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

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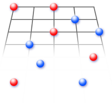
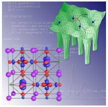


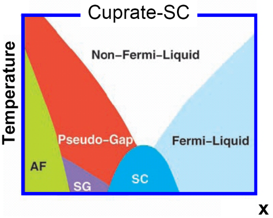
TR 49: *Condensed matter systems with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

FOR 1346
LDA+DMFT
Augsburg *et al.*

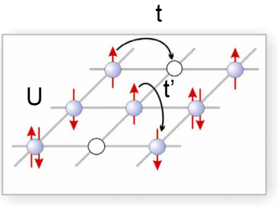


Motivation: Ultracold lattice fermions as quantum simulators?

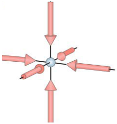
Correlated materials

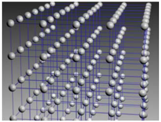


Fermionic Hubbard model



Ultracold fermions on optical lattices



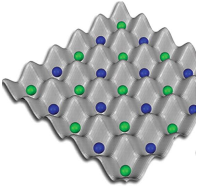


$\mathcal{O}(10^5)$ atoms

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:

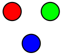
(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of AF order is not straightforward [Gottwald, PvD (2009)]

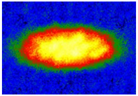
(iii) inhomogeneity, time scale for global (spin) equilibrium

Specifics of ultracold fermions on optical lattices

+ 1-band assumption often accurate, local interaction

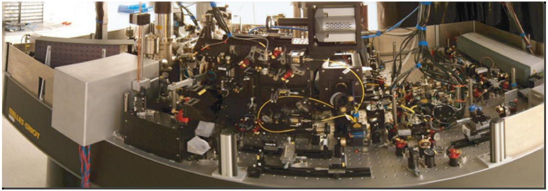
+ Tunability, flexibility, e.g. 3-flavors $\uparrow\downarrow \longrightarrow$ 

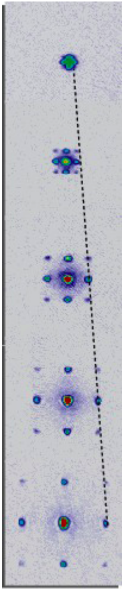
+ Time resolution

− Trap  $\rightsquigarrow$ inhomogeneous systems, finite cloud sizes 

− Preparation complicated and noisy

[Photo courtesy of U. Schneider]





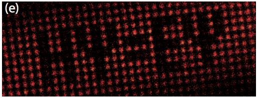
Main measurement: column density (*in situ* / time of flight)
+ spin selectivity + double occupancy

Questions for this talk

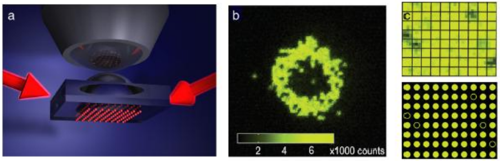
- How to detect AF order/correlations?
- Which entropy range is needed?
- General impact of dimensionality?

Mermin-Wagner: LRO $\leftrightarrow$ $d = 3$

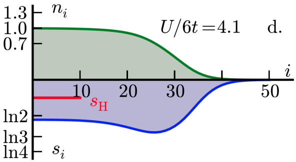
Experimental advantage of 2 dimensions:
single-site resolution (for bosons)



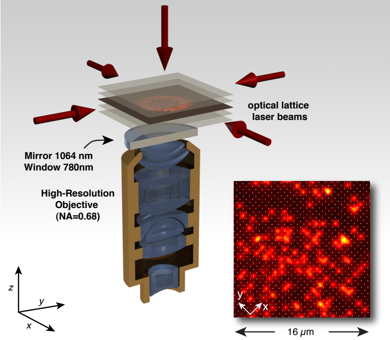
[Würtz et al., PRL **103**, 080404 (2009)]



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



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



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

Outline

Motivation: Ultracold lattice fermions as quantum simulators?

Methods: DMFT + HF-QMC, real-space DMFT

RDMFT study: Néel transition of lattice fermions in a harmonic trap

Effects of non-local correlations? DMFT versus direct QMC + BA

Characteristic temperature of pseudogap in $2d$ Hubbard model?

