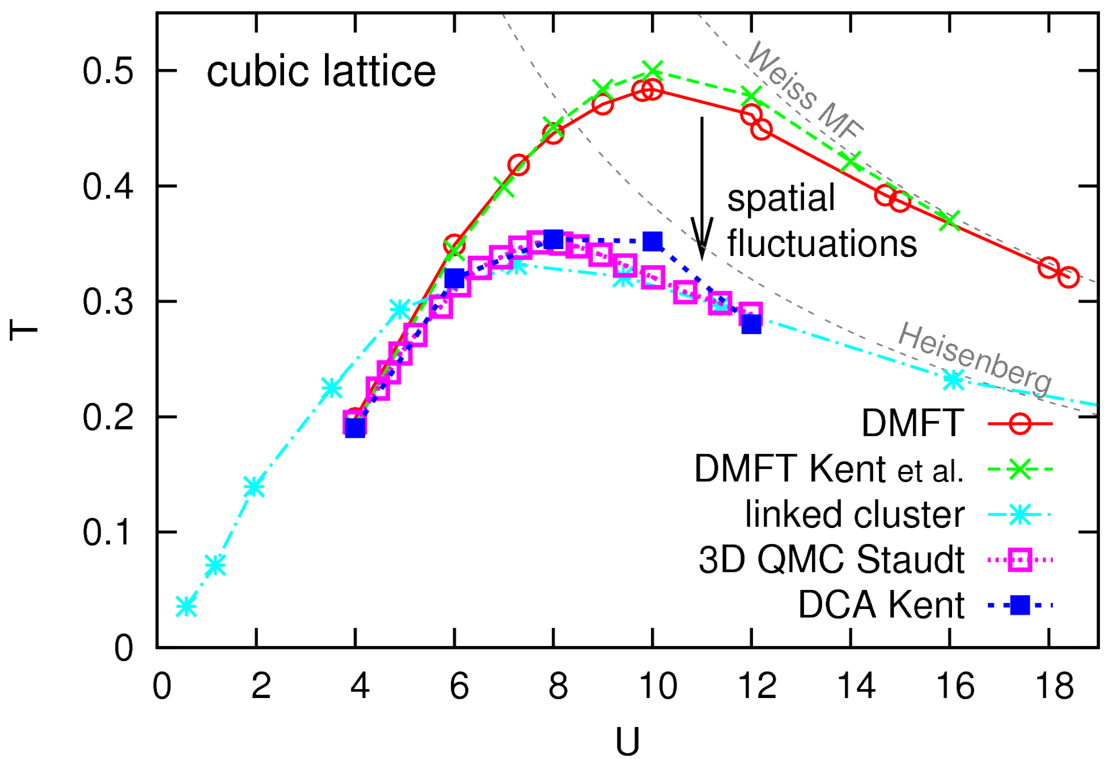


Assumption: measurement along beam with gaussian profile

but: effects of nonlocal correlations?

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

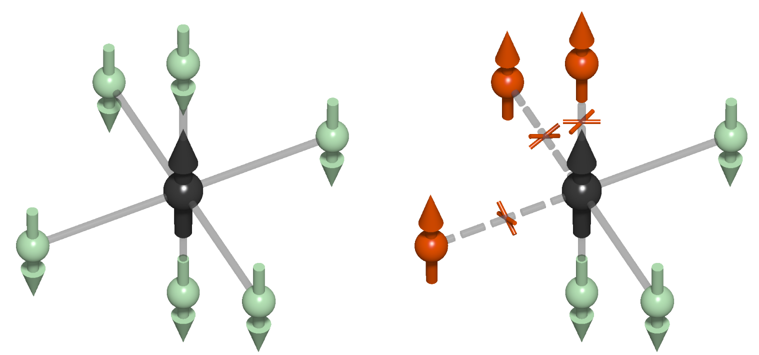




Unavoidable change: kinks cannot remain at $T = T_{\mathrm{N}}^{\mathrm{DMFT}} > T_{\mathrm{N}}$!

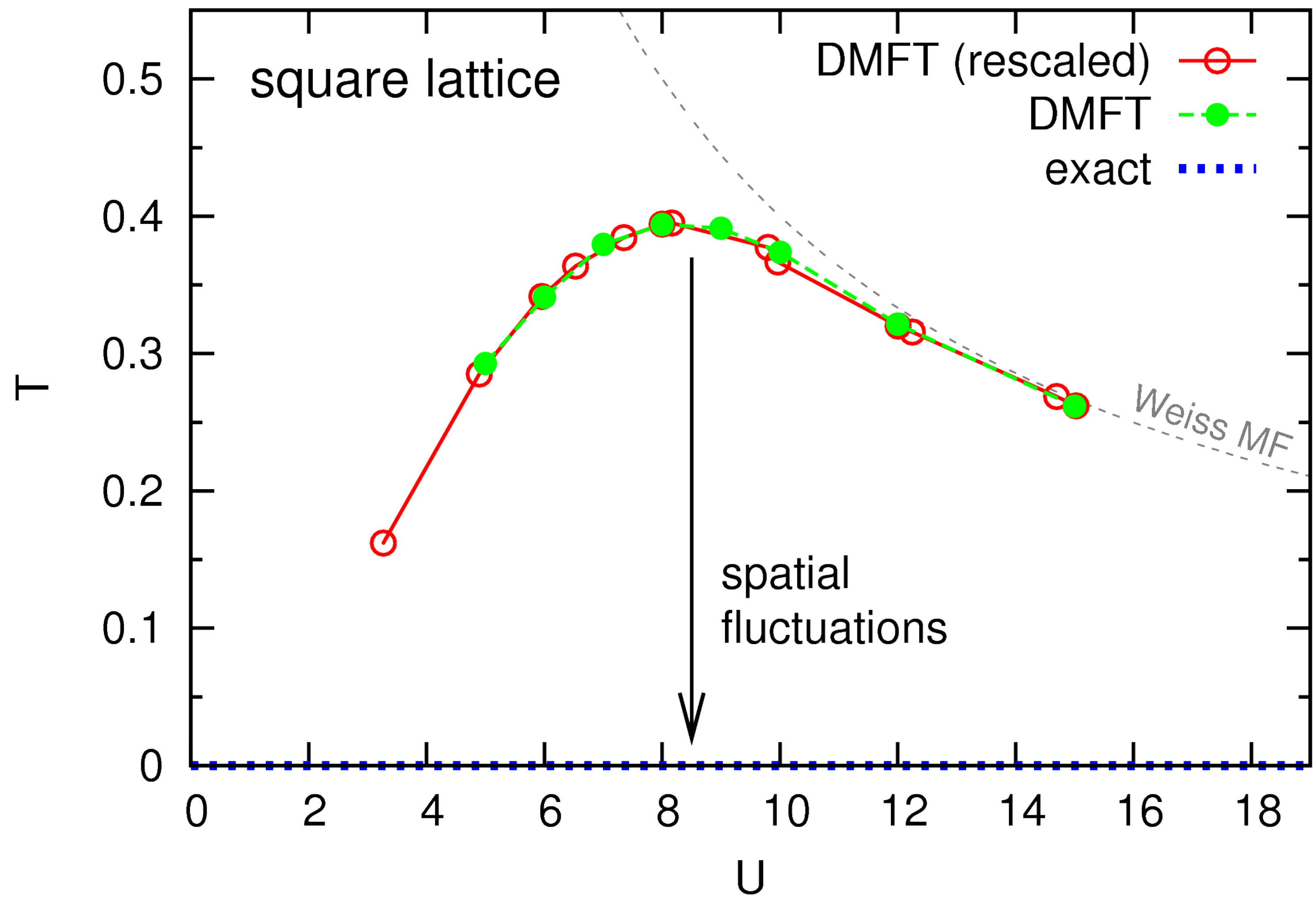
Constraints:

- DMFT results for D(T) agree with high-T expansion at $T >> T_{\mathrm{N}}$ [Jördens et al., PRL (2010)]
- argument for $D_{\mathrm{AF}}/D_{\mathrm{para}} \xrightarrow{U\to\infty} 2$ is not explicitely d-dependent