Collaborators

Postdoc

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Univ. Mainz

Real-space DMFT collaboration

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

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AF in finite dimensions [Gorelik et al., arXiv:1105.3356]

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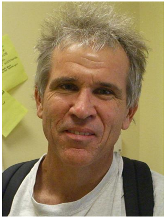

Richard Scalettar
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Diploma student

Daniel Rost
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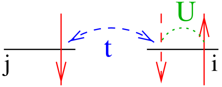
Methods: Approaches for Hubbard-type models

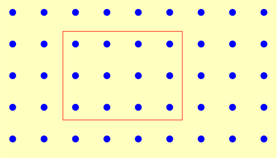
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



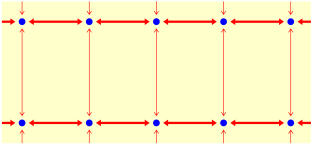
Perturbation theory

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

finite clusters: ED, QMC



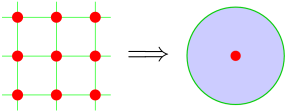
$d \to 1$: Bethe ansatz, DMRG



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

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

+	non-perturbative $\rightsquigarrow$ valid at MIT
+	in thermodynamic limit
+/−	exact for coordination $Z \to \infty$
	(questionable for $d \leq 2 \rightsquigarrow$ DCA, CDMFT)



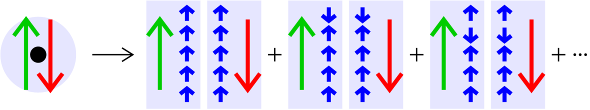
Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

$$G_\sigma(\tau) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \psi^*] \;\psi_\sigma(\tau)\,\psi^*_\sigma(0)\; \exp\Big[\mathcal{A}_0 - U \sum_{\sigma\sigma'} \int_0^\beta d\tau\, \psi^*_\sigma \psi_\sigma \psi^*_{\sigma'} \psi_{\sigma'}\Big]$$

(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

+ exact (after extrapol. $\Delta\tau \to 0$) + no sign problem (density-type interactions)

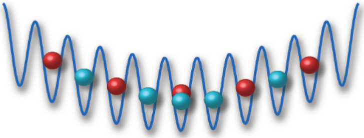
Alternative to DMFT + HF-QMC: Determinantal QMC [BSS (1981)]

+ accurate for low Z − sign problem for $n \neq 1$ − finite-size effects

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

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

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



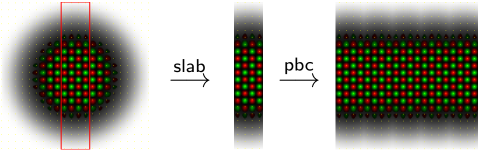
$\rightsquigarrow$ N single-site impurities, coupled by real-space lattice Dyson equation:

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

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

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

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



Néel transition of trapped fermions on cubic optical lattice at (real-space) DMFT level

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

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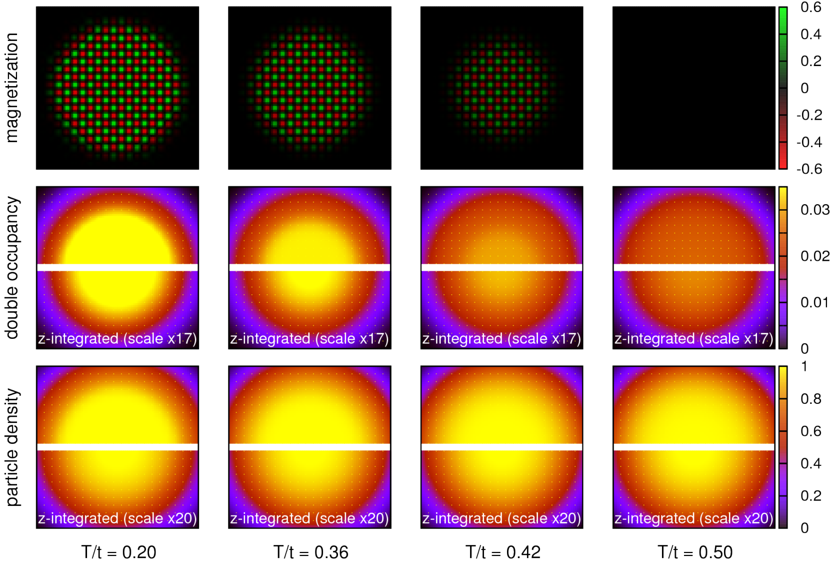
Results: RDMFT-QMC (cubic lattice, $V = 0.05t$, $U = W = 12t$)