and independ. of long-range order

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



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

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

PRL 104, 066406 (2010) PHYSICAL REVIEW LETTERS week ending 12 FEBRUARY 2010

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

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

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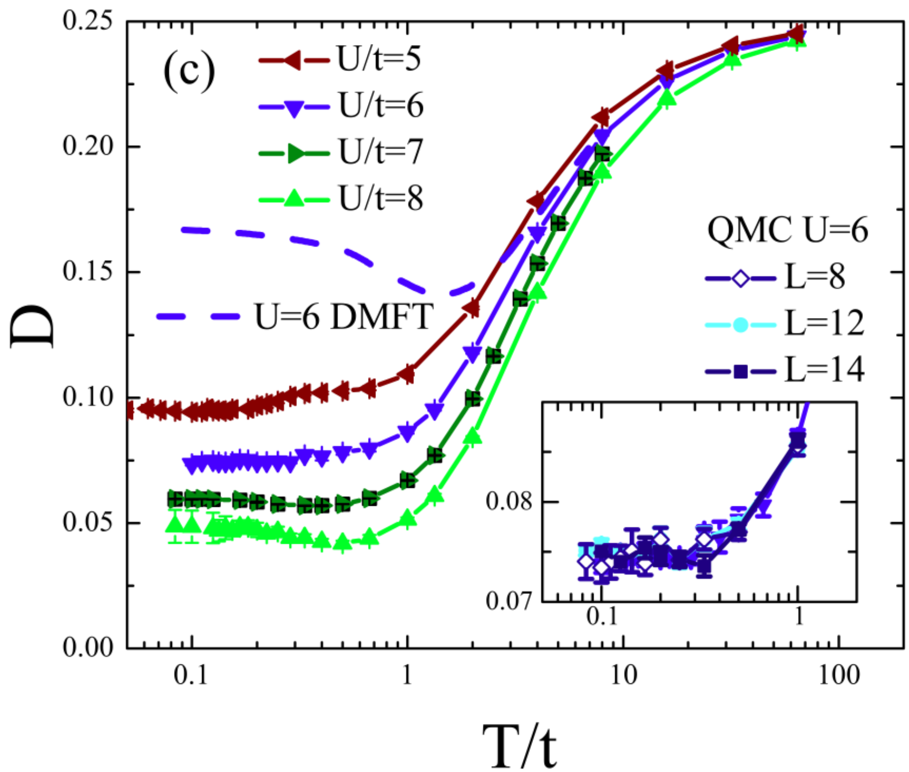
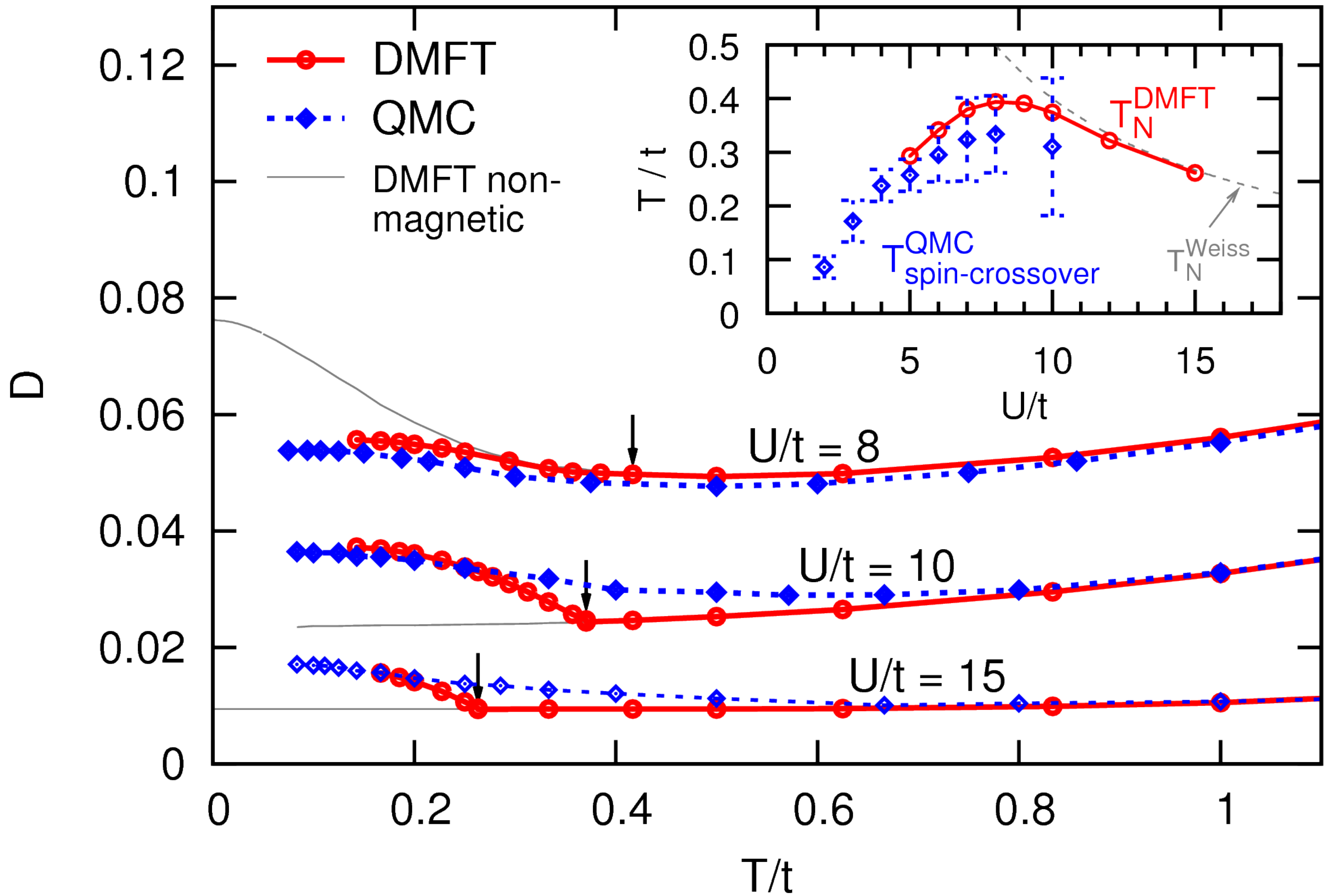
(Received 18 June 2009; published 11 February 2010)



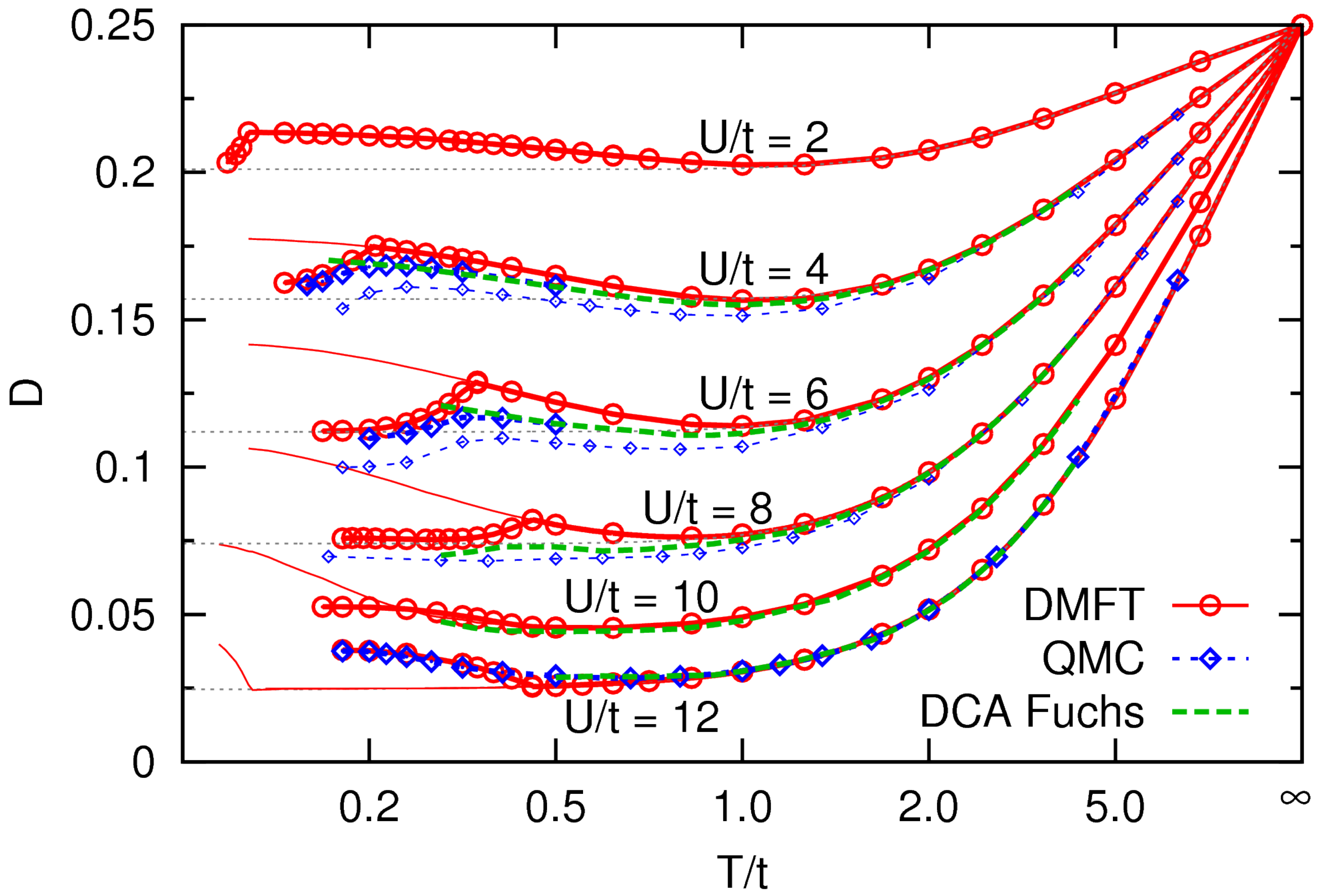
Comparison DMFT – direct QMC for the 2d square lattice ($n = 1$)