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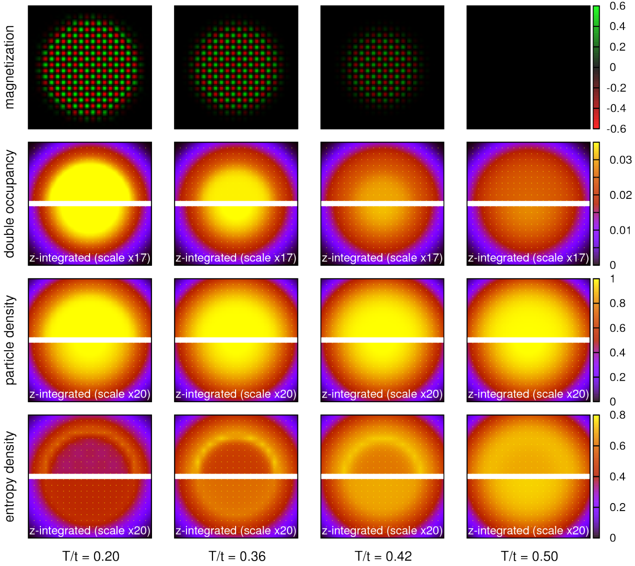


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!
observable only for cold atoms!

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

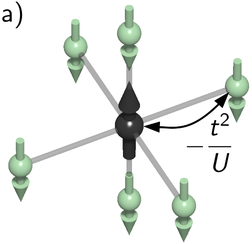
Entropy

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

Enhanced double occupancy: a signature of AF order

Illustration of strong-coupling mechanism for enhanced double occupancy

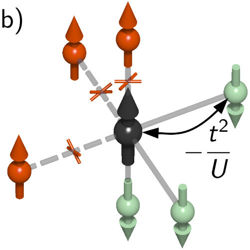
(a)



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

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

(b)



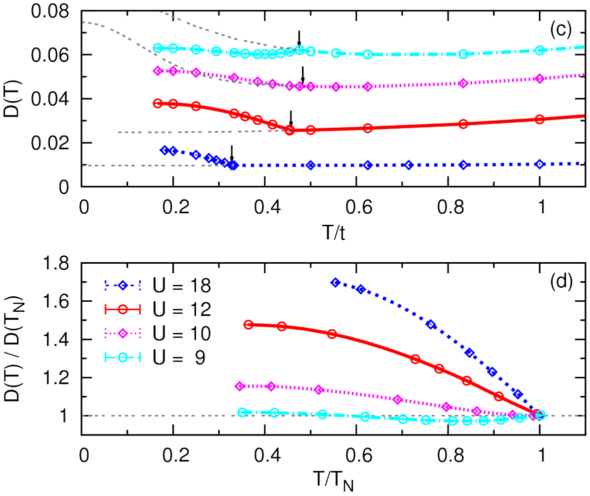
Para/nonmagnetic state: 1/2 of neighbors Pauli forbidden

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

$D = dE/dU$ (at $T = 0$) $\rightsquigarrow$ $D_{\mathbf{AF}}/D_{\mathbf{p}} \stackrel{U\to\infty}{\longrightarrow} 2$

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 double occupancy D at half filling



At $U \gtrsim 10t$:
D enhanced below Néel temperature T_N (arrows)

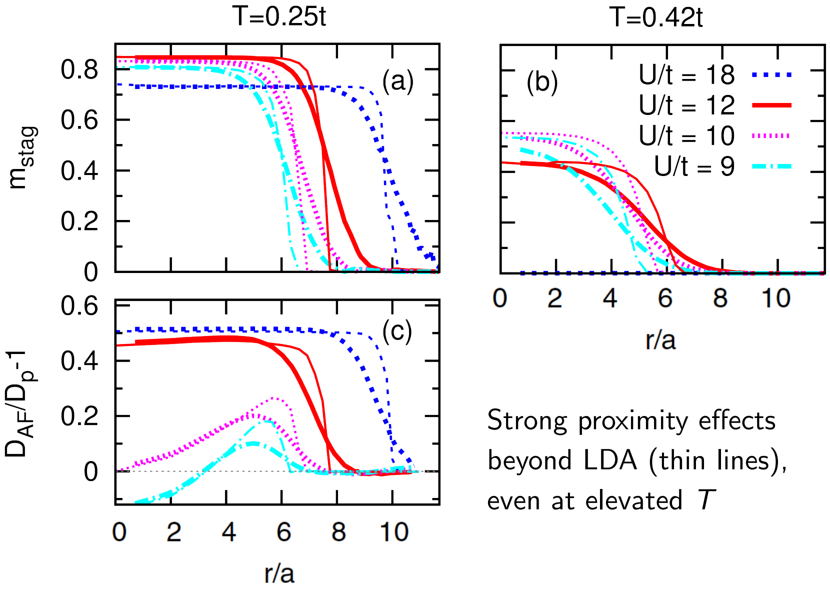
Thin lines: metastable nonmagnetic phase