Excellent agreement at large T and low T, rounding off at $T \approx T_N^{\mathrm{DMFT}}$

T_N^{DMFT} is relevant temperature scale for AF correlations!

Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)

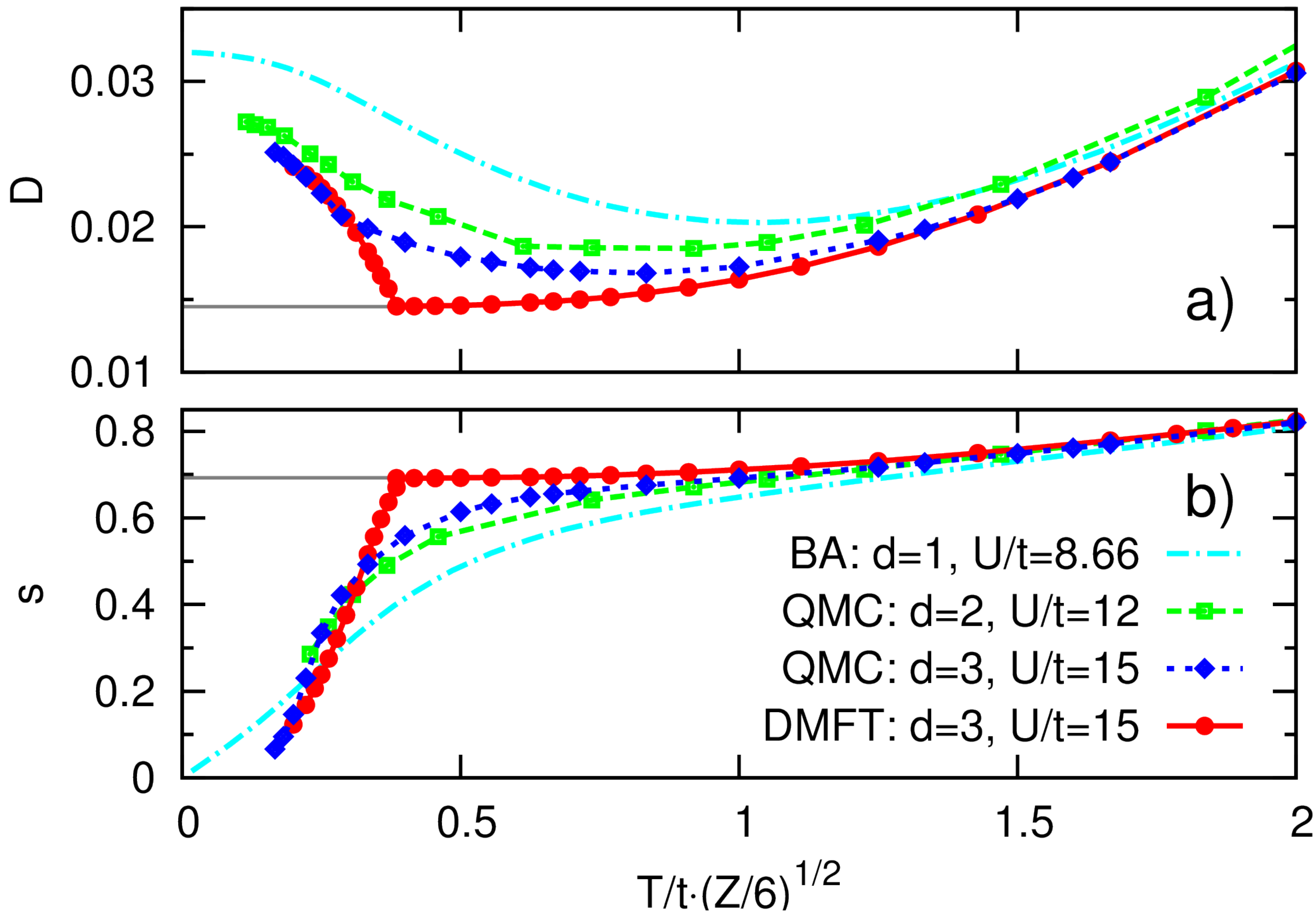


Excellent general agreement, even at small U (reduction of D by AF)

Dynamical cluster approximation (DCA) misses AF signatures in D

Typical QMC discretization errors (thin lines) larger than DMFT deviations

Dimensional comparison at $n = 1$: DMFT ($d = \infty$) vs. $d = 3, 2, 1$



Regular dimensional convergence (only for proper scaling $\propto \sqrt{Z}t$)

But: minimum in $D(T)$ shifts with d – offset by $s(T)$?

PHYSICAL REVIEW A **83**, 023606 (2011)

Thermodynamics of the three-dimensional Hubbard model: Implications for cooling cold atomic gases in optical lattices

Lorenzo De Leo,[1] Jean-Sébastien Bernier,[1] Corinna Kollath,[1,2] Antoine Georges,[1,3] and Vito W. Scarola[4]
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[2] *Département de Physique Théorique, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genéve 4, Switzerland*
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(Received 15 September 2010; published 10 February 2011)

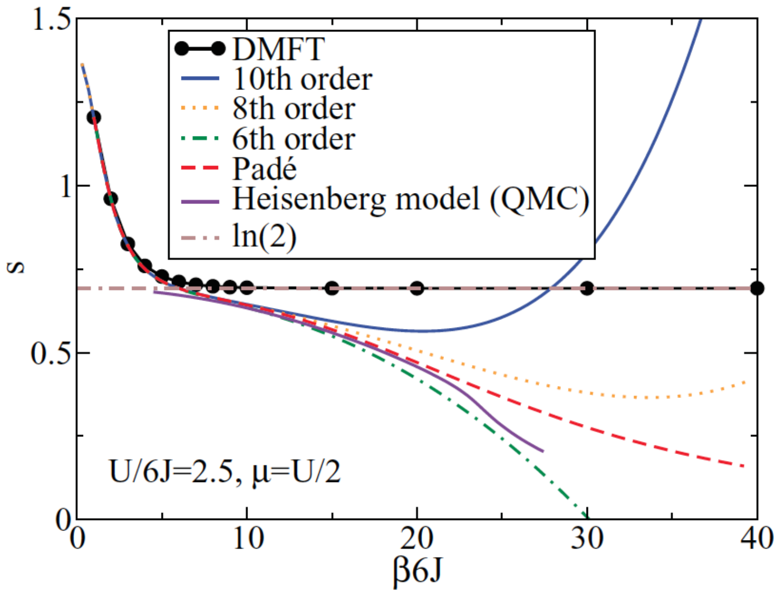
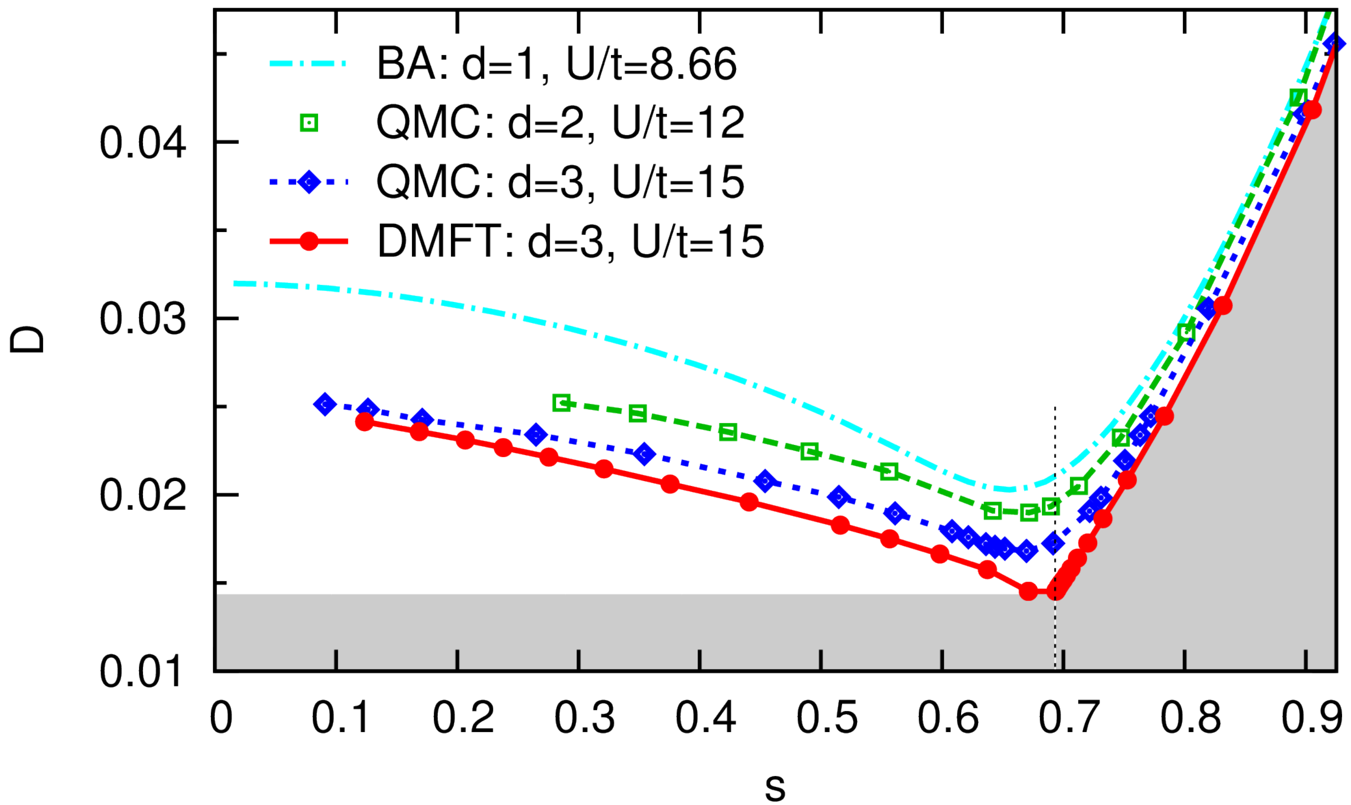