Data scaled to values of critical point:

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

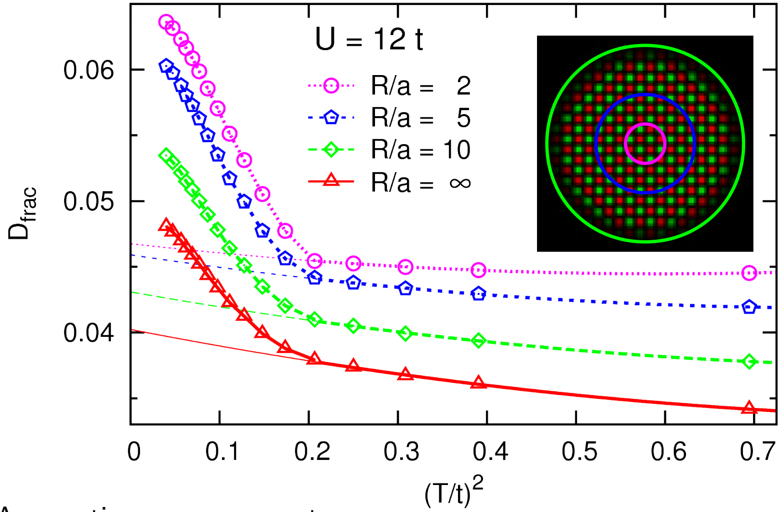
Note: AF kills Pomeranchuk cooling [Werner, Parcollet, Georges, Hassan, PRL (2005)]

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



Strong proximity effects beyond LDA (thin lines), even at elevated T

Néel transition visible in integrated quantities? Yes!



Assumption: measurement along gaussian beam

But: effects of nonlocal correlations?

Effects of non-local correlations?
Comparisons with direct QMC + BA

[Gorelik, Rost, Paiva, Scalettar, Klümper, NB, arXiv:1105.3356]

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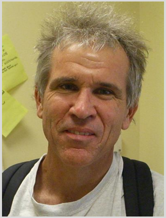

Richard Scalettar
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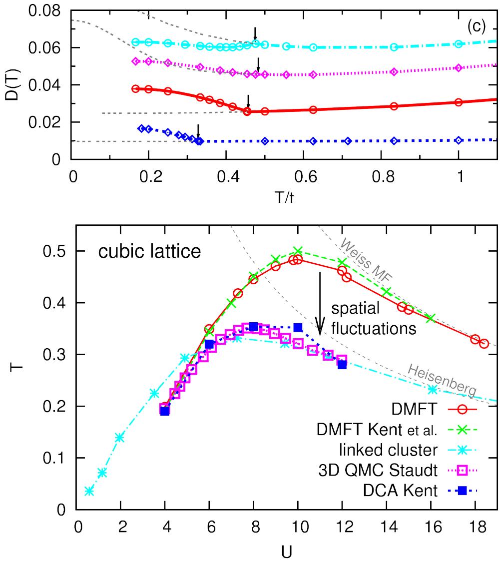
Modification of DMFT predictions by spatial fluctuations in 3d: how?

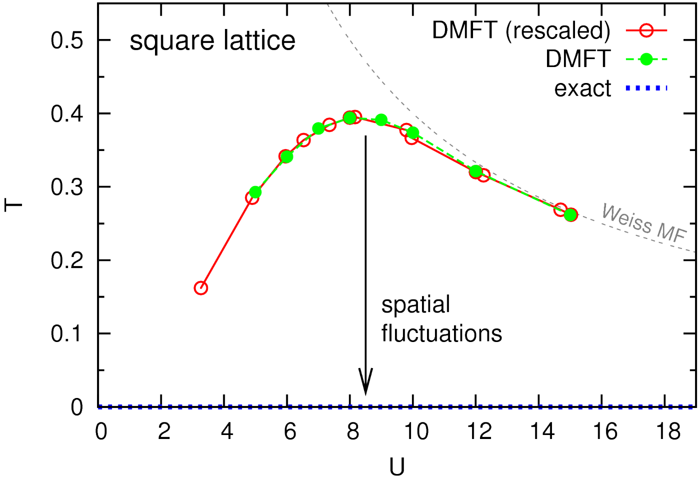


Unavoidable change: kinks cannot remain at $T = T_{\mathrm{N}}^{\mathrm{DMFT}} > T_{\mathrm{N}}$!