FIG. 14. (Color online) Entropy per particle in a system at half filling and intermediate interaction strength $U/6J = 2.5$ obtained by series expansion, DMFT, and QMC (for the Heisenberg model) [26].

Double occupancy as a universal measure of AF correlations + entropy



For all dimensions: $\min\{D(s)\}$ at $s \approx \log 2$

No significant features in $d = 3$ at Néel transition

Effect is larger for lower dimensions:

$$\langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle_0 = \begin{cases} -1.00 & DMFT \\ -1.20 & (d=3) \\ -1.34 & (d=2) \\ -1.77 & (d=1) \end{cases}$$

$$D_0 = \left(1 - \langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle\right) Zt^2/(2U^2) + \mathcal{O}\left(t^4/U^4\right)$$

PRL **106,** 145302 (2011) PHYSICAL REVIEW LETTERS week ending 8 APRIL 2011

Probing Nearest-Neighbor Correlations of Ultracold Fermions in an Optical Lattice

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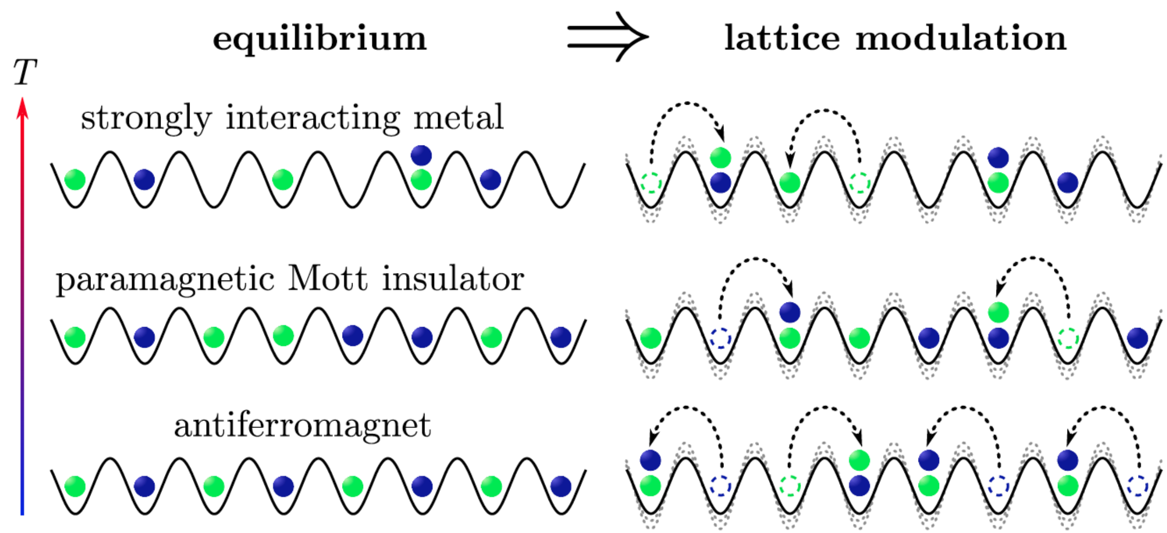
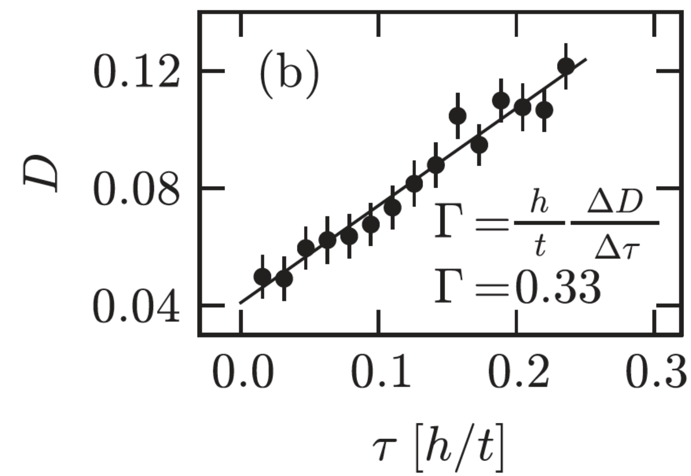
Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland

(Received 2 December 2010; revised manuscript received 1 February 2011; published 5 April 2011)

We demonstrate a probe for nearest-neighbor correlations of fermionic quantum gases in optical lattices. It gives access to spin and density configurations of adjacent sites and relies on creating additional doubly occupied sites by perturbative lattice modulation. The measured correlations for different lattice temperatures are in good agreement with an *ab initio* calculation without any fitting parameters. This probe opens new prospects for studying the approach to magnetically ordered phases.





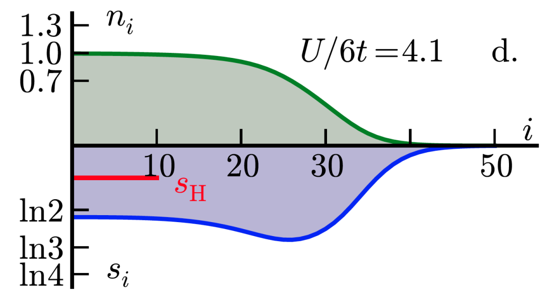
Correlator $\mathcal{P}_{i,i+1} = \sum_\sigma \langle n_{i,\sigma}(1 - n_{i,\bar\sigma})\, n_{i+1,\bar\sigma}(1 - n_{i+1,\sigma})\rangle \xrightarrow{n\to 1} (1 - \langle \sigma_i^z \sigma_{i+1}^z \rangle)/2$ MF?

Summary

QMC based implementation of real-space DMFT

Efficient for cold-atom temperatures, flexible

$\mathcal{O}(10^5)$ particles within slab approximation ($\sim$ GGA)

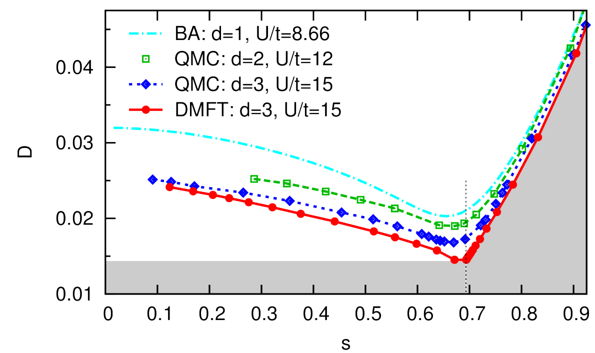


Real-space DMFT study of antiferromagnetism

AF correlations at finite T signaled by enhanced D

Proximity effects important – LDA deficient

[Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]



DMFT surprisingly accurate in low dimensions

Double occupancy: universal probe of AF correlations and entropy

[E. V. Gorelik, T. Paiva, R. Scalettar, A. Klümper, N. Blümer, arXiv:1105.3356]

D quantifies frustration effects (square – triangular – cubic lattice)