Constraint:

- DMFT results for D(T) agree with high-T expansion at $T \gg T_{\mathrm{N}}$ [Jördens et al., PRL (2010)]

Situation "worse" in 2 dimensions: $T_N = 0 \ll T_N^{DMFT}$!



Mermin-Wagner theorem excludes AF long-range order at finite temperatures

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

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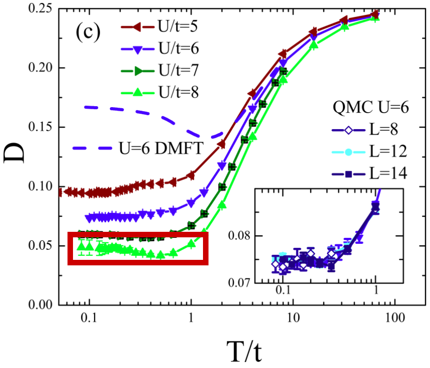


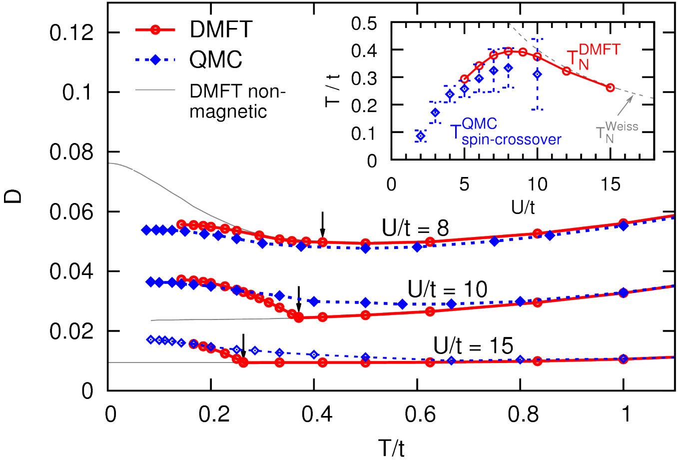
Low $-T$ enhancement of D at $U/t = 8$, "right" T scale!

Note: $U = 6$ "DMFT" curve completely off (wrong phase, wrong scaling)

Correct scaling: $\propto \sqrt{Z}$

[Metzner, Vollhardt, PRL (1989)]

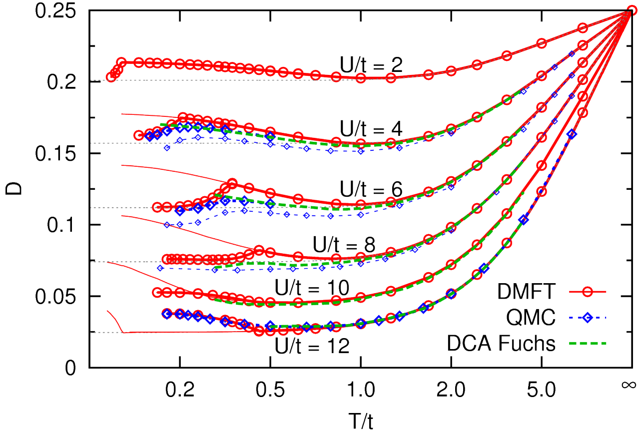
Comparison DMFT – direct QMC for the 2d square lattice ($n = 1$)



AF DMFT confirmed at high T and at low T, rounding off at $T \approx T_N^{\text{DMFT}}$

Nonmagnetic DMFT completely off at low T!!!

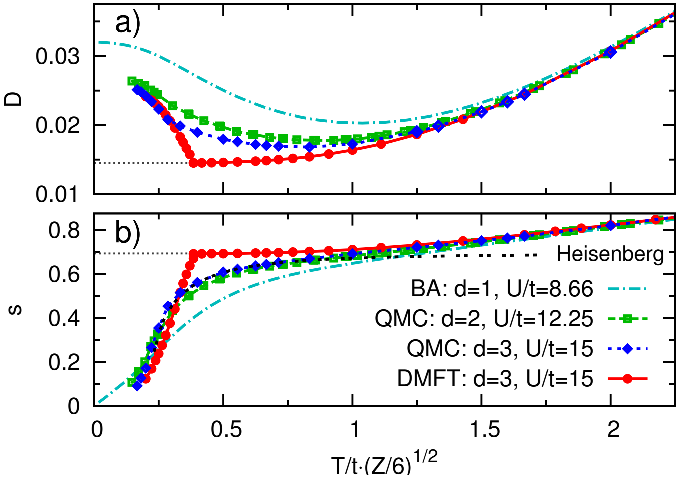
Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)



Excellent general agreement DMFT ↔ QMC, even at small U

DCA study [Fuchs et al., PRL (2011)] misses AF signatures

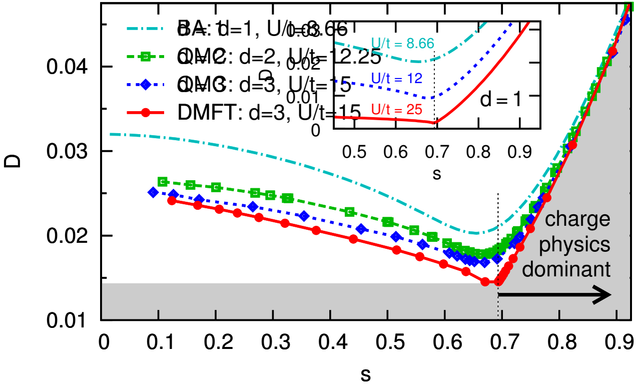
Typical QMC discretization errors (thin lines) larger than DMFT deviations!



Regular dimensional convergence (for proper scaling $\propto \sqrt{Z}t$), fast at high T

First high-precision data for entropy?

Double occupancy as a universal measure of AF correlations + entropy



Minimum of $D(s)$ at $s \approx \log 2$ for all d!

No features seen at $d = 3$ Néel transition

Local probes see only short-range AF $\rightsquigarrow$ needed: $s \lesssim log(2)$, not $s \lesssim log(2)/2$

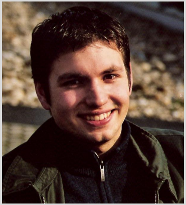
AF enhancement of D is larger in lower dimensions:

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

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

Characteristic temperature of pseudogap in the two-dimensional Hubbard model?

[Preliminary results]



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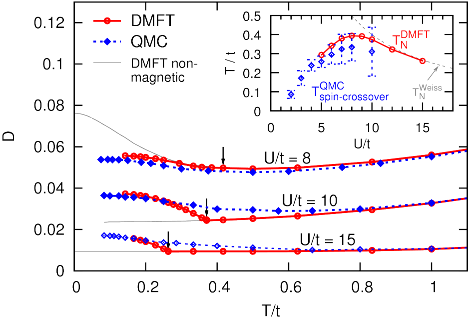
Pseudogap in square lattice Hubbard model from DQMC



Double occupancy "sees" T_N^{DMFT}
– how about less local properties?

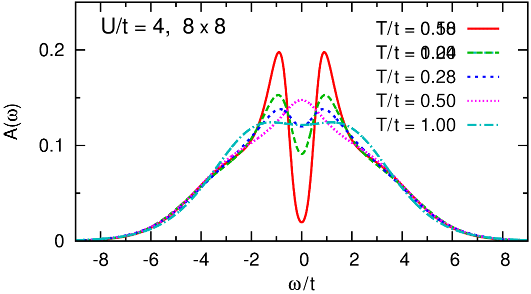
Spectral function (test case for multigrid DQMC and MEM)

At weak coupling ($U = 4t$):

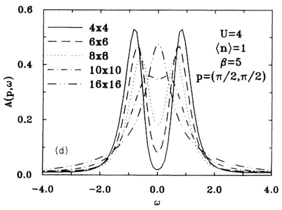
FL peak at intermediate T

Pseudogap for $T \lesssim T_N^{\mathrm{DMFT}}$

– coincidence?

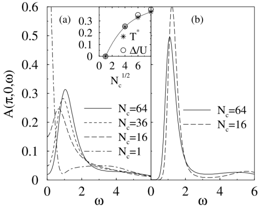


Existence and nature of pseudogap: long controversy!



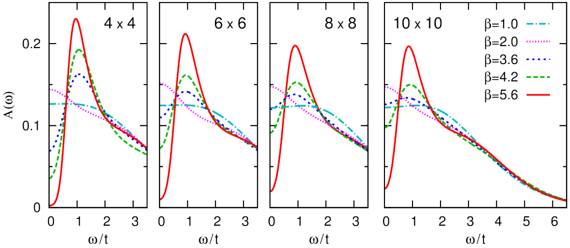
Gap is finite-size effect

[White, PRB (1992)]

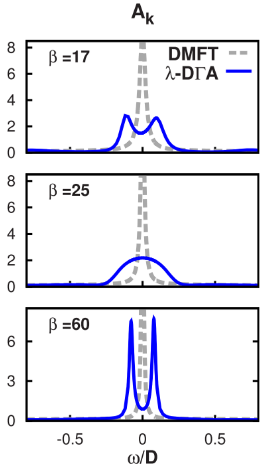


DCA/QMC $\rightsquigarrow$ gap

[Huscroft et al., PRL (2001)]



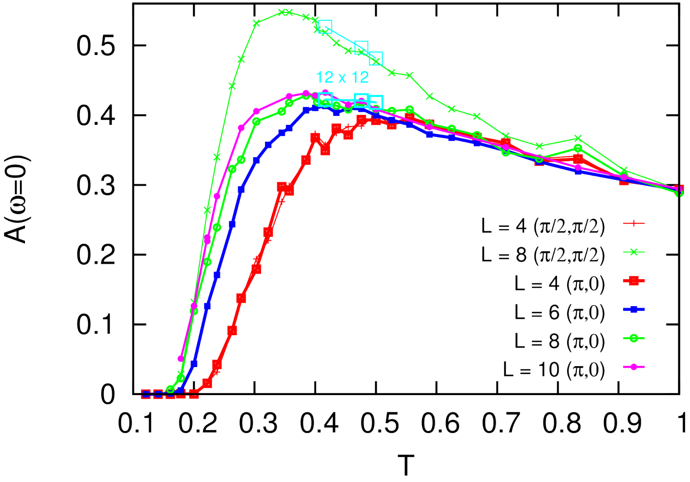
Sweeps + $\Delta\tau$ important; moderate finite-size effects



DΓA: reentrant behavior

[Katanin et al., PRB (2009)]

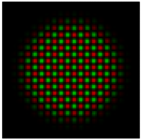
Clue to finite-size extrapolation: shifting cross-over temperature

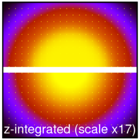


Crossover-temperature seems to converge to $T \gtrsim T_N^{\mathrm{DMFT}} \approx 0.25t$!

Same picture as for double occupancy!

Summary

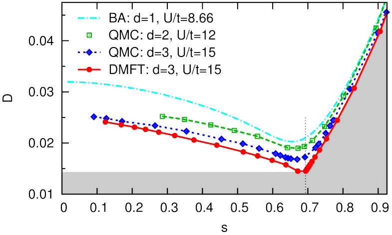


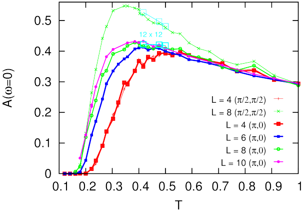


RDMFT: accurate approach for inhomogeneous correlated Fermi systems (cold atoms or materials)

Double occupancy: universal probe of AF correlations and entropy

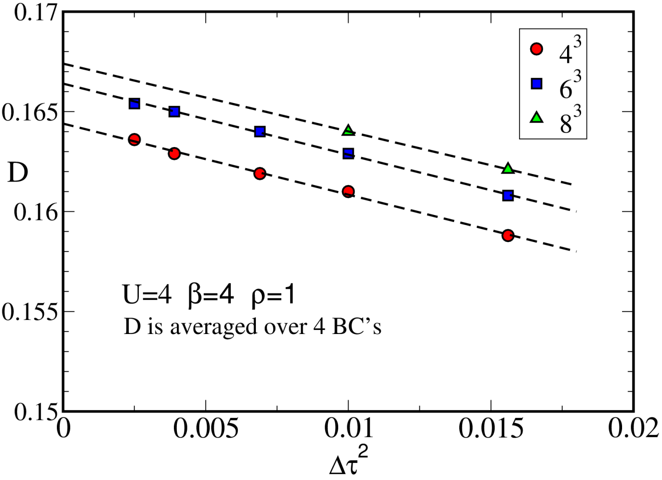
Relevant entropy scale for ultracold experiments (local probes): $s \approx \log(2)$





Characteristic pseudogap temperature in half-filled 2-dimensional Hubbard model

Finite-size effects on D in DQMC (cubic lattice)?



[R. Scalettar, 2011/09/14]

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

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

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(Received 15 September 2010; published 10 February 2011)

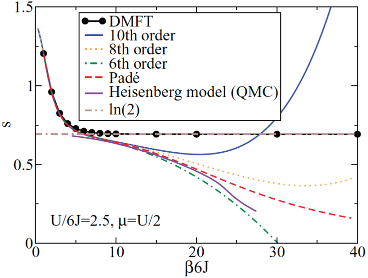

FIG. 14. (Color online) Entropy per particle in a system at half filling and intermediate interaction strength $U/6J = 2.5$ obtained by series expansion, DMFT, and QMC (for the Heisenberg model) [26].

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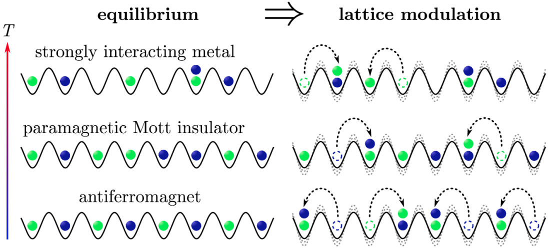
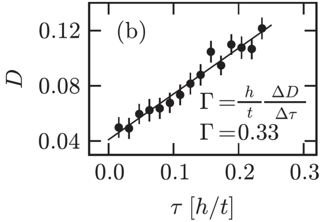
(Received 2 December 2010; revised manuscript received 1 February 2011; published 5 April 2011)

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.



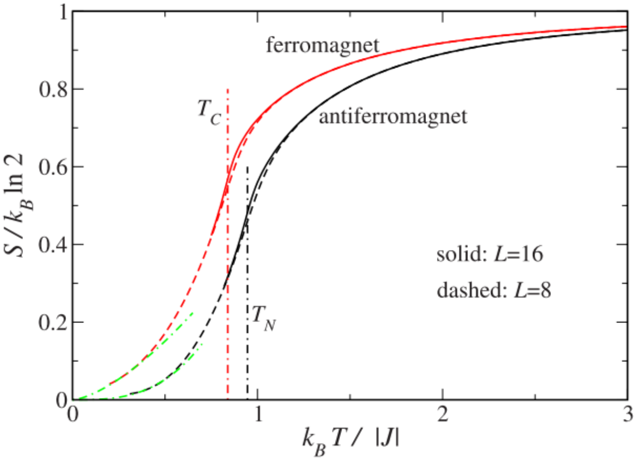


Correlator $\mathcal{P}_{i,i+1} = \sum_\sigma \langle n_{i,\sigma}(1-n_{i,\bar\sigma})\, n_{i+1,\bar\sigma}(1-n_{i+1,\sigma})\rangle \xrightarrow{n\to 1} (1-\langle \sigma_i^z \sigma_{i+1}^z\rangle)/2$

MF?

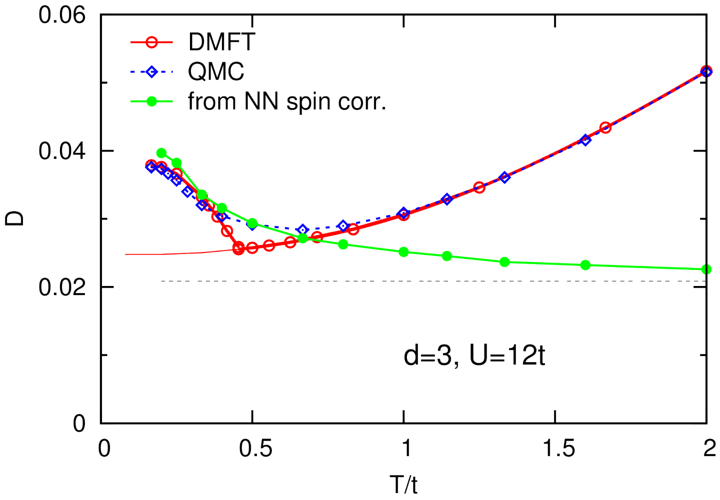
Finite-size rounding of phase transition relevant beyond 16^3

Example: Spin-1/2 Heisenberg model on cubic lattice



[Wessel, PRB (2010)]

Direct test of strong coupling picture ($d = 3$)



Good agreement at low T; AF signal in D stronger than expected from $\langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle$