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

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Outline

Introduction: strong correlations in electrons and cold atoms

Theory: (R)DMFT, LDA, slab approximation, (multigrid) HF-QMC

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

Néel transition of lattice fermions in a harmonic trap

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Effect of nonlocal correlations? Comparisons with direct QMC + BA

[ongoing collaboration with T. Paiva, R. Scalettar, and A. Klümper]

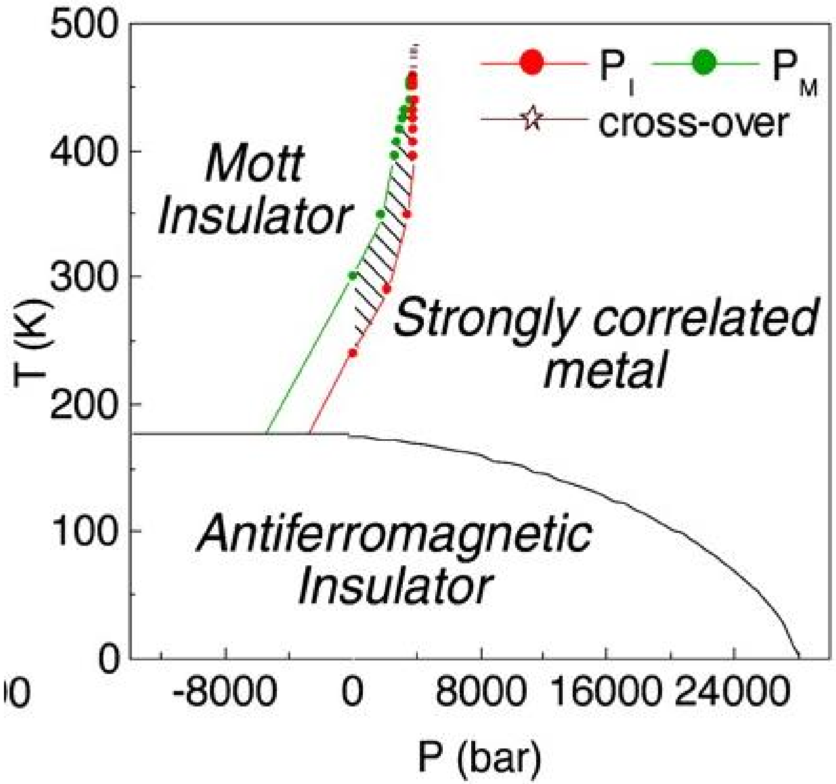
Impact of frustration, triangular lattice

Summary and outlook

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

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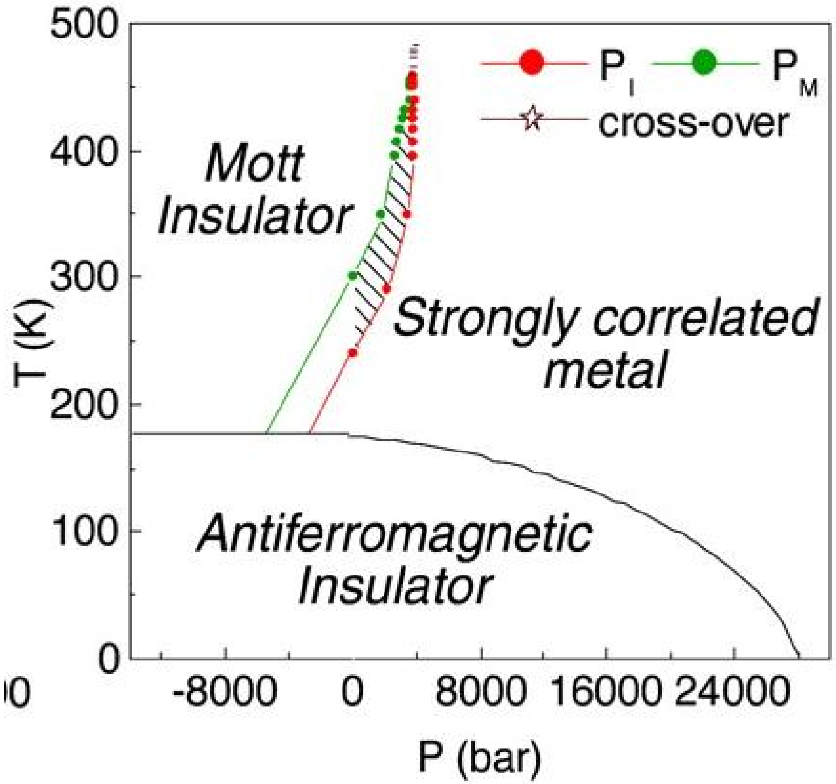

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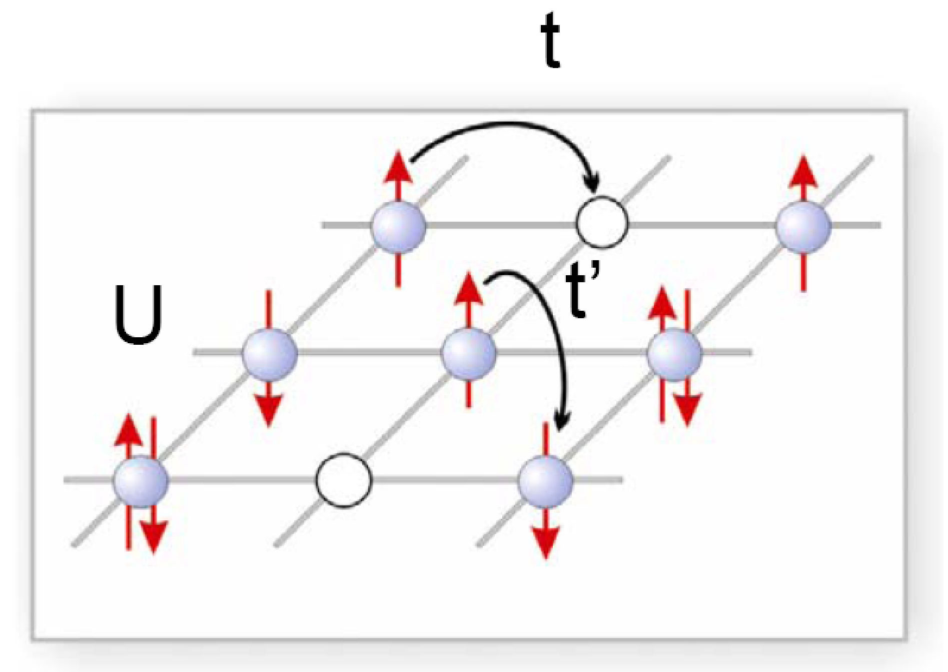

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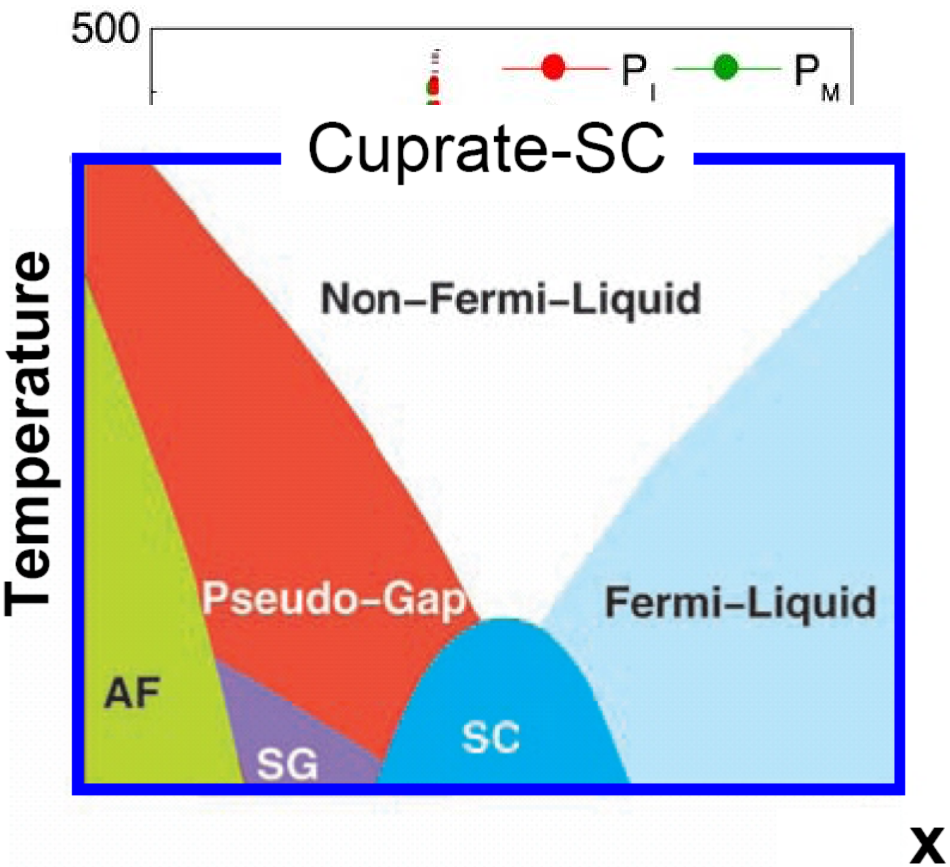

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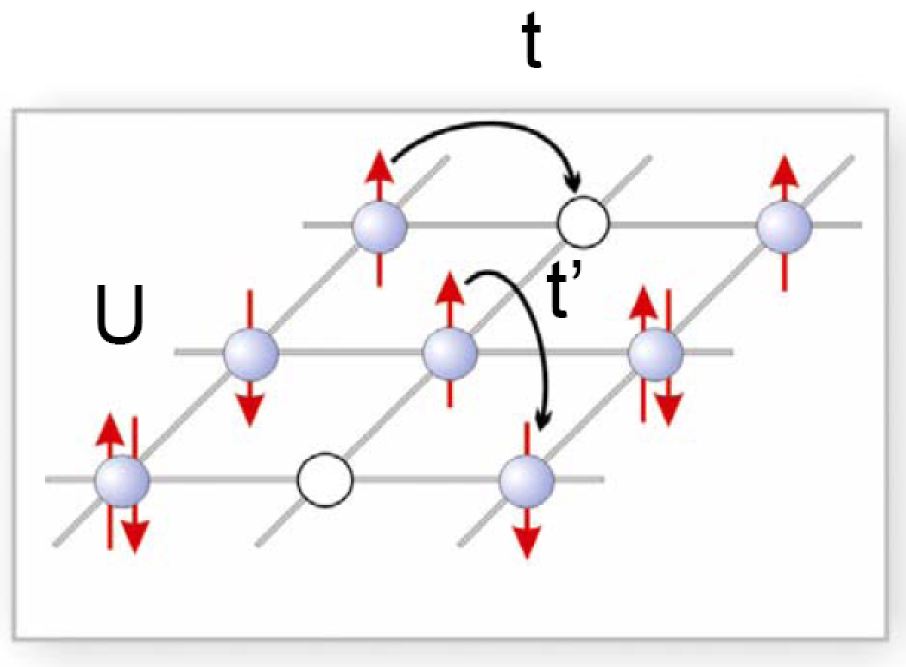

Are AF and Mott phases essential for superconductivity?

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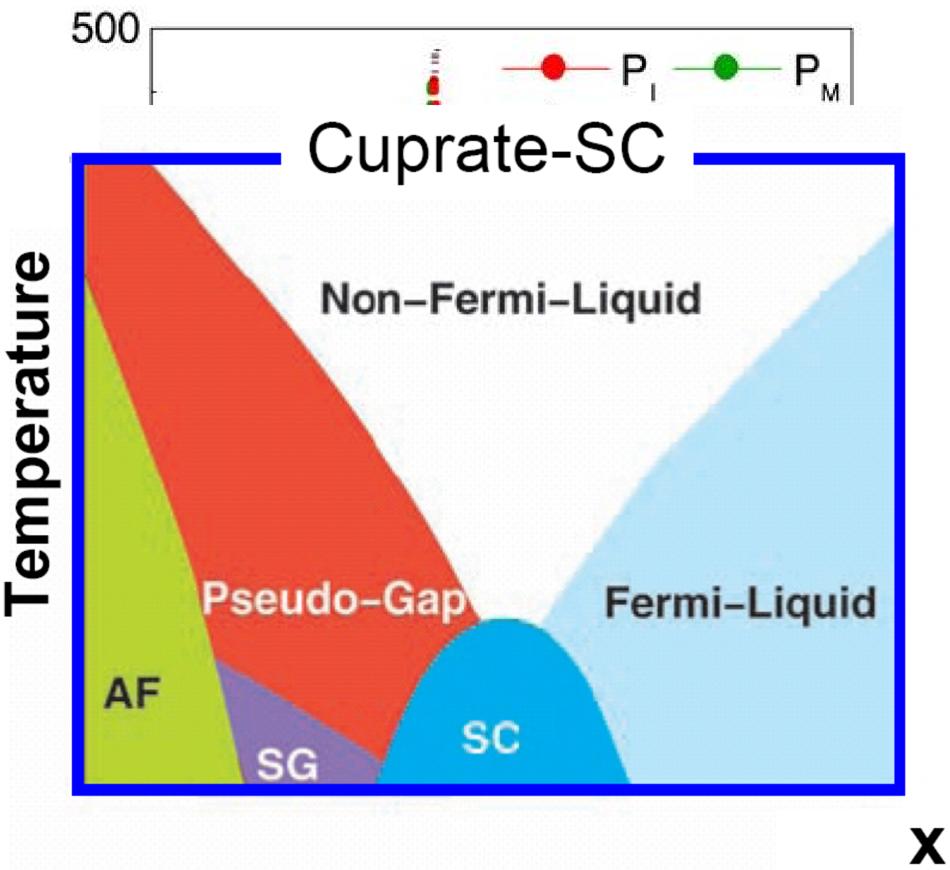

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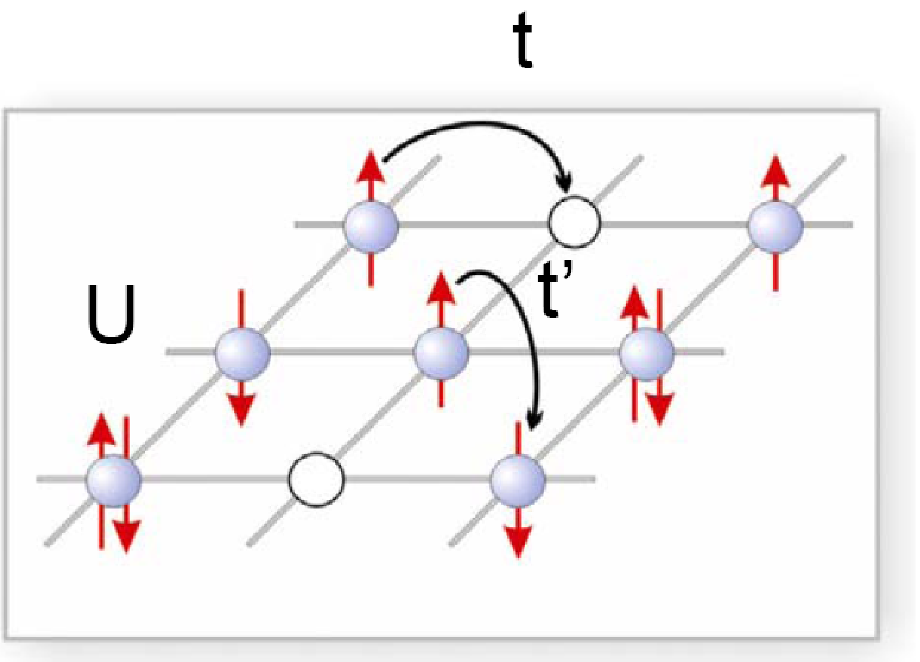


Are AF and Mott phases essential for superconductivity?

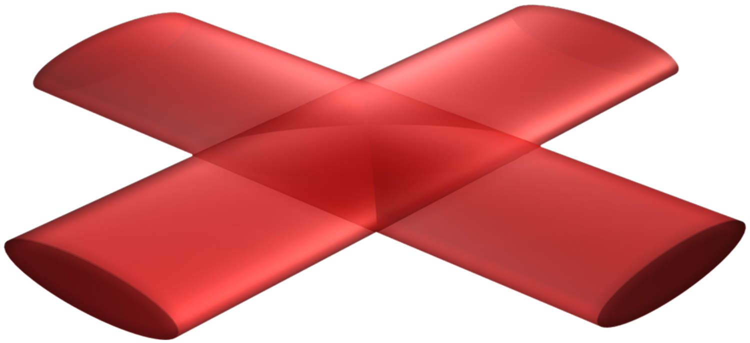
Claim: cold atoms ⇝ quantum simulators

Correlated ultracold quantum gases on optical lattices: basics

Experimental systems: small dilute clouds of about 10^5 ultracold atoms $\rightsquigarrow$ need trap

Optical dipole trap (2 beams)

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



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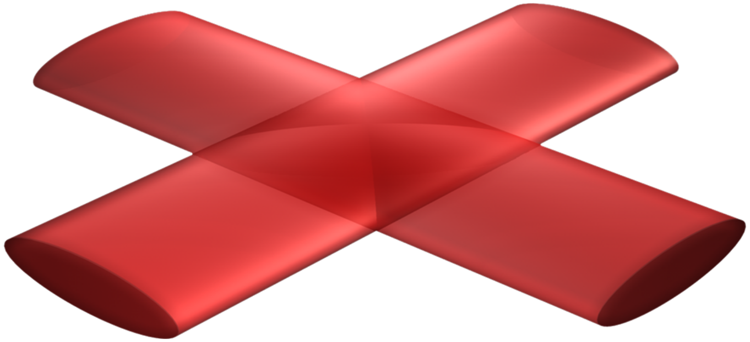

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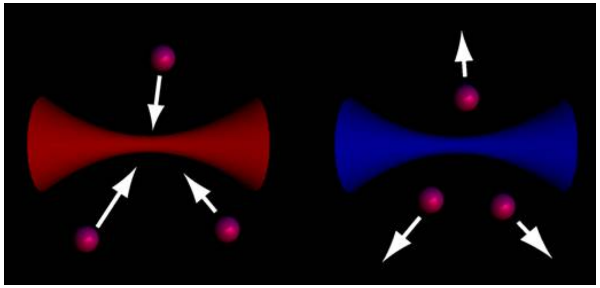

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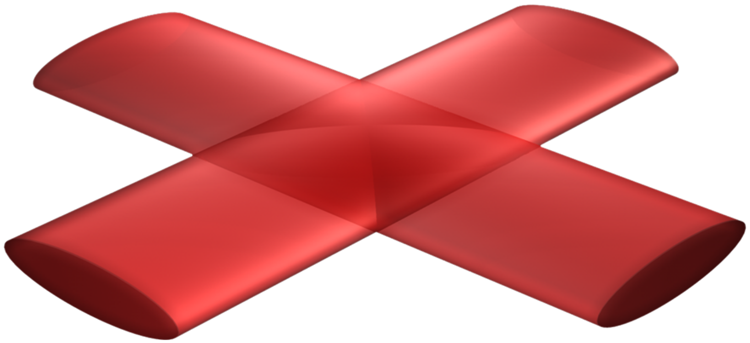

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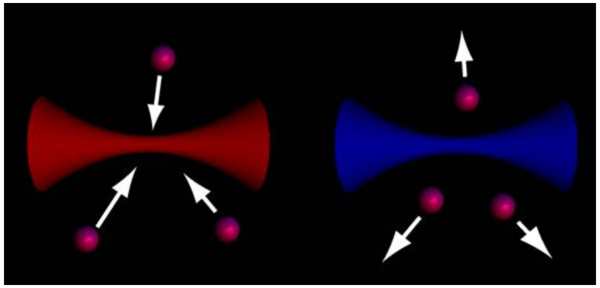
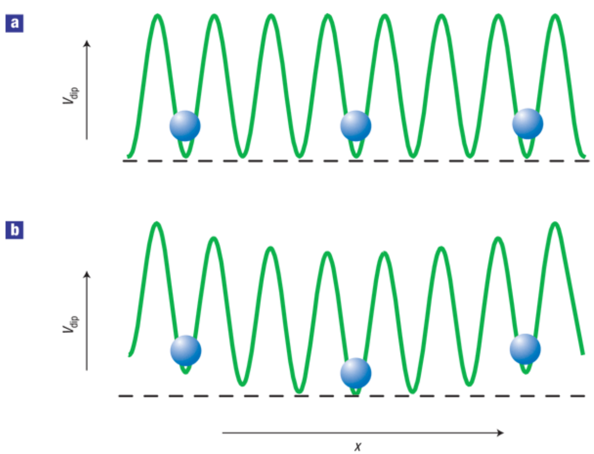


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



Beam profile: (anti) trapping

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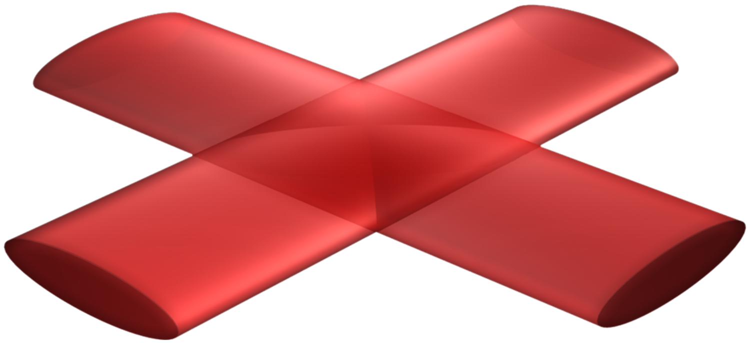

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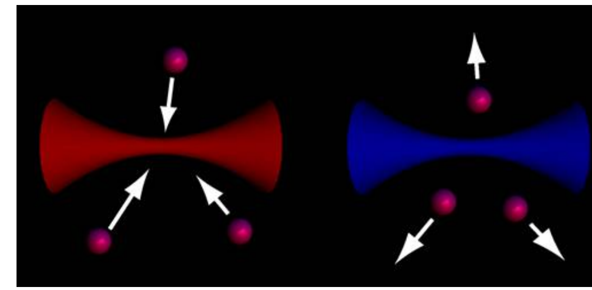

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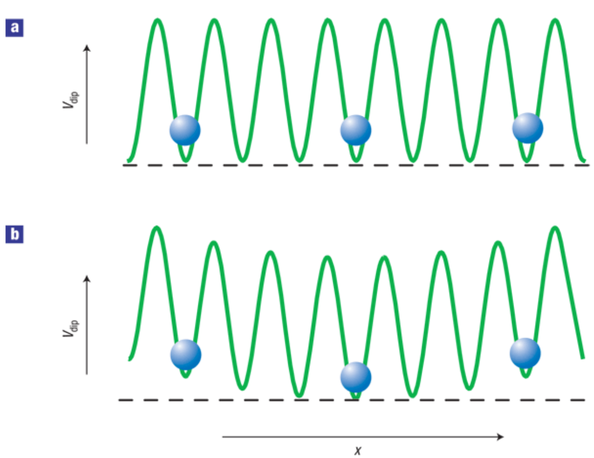


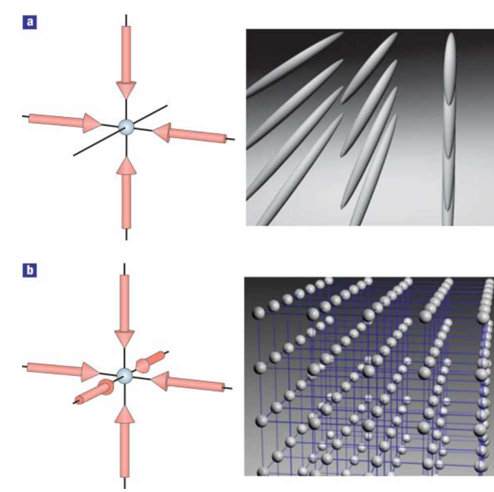
Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

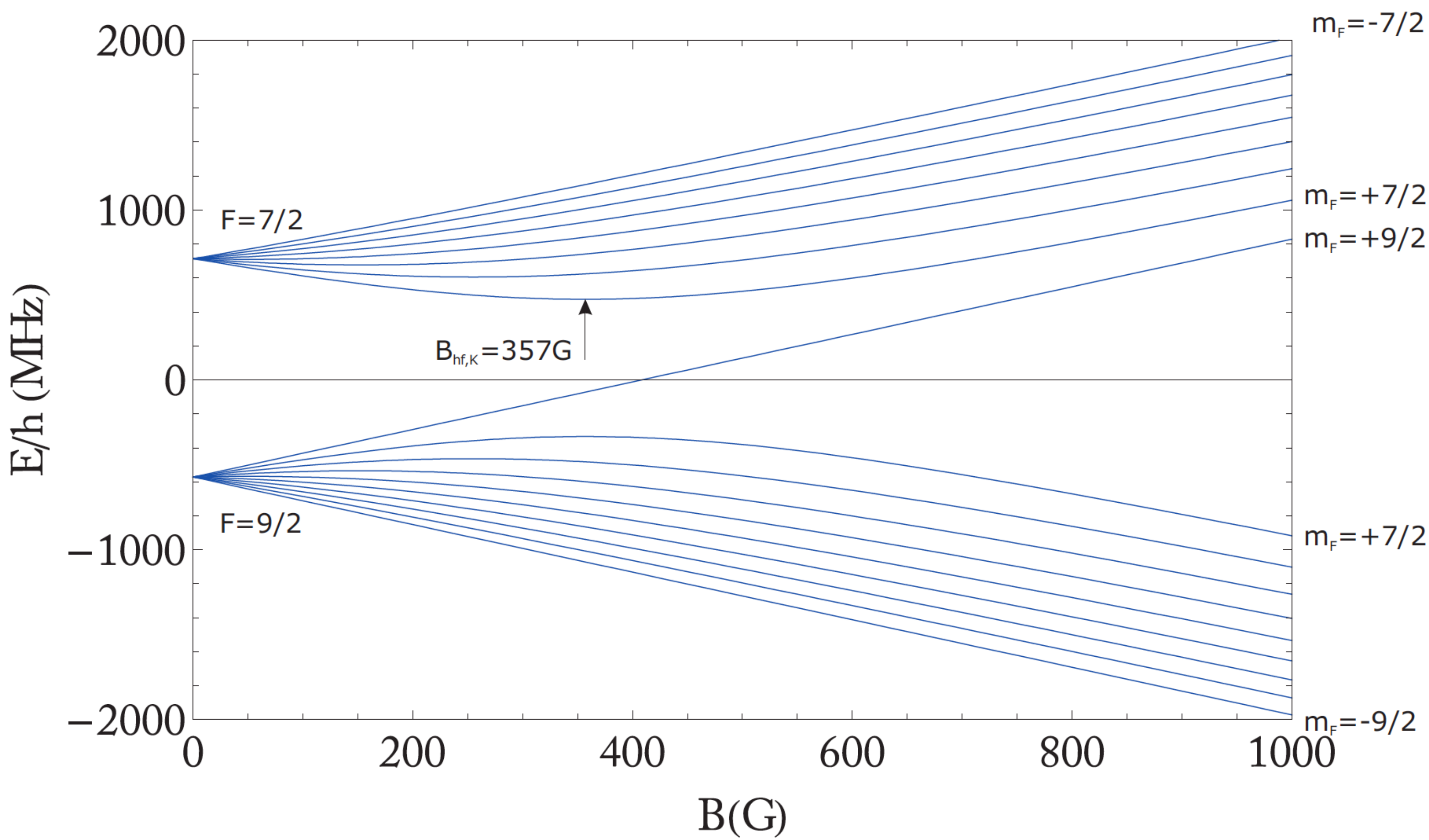
2 pairs of lasers $\rightsquigarrow$ tubes

3 pairs of lasers $\rightsquigarrow$ 3D lattice

hopping t tunable by laser



Large multiplets: reservoir of "flavors"

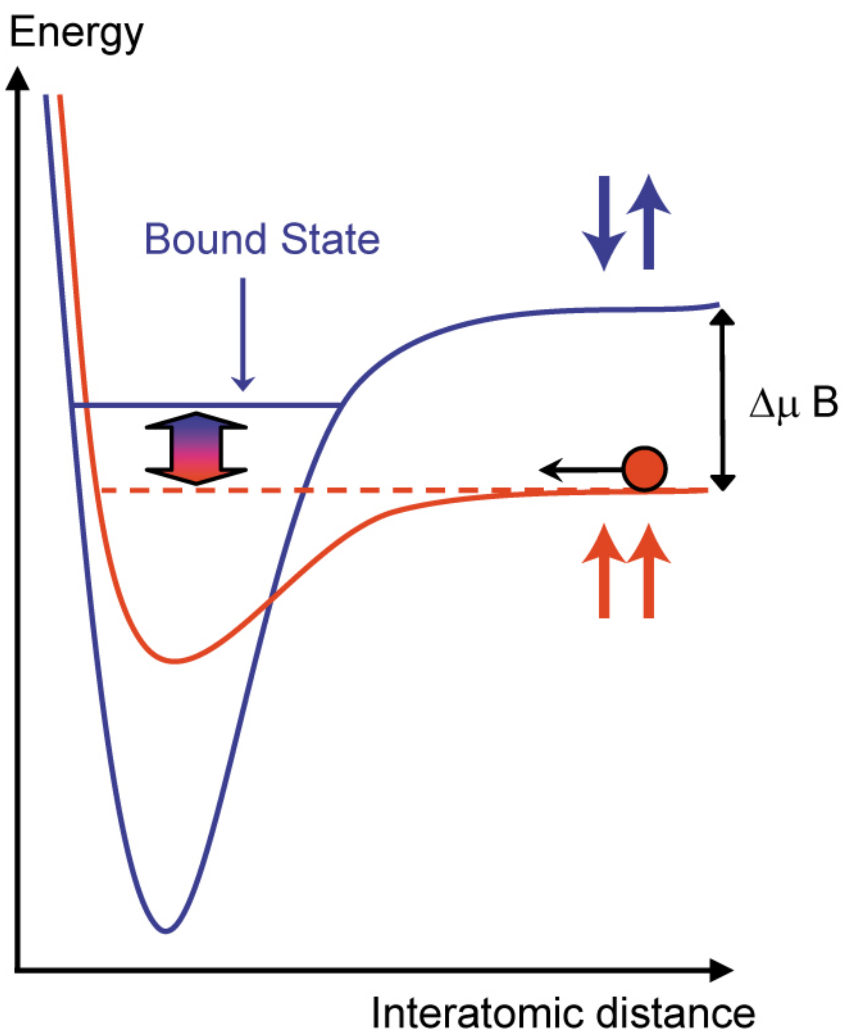


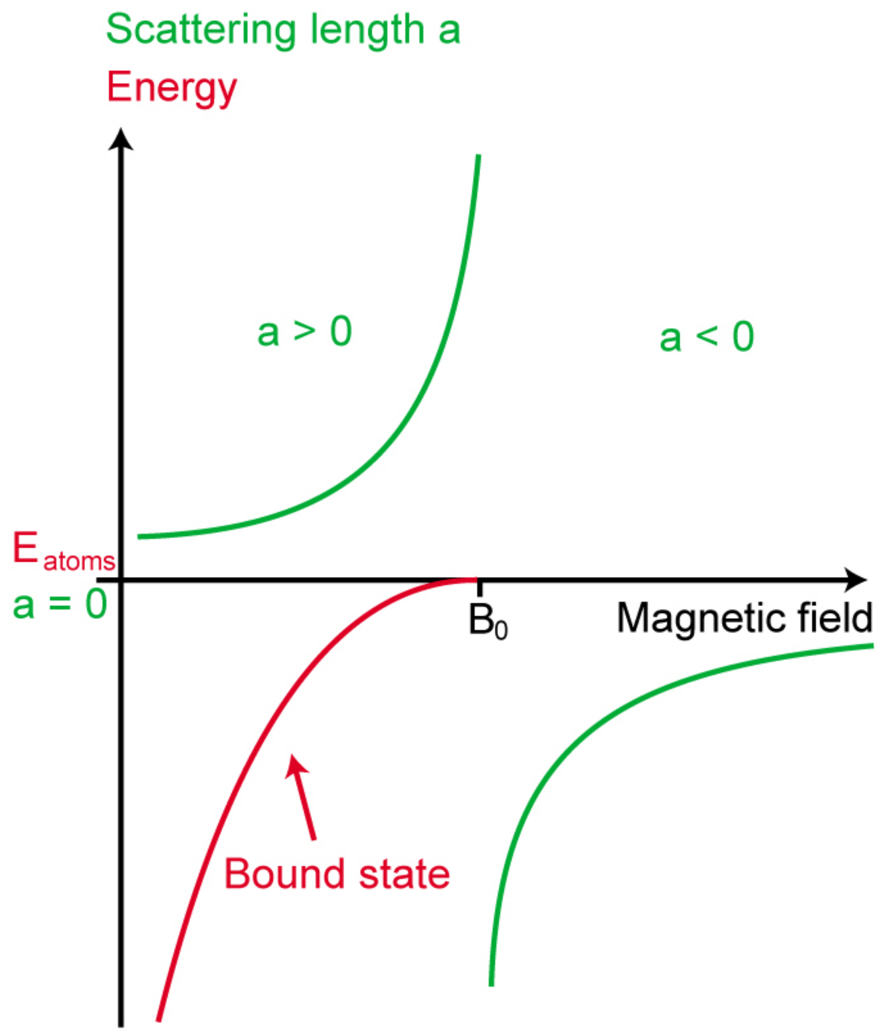
Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

[Tiecke, unpublished]

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

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

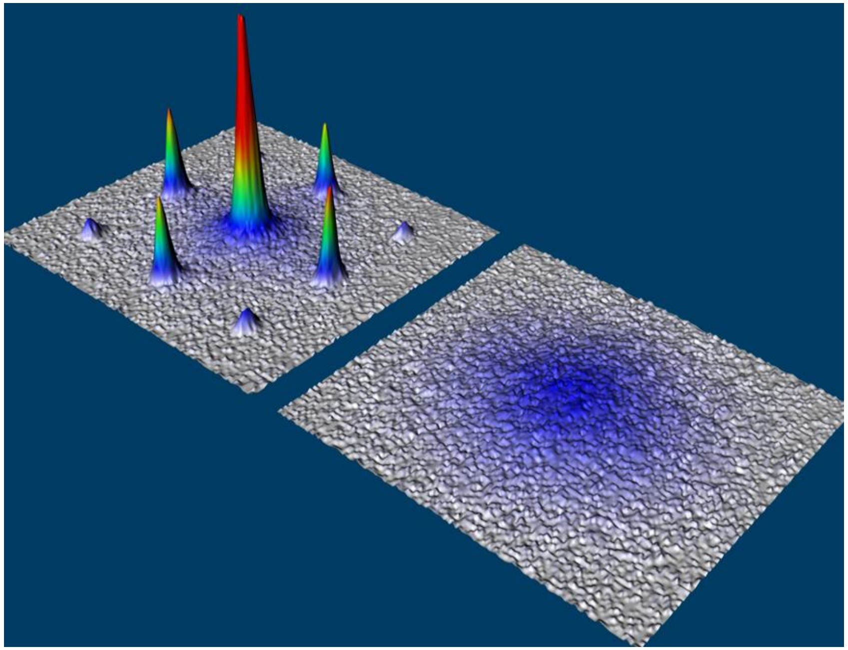




Correlated ultracold quantum gases on optical lattices: bosons

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

Time-of-flight image – $\boldsymbol{k}$ distribution



[Bloch group, 2002]

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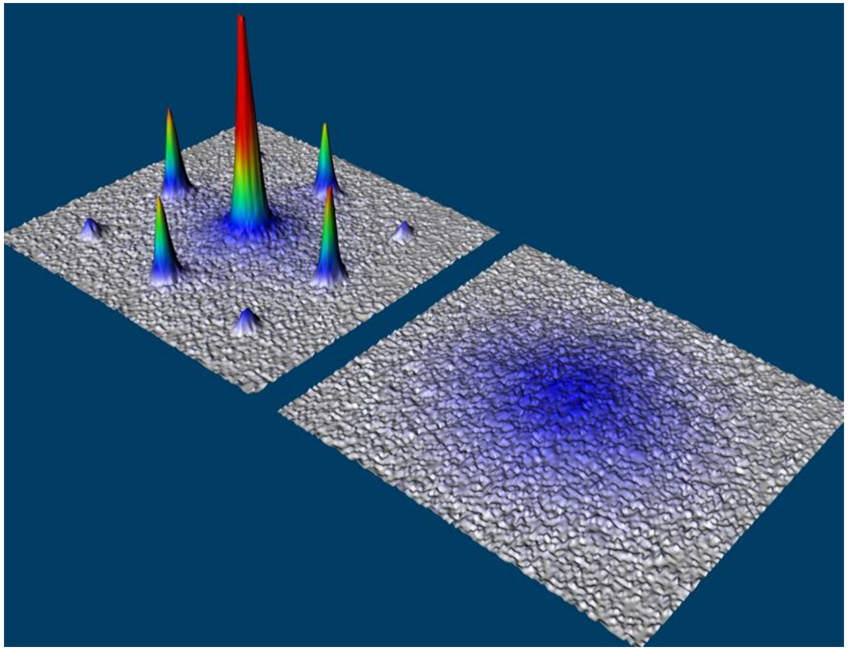

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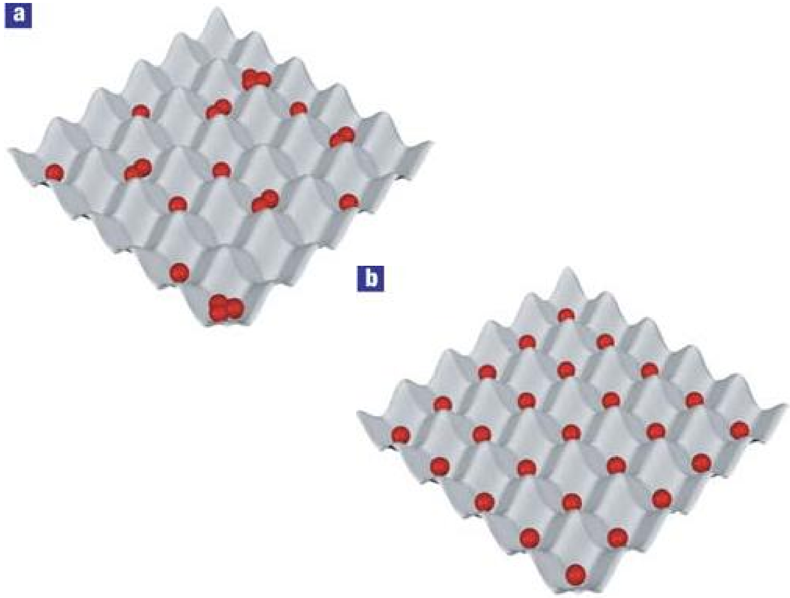
corresponding real-space picture



Superfluidity destroyed by density constraint at large U

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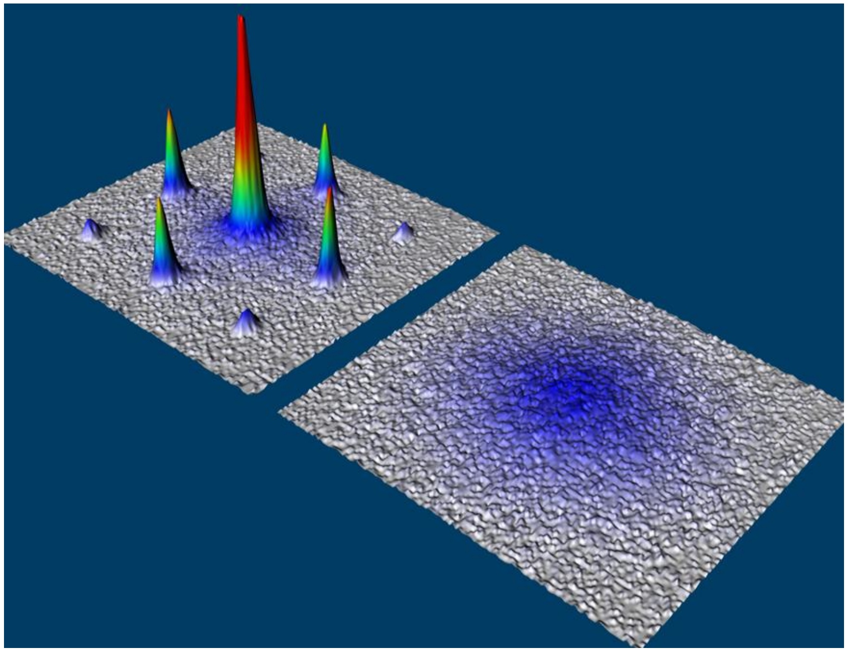

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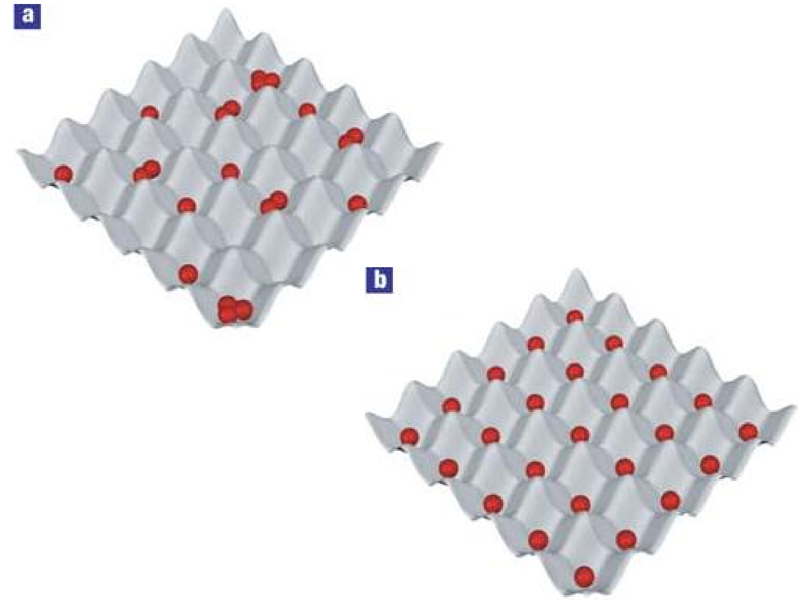

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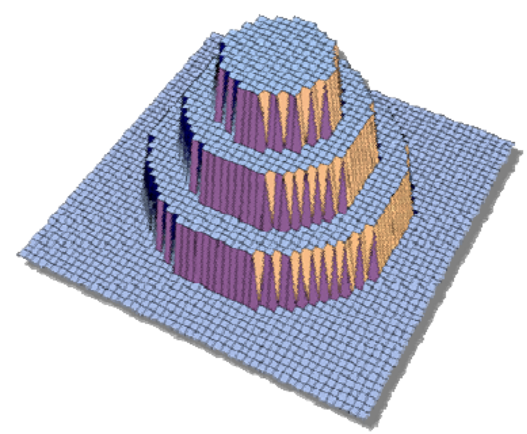
Trapping potential $\rightsquigarrow$ wedding cake structure



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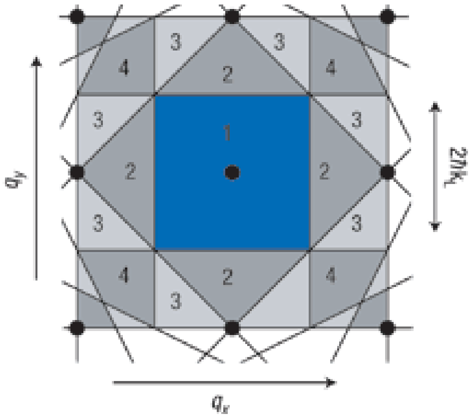

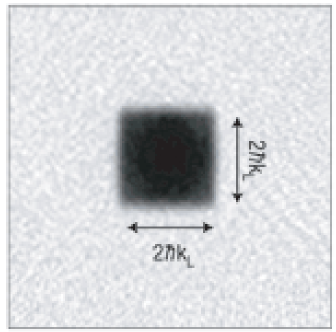

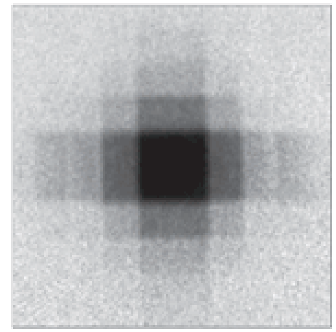

1 species: band insulator for filled 1st Brillouin zone:

[Köhl et al, PRL (2005)]

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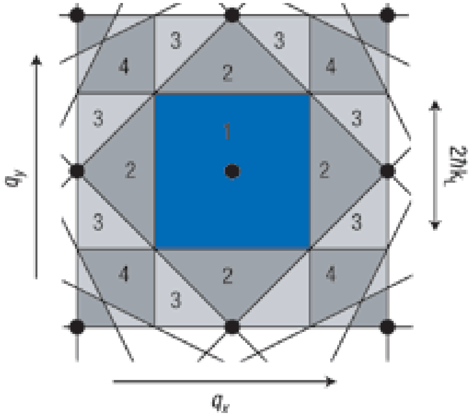

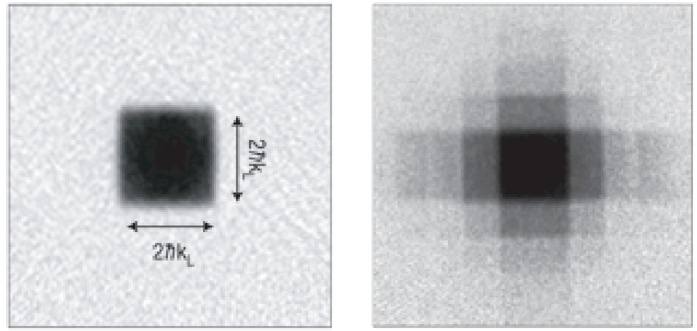

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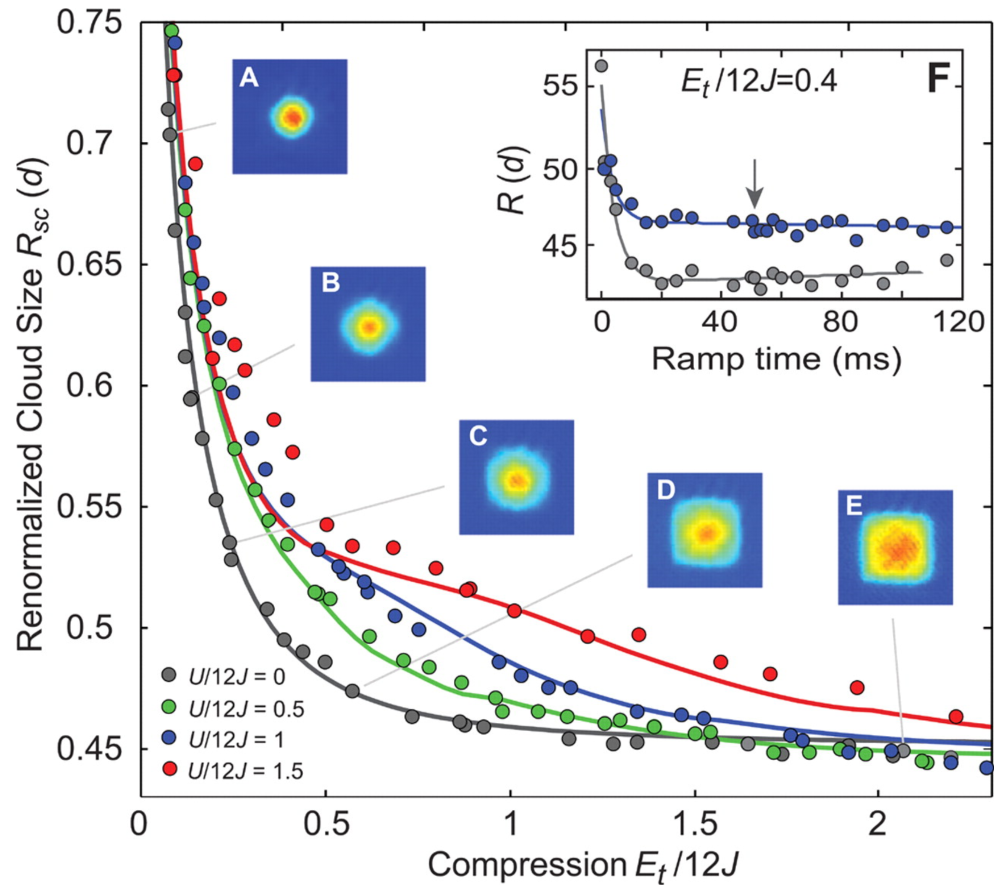
Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

Detection method: measure cloud diameter vs. trap strength

MIT signature: plateau in $R_{SC}(E_t)$

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

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



Further MIT observable: fraction of atoms with double occupations

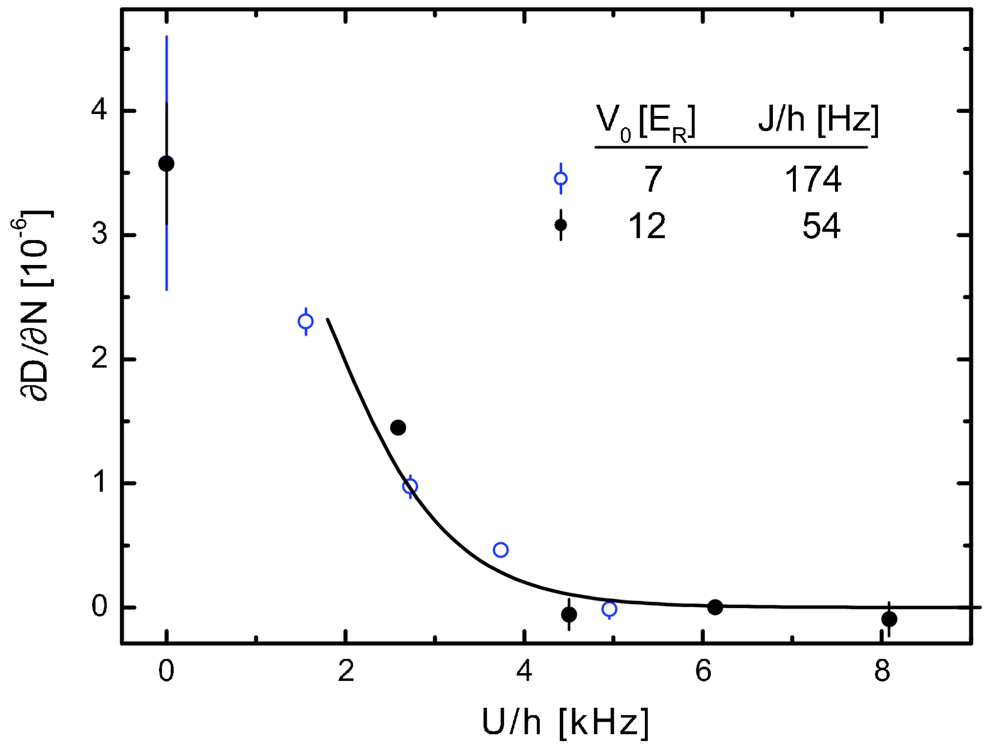
Extension of TOF technique:

- switch off hopping

- transfer atoms on doubly occupied sites to extra state (initially empty)

- expand in magnetic field ($\sim$ Stern-Gerlach)

MIT signature: suppression of D



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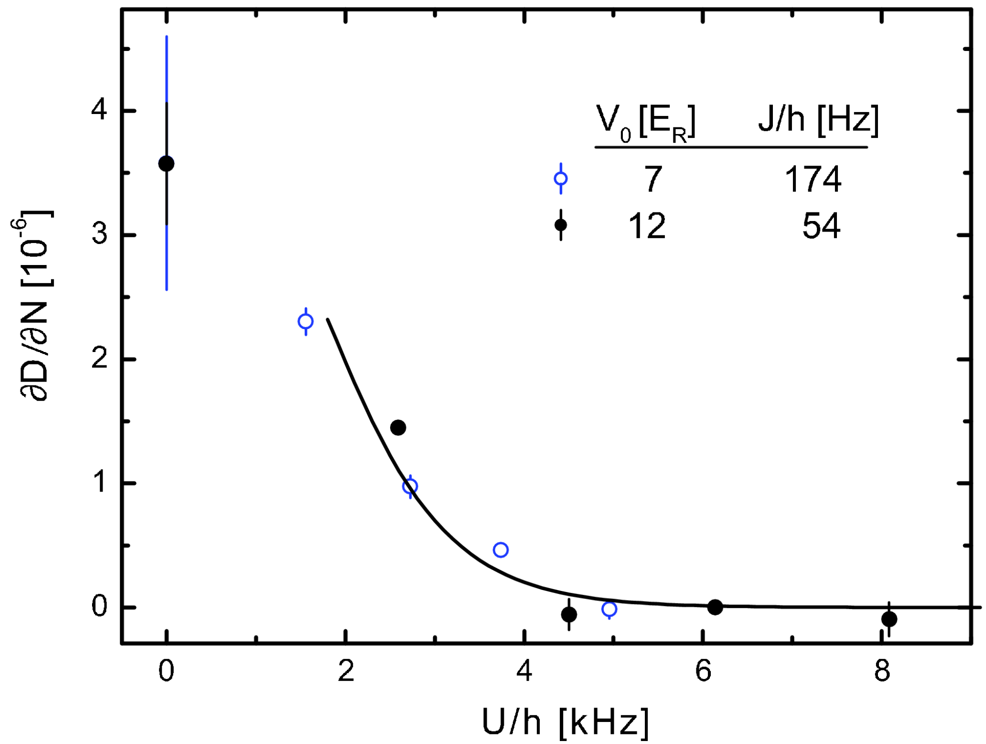

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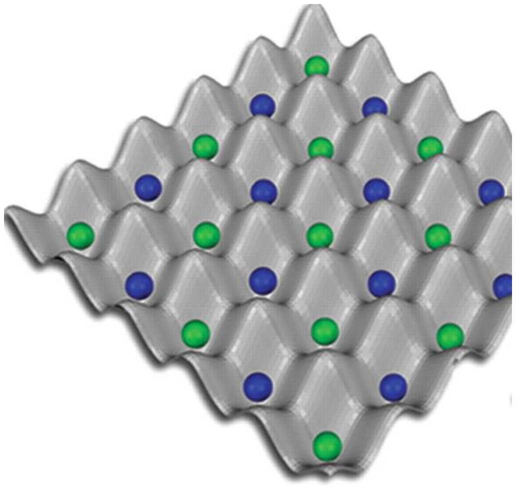
Many other phenomena seen: superconductivity, vortices, BEC-BCS crossover, . . .

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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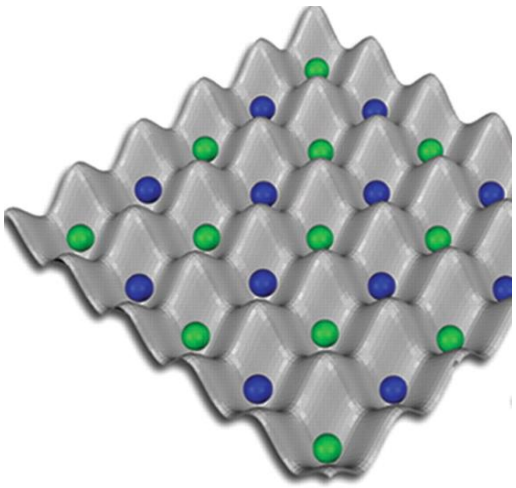

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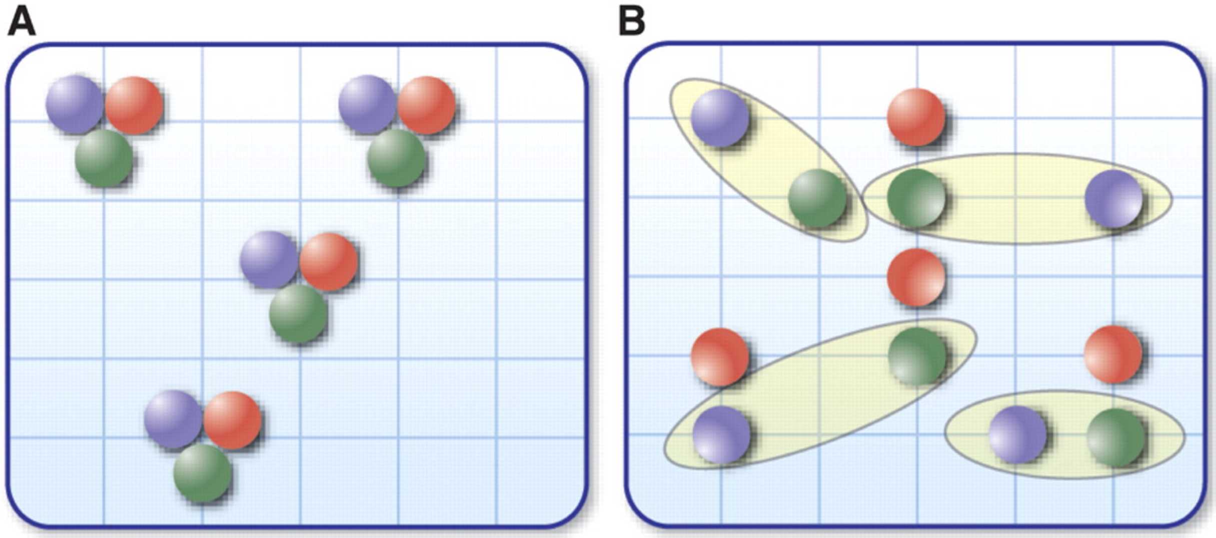
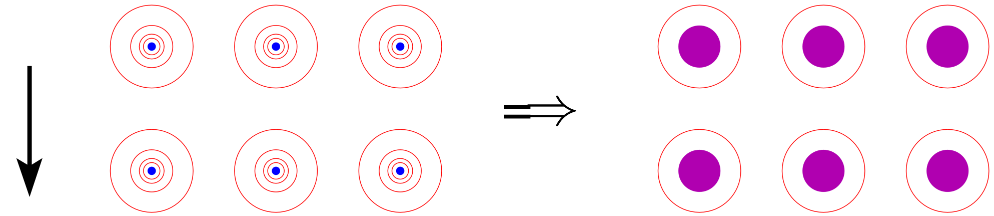
Multiflavor phenomena, e.g. trions versus color superconductivity



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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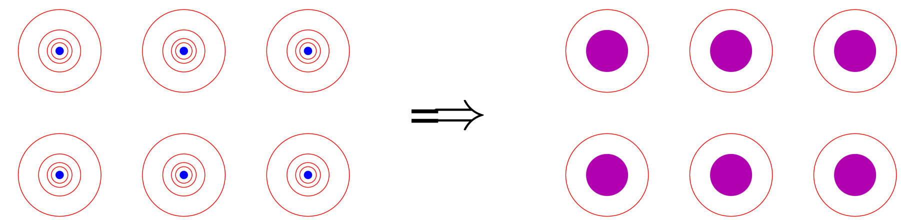

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occupation number formalism $\downarrow$ Wannier orbitals

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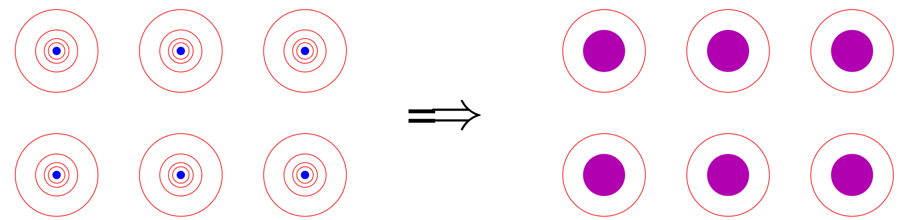

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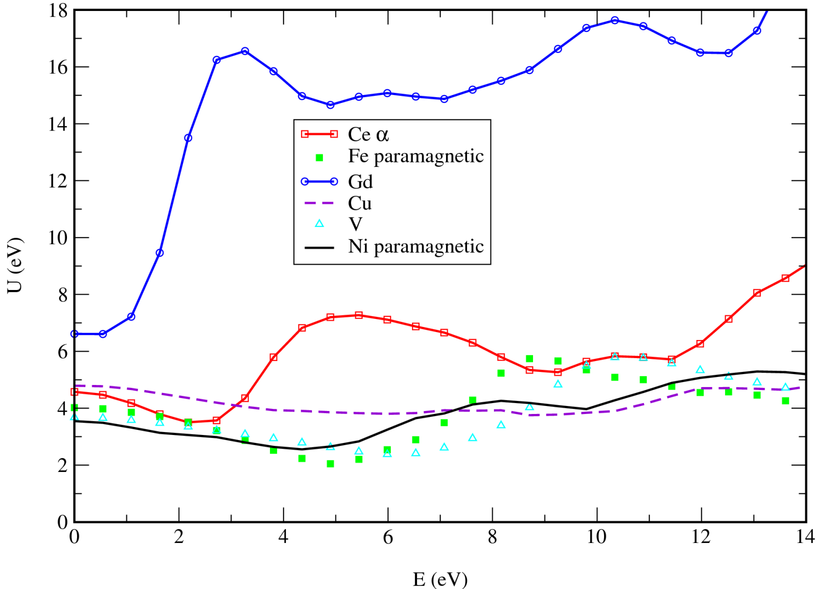
...elated lattice Fermi systems



[Aryasetiawan et al., PRB 2006]

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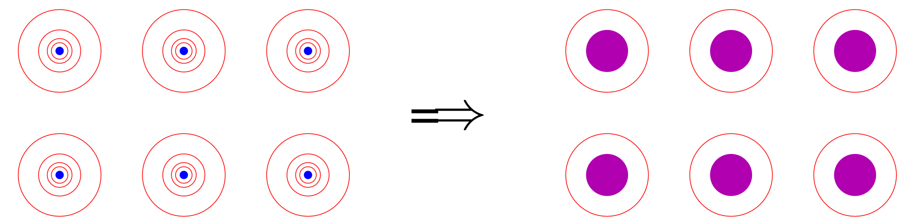
...trons ↓



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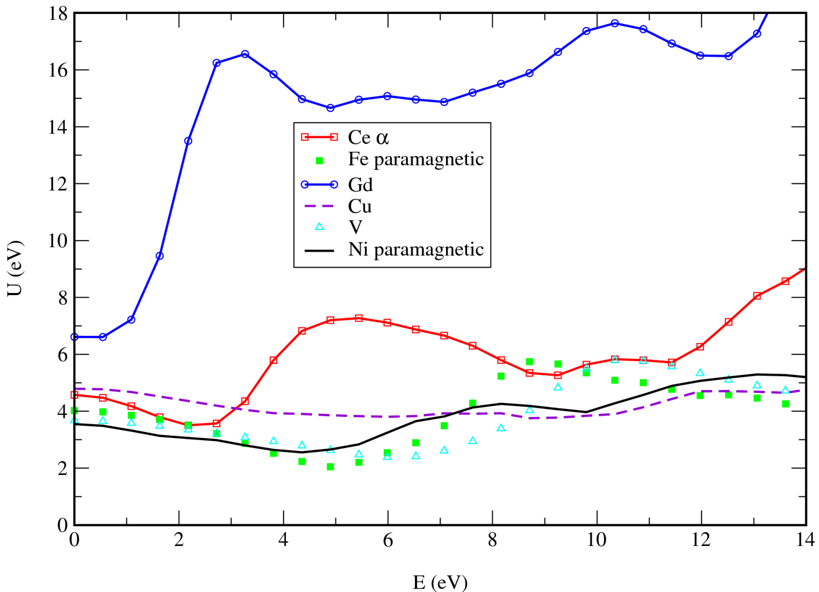

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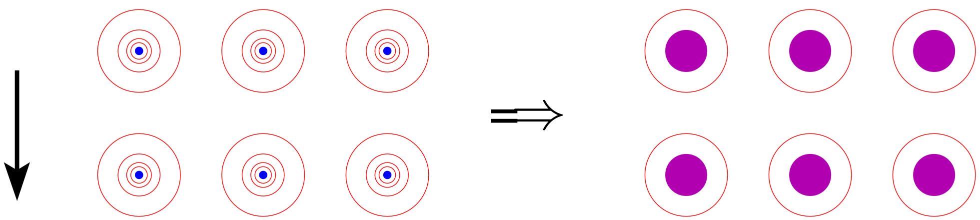
trons



$$H = \sum_{i=1}^{N_v} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\mathbf{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\mathbf{r}_i, \mathbf{r}_j)[\omega]$$

occupation number formalism ↓ Wannier orbitals

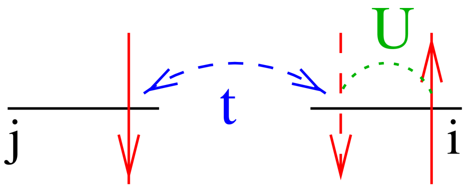
$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu'\sigma'}^{\dagger}\, \hat{c}_{n\mu'\sigma'}\,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

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

Note: no core states in quantum gas case!

Approaches for Hubbard-type models

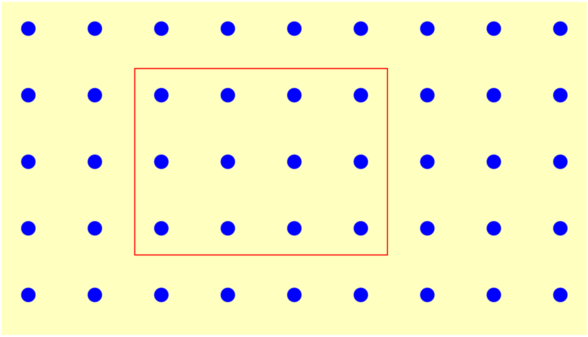
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



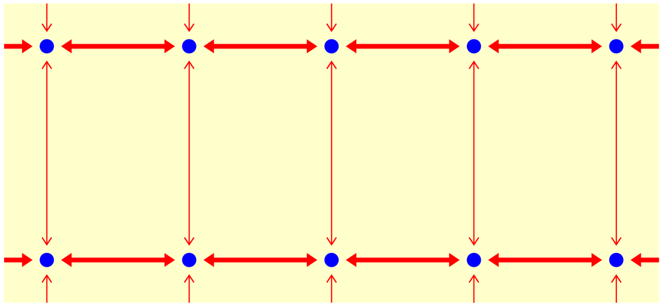
Perturbation theory

- $U \to 0$: 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



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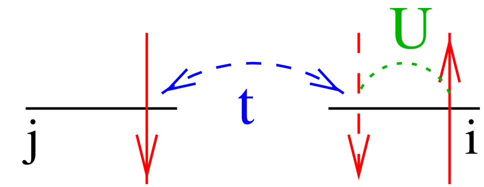

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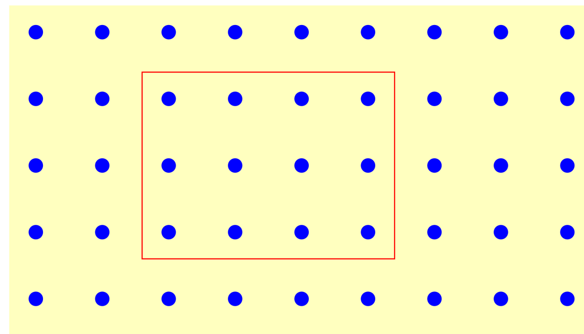

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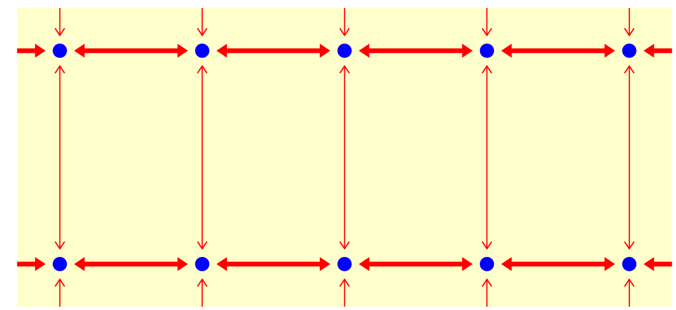
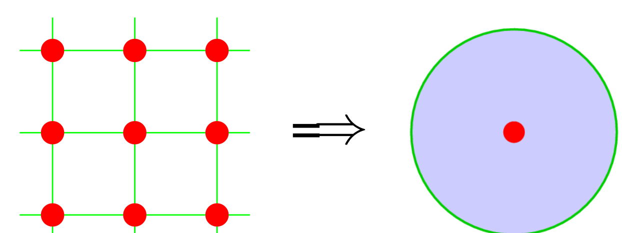


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\mathbf{k}, \omega) \equiv \Sigma(\omega)$

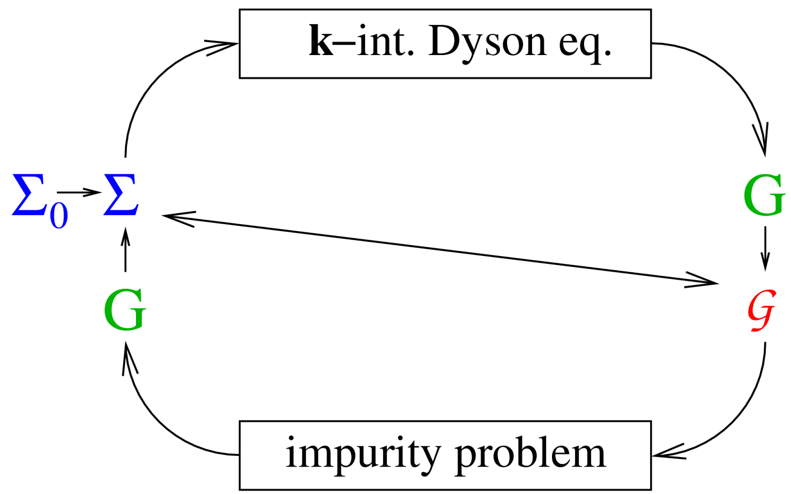
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

- \+ non-perturbative $\rightsquigarrow$ valid at MIT
- \+ 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

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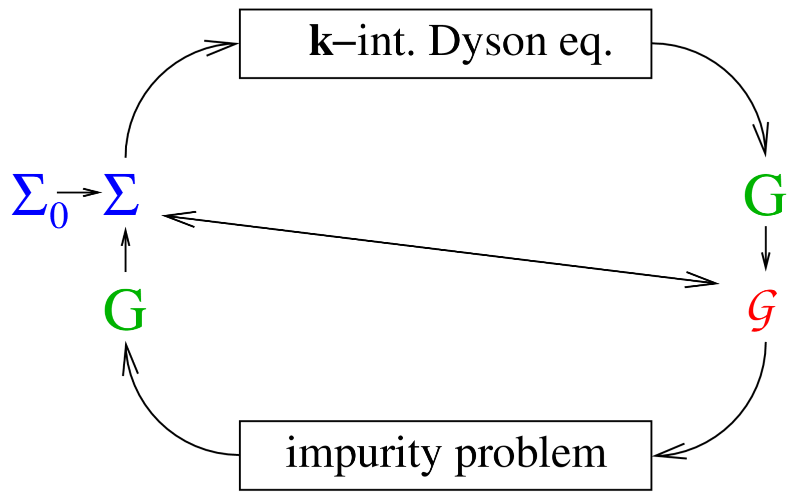
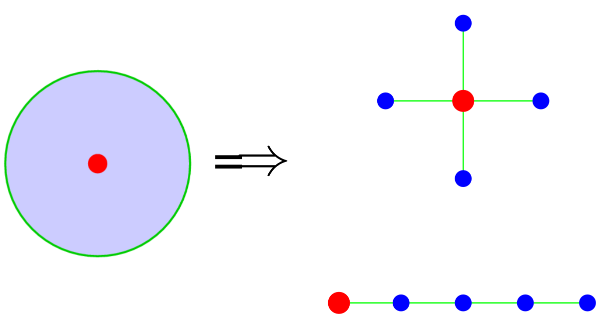


$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu \boldsymbol{k}}$

$\longleftarrow$ local interactions

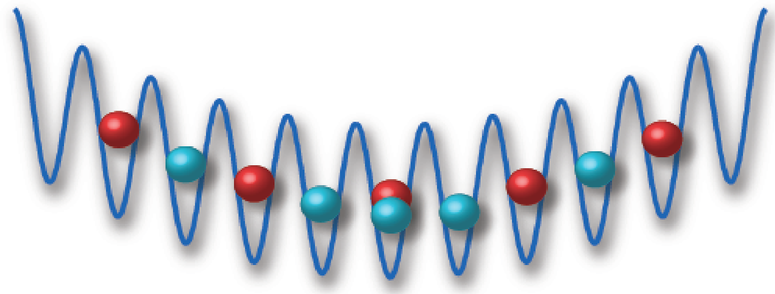
Impurity solver:

- 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)
- Self-energy functional theory (SFT) + ED



Generalization for inhomogeneous (finite-size) Hubbard type systems

Here: 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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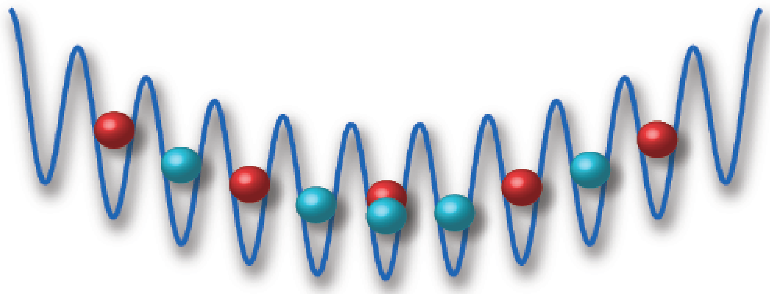

Real-space DMFT: use local, but site-dependent, self-energy

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

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

[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]

RDMFT algorithm

0) Choose $\Sigma_i(i\omega_n) \rightsquigarrow z_i(i\omega_n)$

1) For each ω_n evaluate lattice Dyson equation ($z_i \equiv z_i(i\omega_n)$):

Example: 1d chain with open bc

$$\begin{pmatrix} G_{-2,-2} & G_{-2,-1} & G_{-2,0} & G_{-2,1} & G_{-2,2} \\ G_{-1,-2} & G_{-1,-1} & G_{-1,0} & G_{-1,1} & G_{-1,2} \\ G_{0,-2} & G_{0,-1} & G_{0,0} & G_{0,1} & G_{0,2} \\ G_{1,-2} & G_{1,-1} & G_{1,0} & G_{1,1} & G_{1,2} \\ G_{2,-2} & G_{2,-1} & G_{2,0} & G_{2,1} & G_{2,2} \end{pmatrix} = \begin{pmatrix} z_{-2} & -t & 0 & 0 & 0 \\ -t & z_{-1} & -t & 0 & 0 \\ 0 & -t & z_0 & -t & 0 \\ 0 & 0 & -t & z_1 & -t \\ 0 & 0 & 0 & -t & z_2 \end{pmatrix}^{-1}$$

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2) Compute bath Green function: $\mathcal{G}_i^{-1}(i\omega_n) = G_{ii}^{-1} + \Sigma_i(i\omega_n) \quad \forall i, \omega_n$

3) Solve impurity model ($\mathcal{G}_i$, U_i, V_i, μ, T) for each inequivalent site i

4) Compute new self-energy $\Sigma_i(i\omega_n) = \mathcal{G}_i^{-1}(i\omega_n) - G_{ii}^{-1} \quad \forall i, \omega_n$

Repeat steps 1) – 4) until convergence

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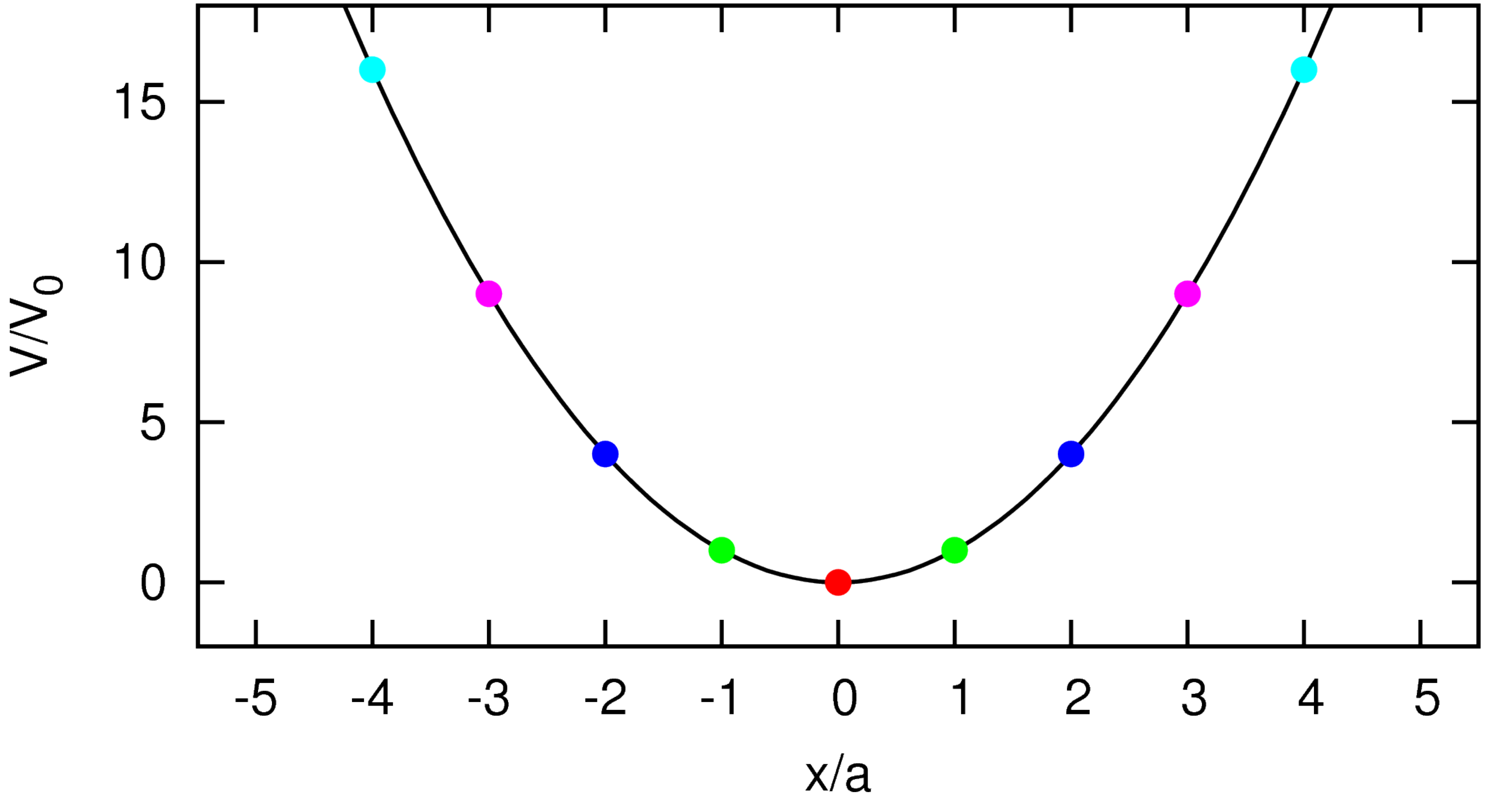
Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

All previous implementations: RDMFT+NRG

Simple approximation: "local density approximation (LDA)"

Approximate properties of each site by properties of homogeneous system with same effective chemical potential ($\rightsquigarrow$ standard DMFT)

Example: 1d chain



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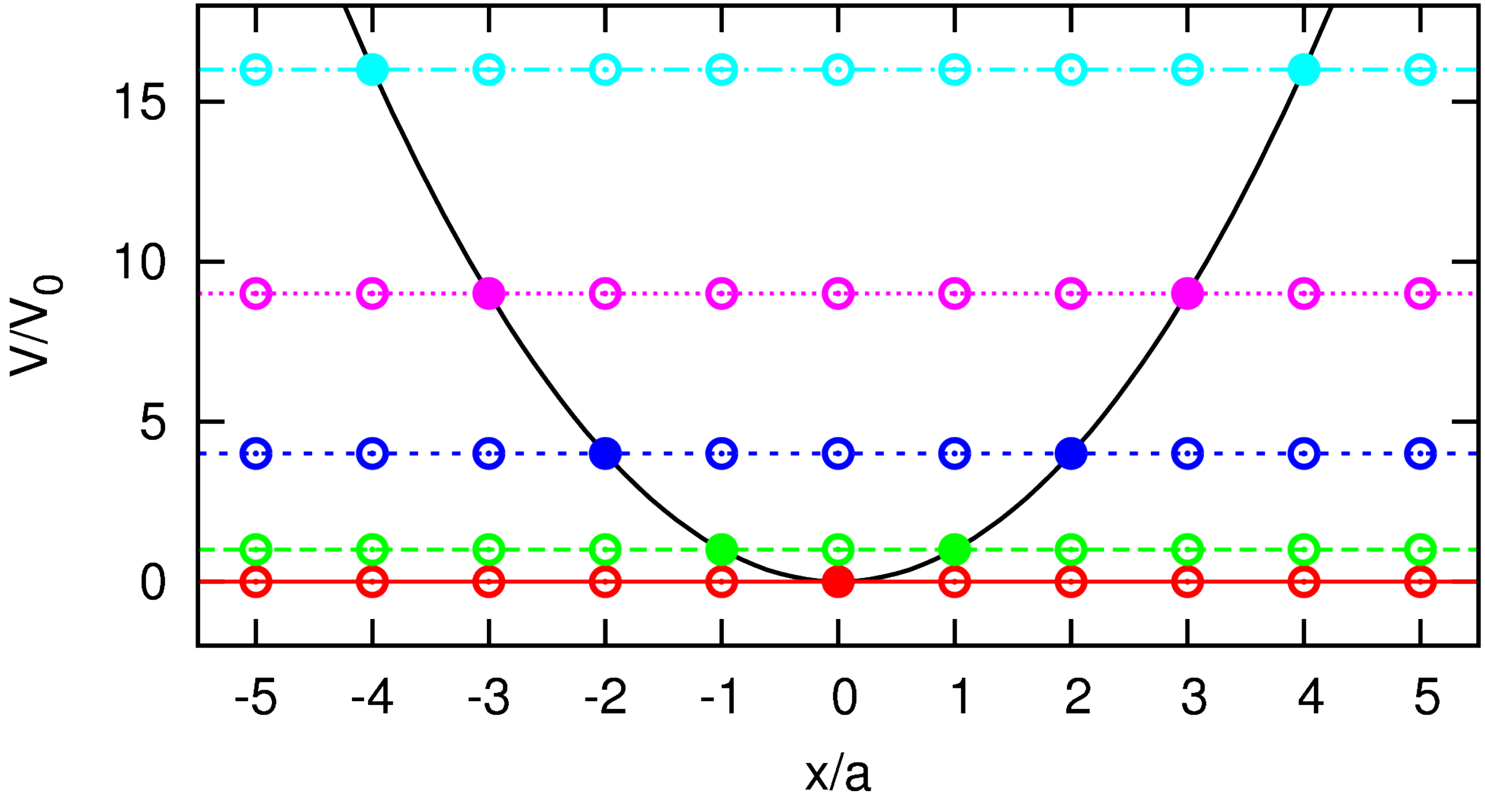

. . . will be used for comparison to RDMFT

Much better: "slab approximation" ($\longrightarrow$ discussion)

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

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

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

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

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

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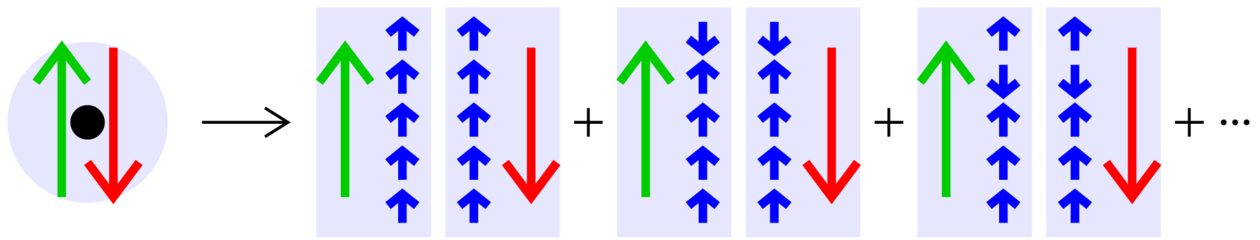

Wick theorem:

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

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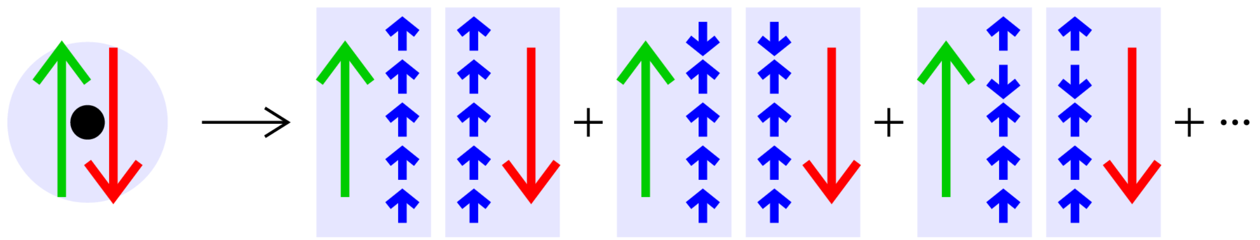


Wick theorem:

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

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

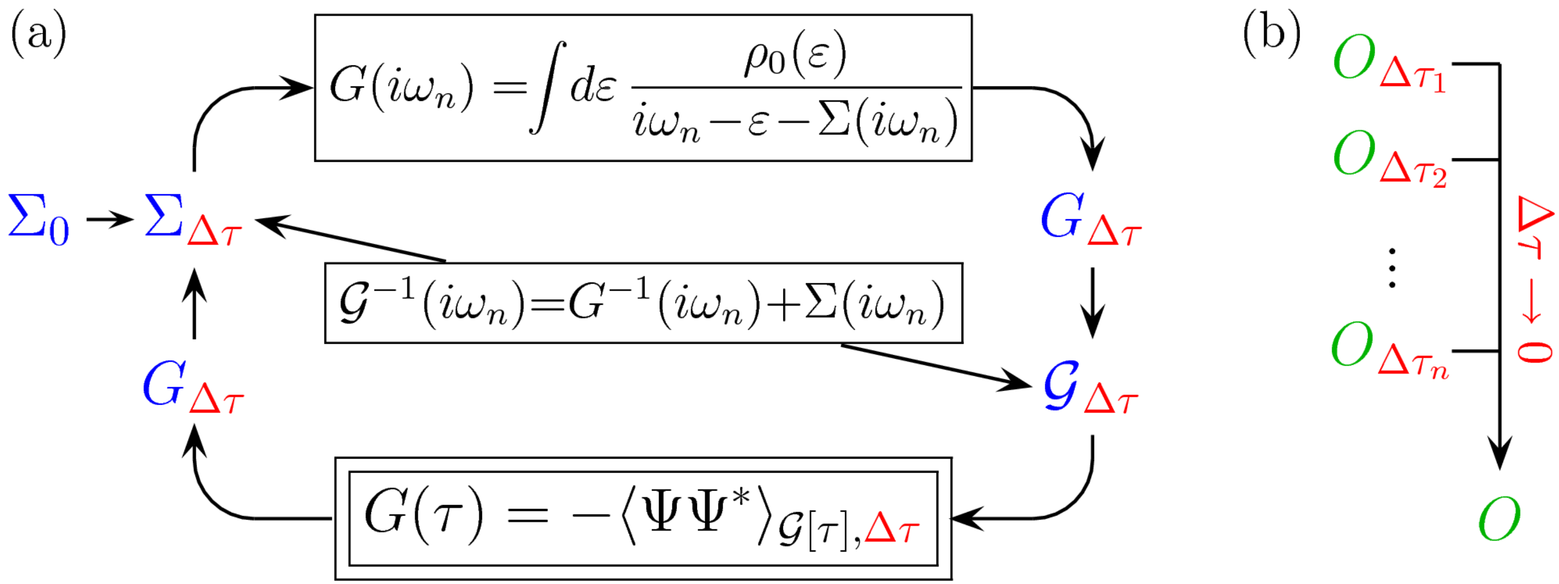
+ numerically exact, + no sign problem, − effort scales as T^{-3}

(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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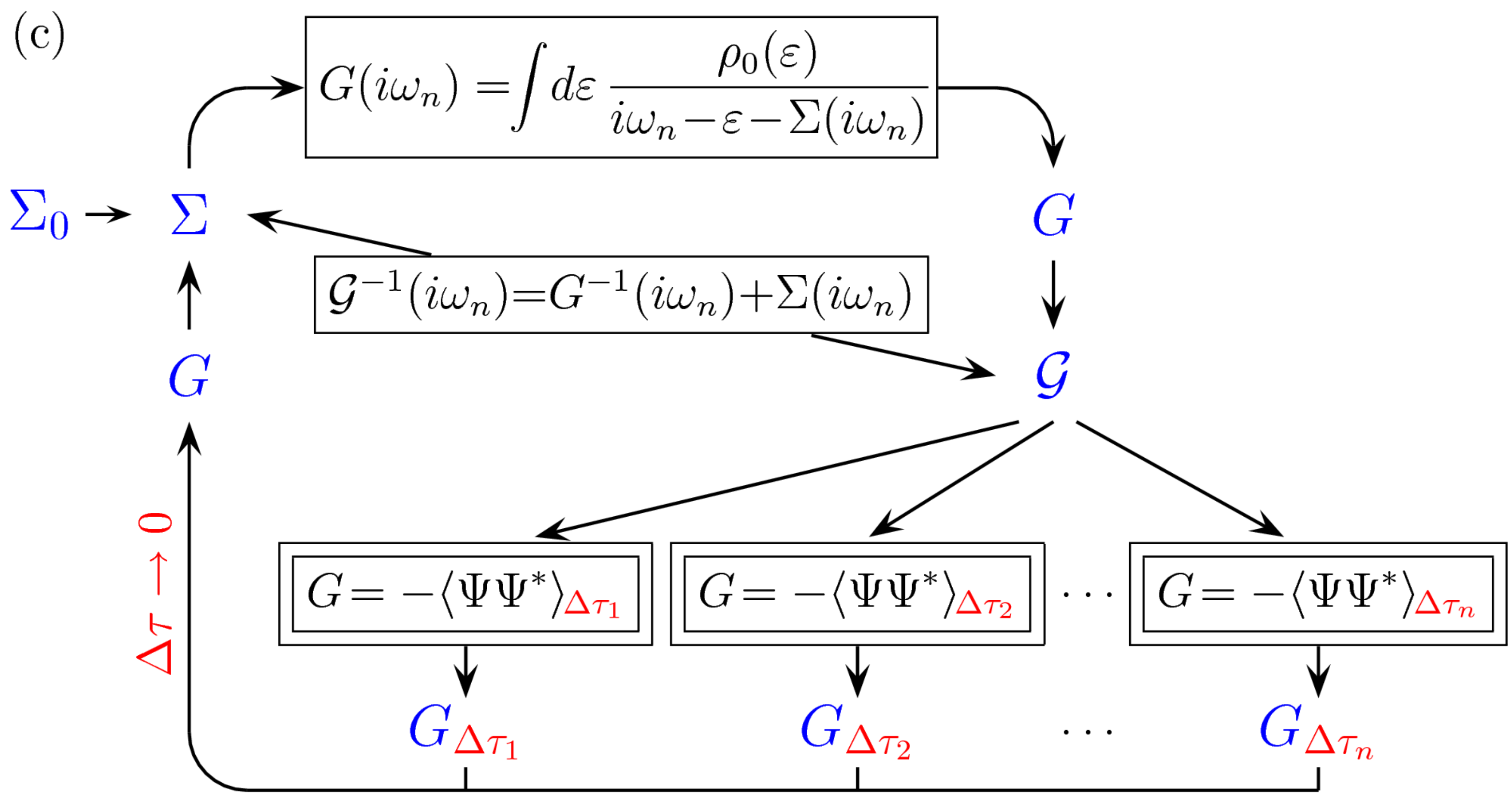


(c) Multigrid HF-QMC: internal elimination of Trotter error

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

Antiferromagnetic order at finite T in an optical trap

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

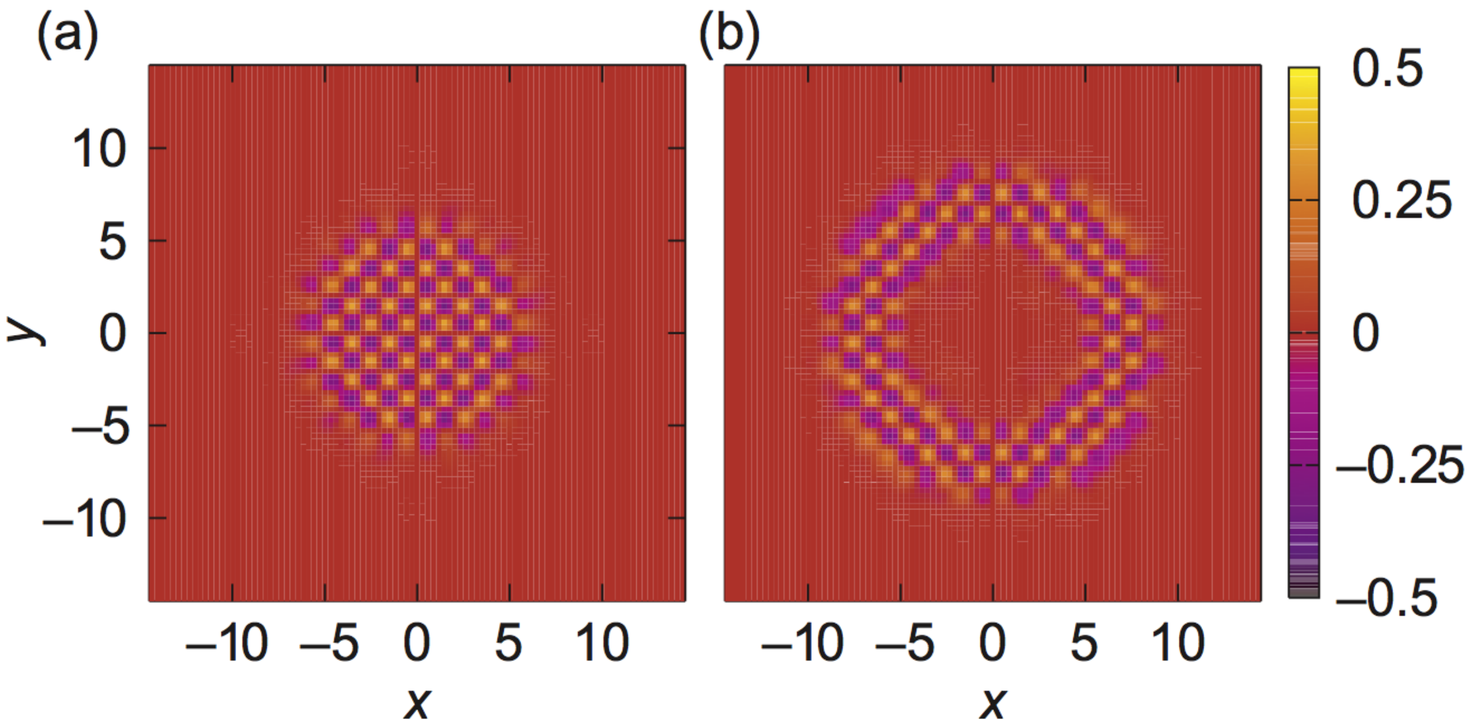
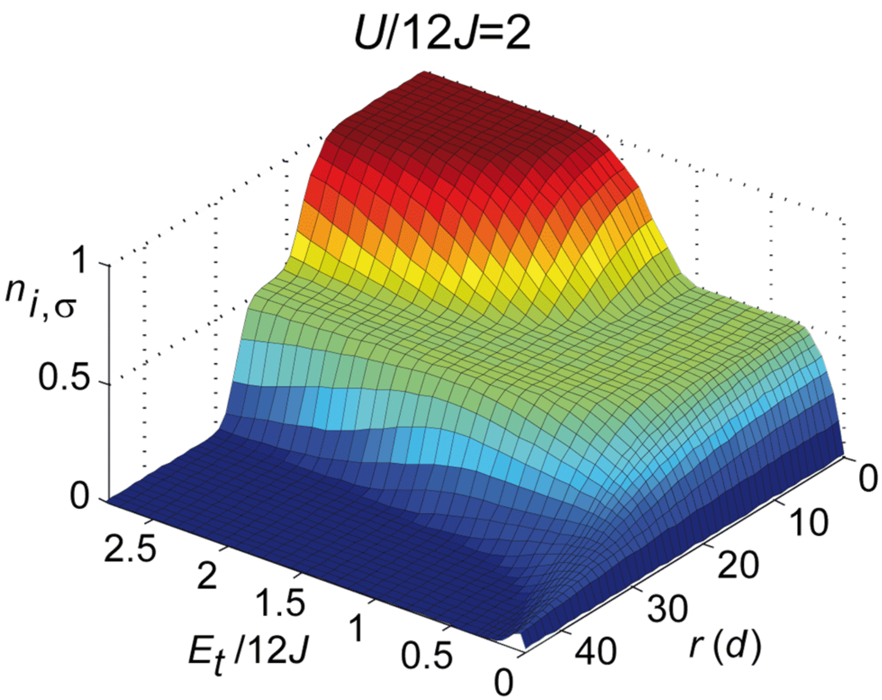


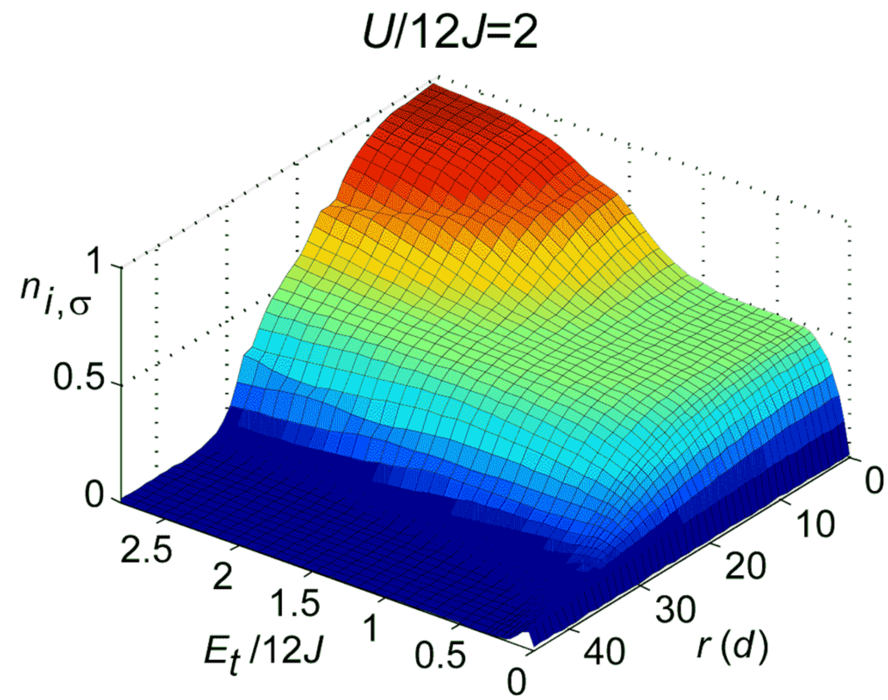
Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_\uparrow = \mu_\downarrow = 5$; (b) $V = 0.2$ and $\mu_\uparrow = \mu_\downarrow = 15$. Energies are expressed in units of the hopping parameter J.

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

But: NRG problematic at elevated temperatures



$T = 0.07t$

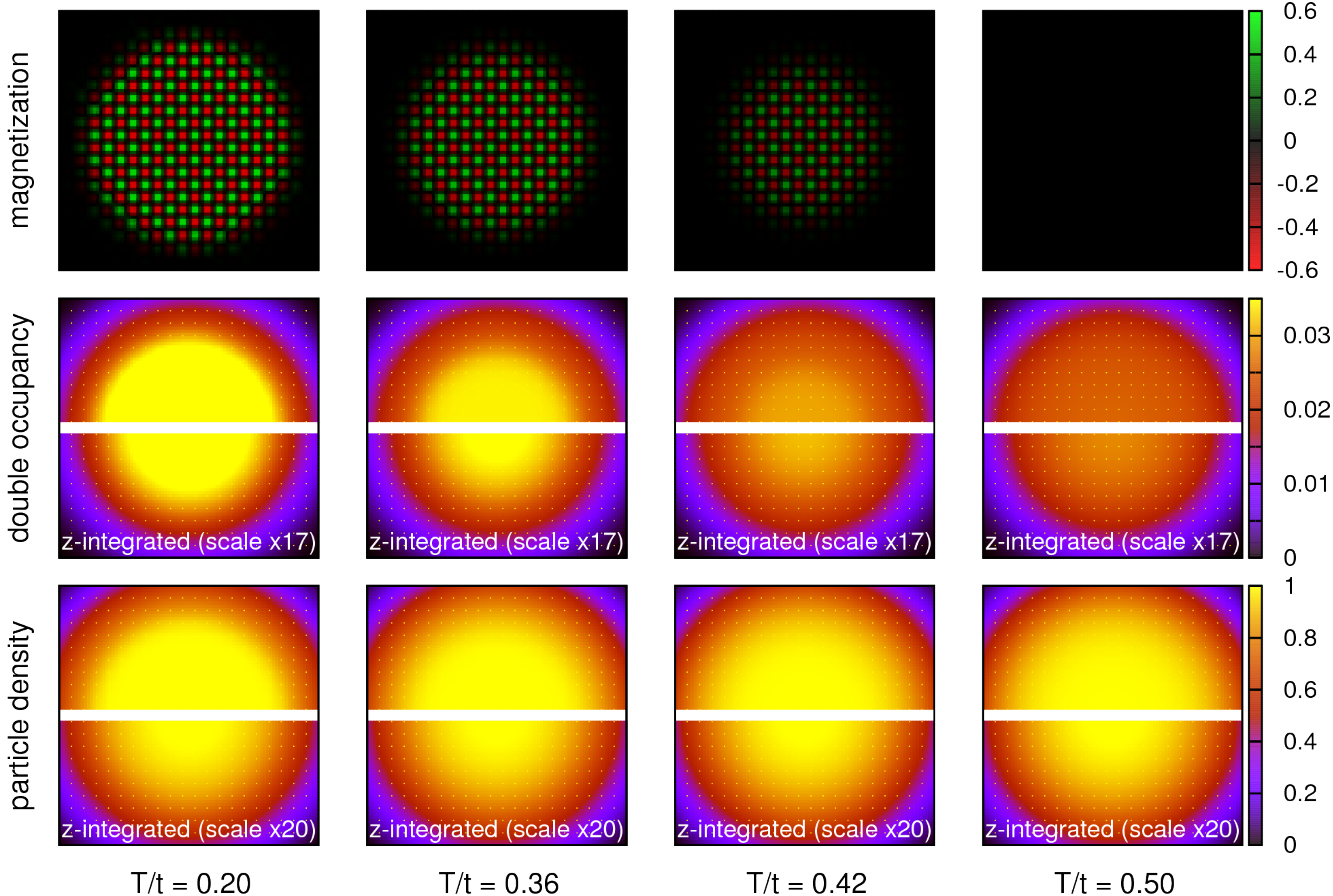


$T = 0.15t$

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!

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



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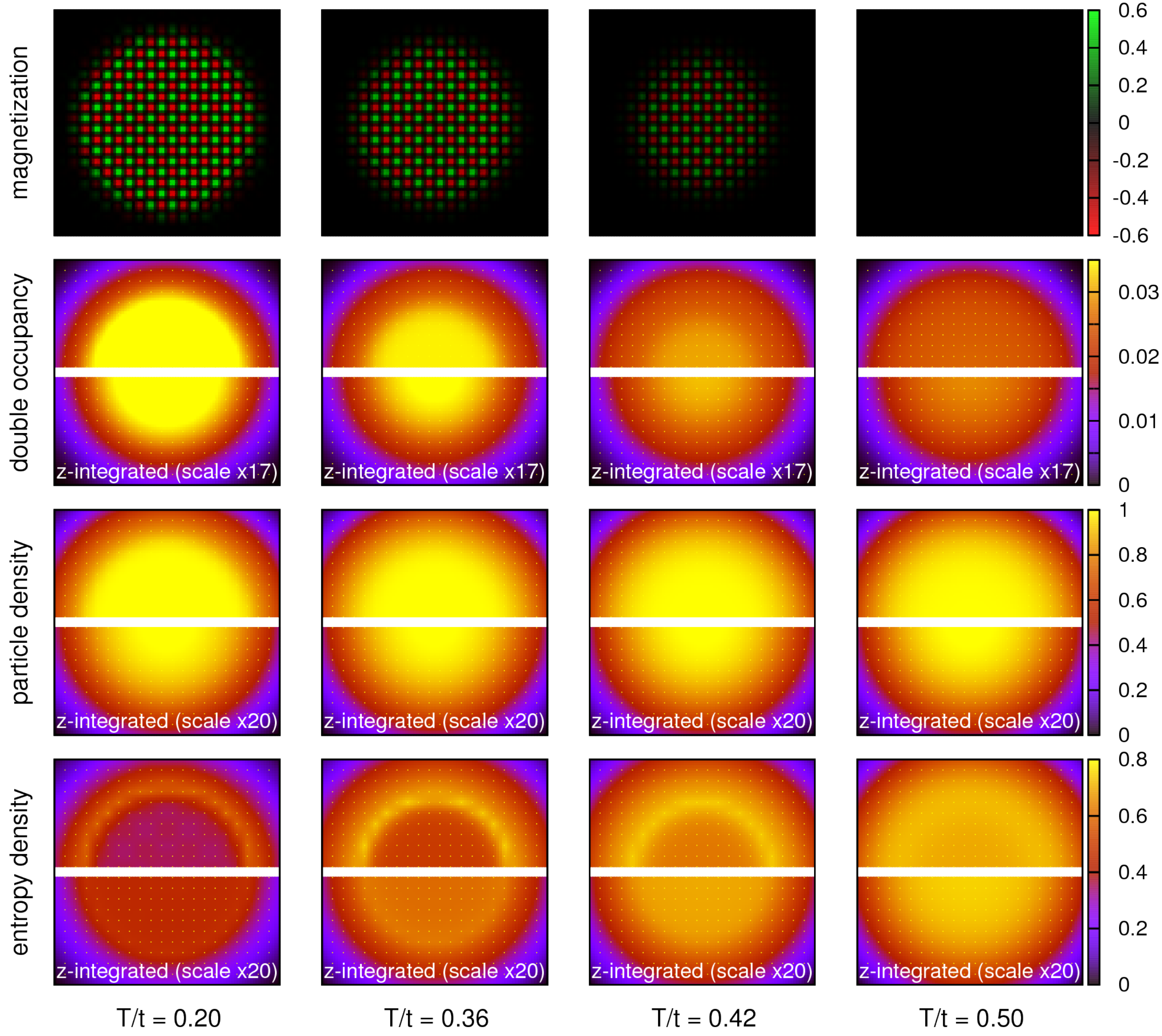


AF core:

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)

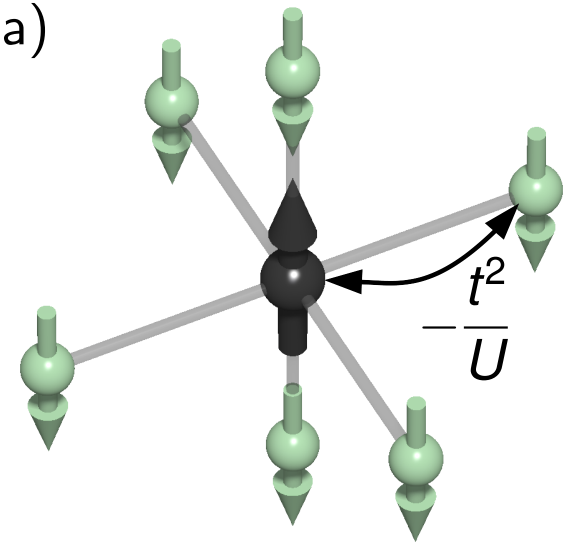
Entropy

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

Enhanced double occupancy: a signature of AF order

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

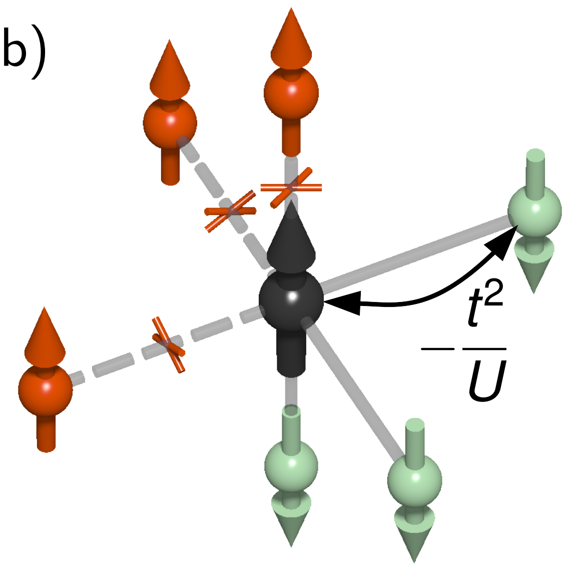
(a)



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

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

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

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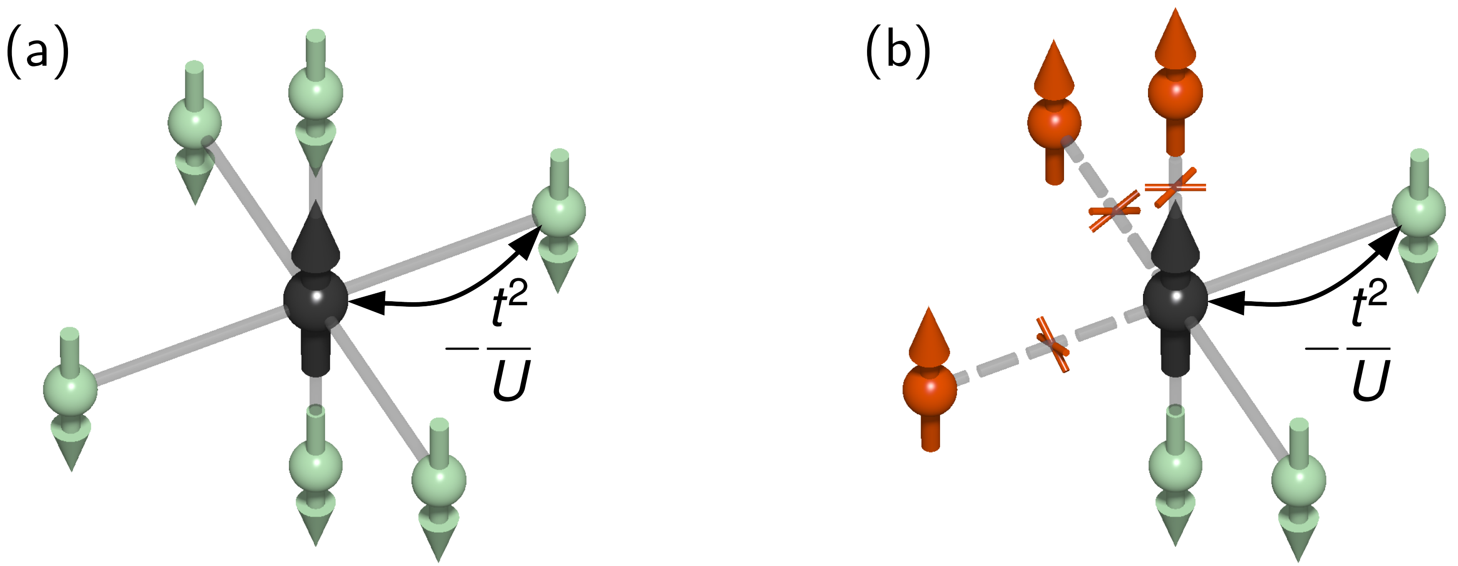

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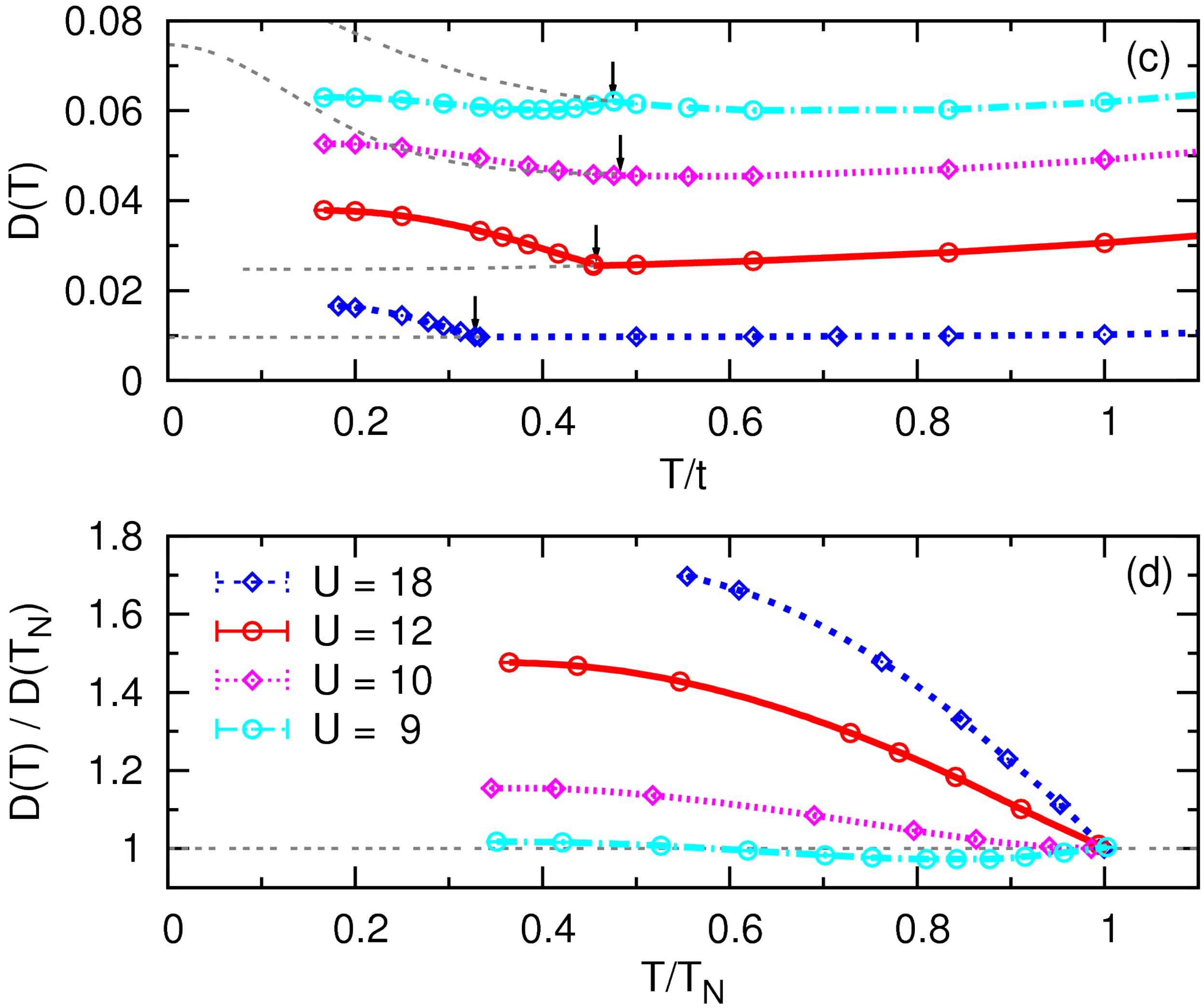
By $D = dE/dU$ (at $T = 0$), the argument implies $D_{\mathbf{AF}}/D_{\mathbf{p}} \stackrel{U\to\infty}{\longrightarrow} 2$.

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 D at half filling



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

arrows: Néel temperatures

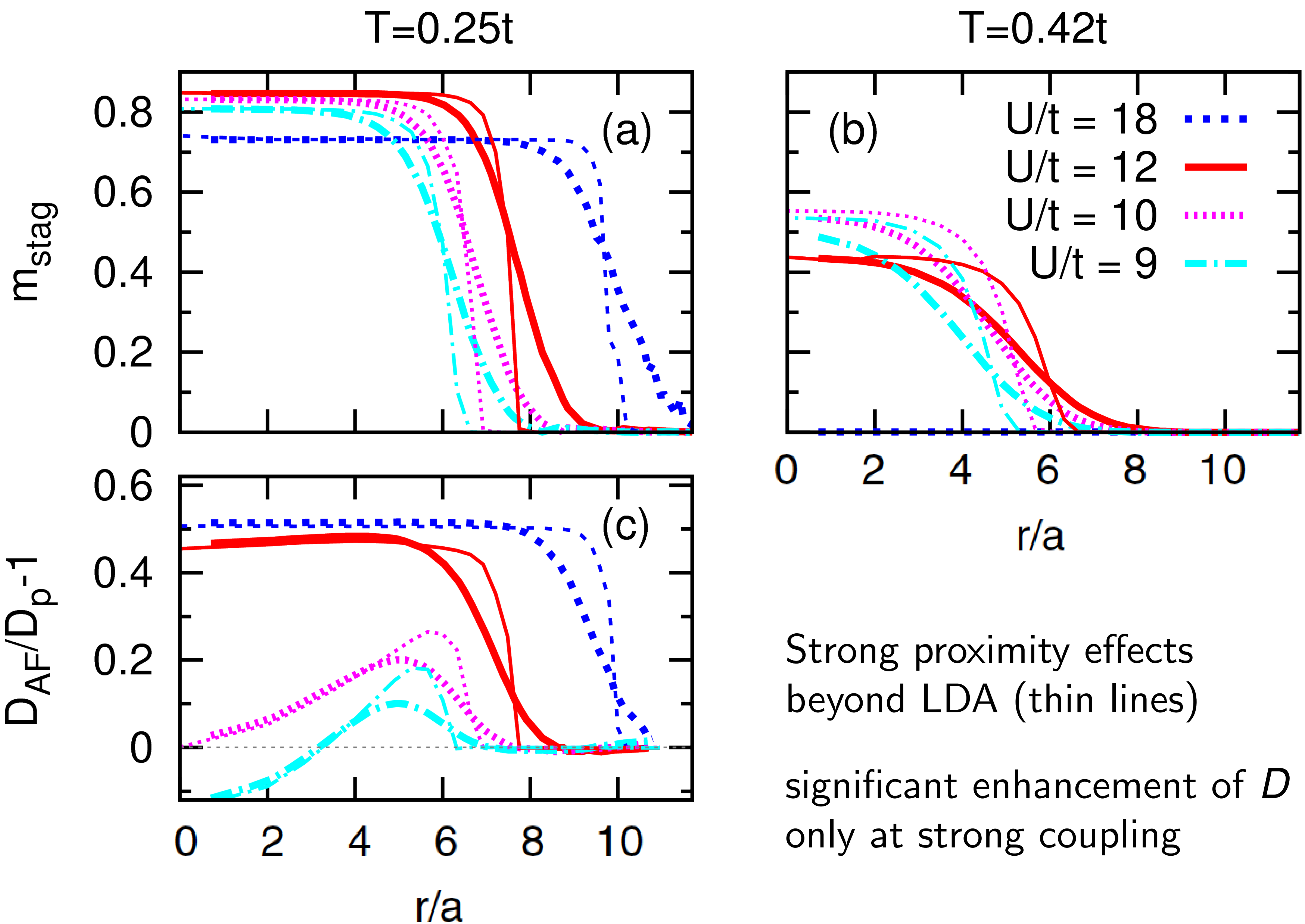
thin lines: metastable paramagnetic phase.

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)]!

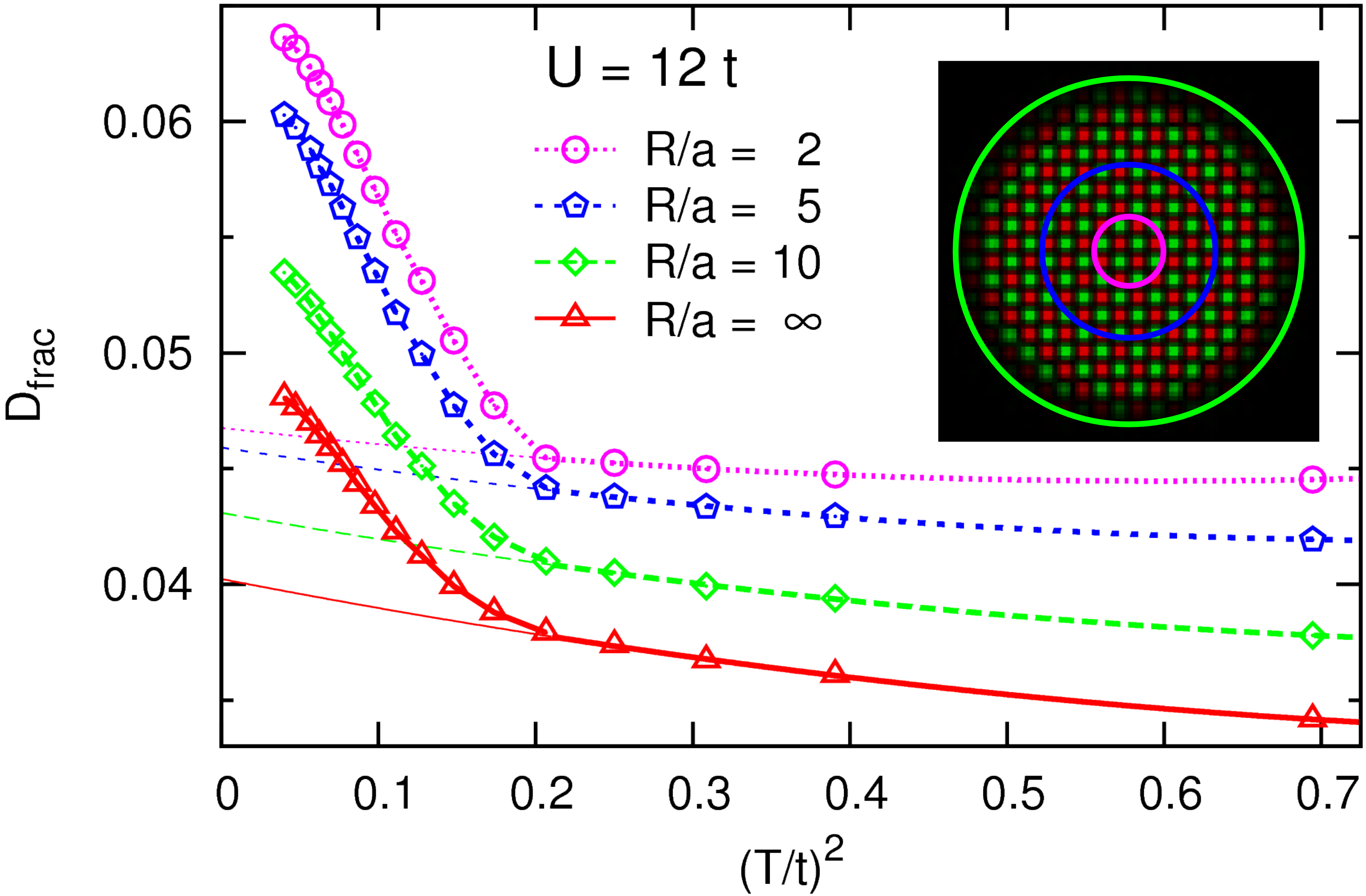
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



Strong proximity effects beyond LDA (thin lines)

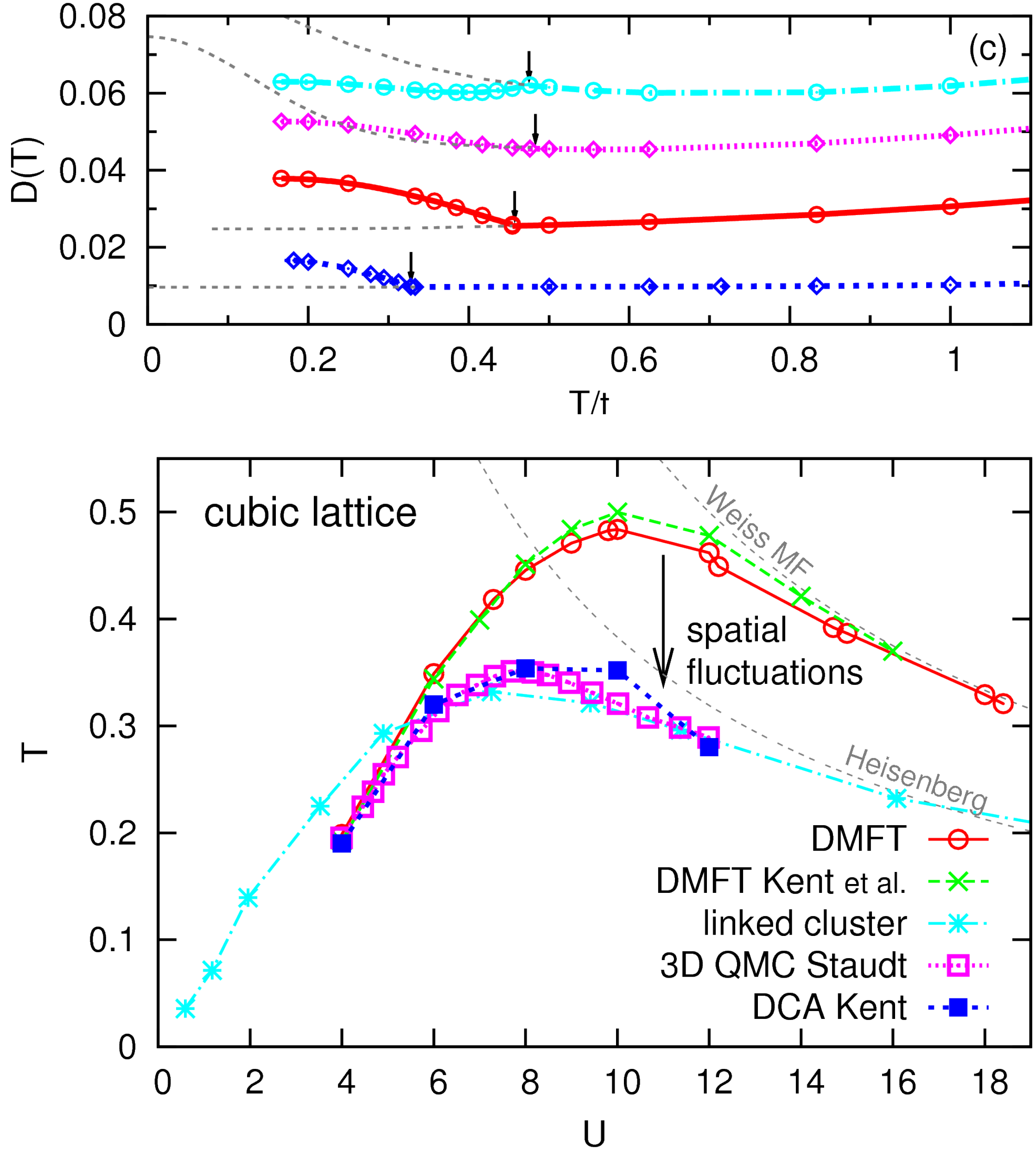
significant enhancement of D only at strong coupling

Néel transition visible in integrated quantities? Yes!



but: effects of nonlocal correlations?

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



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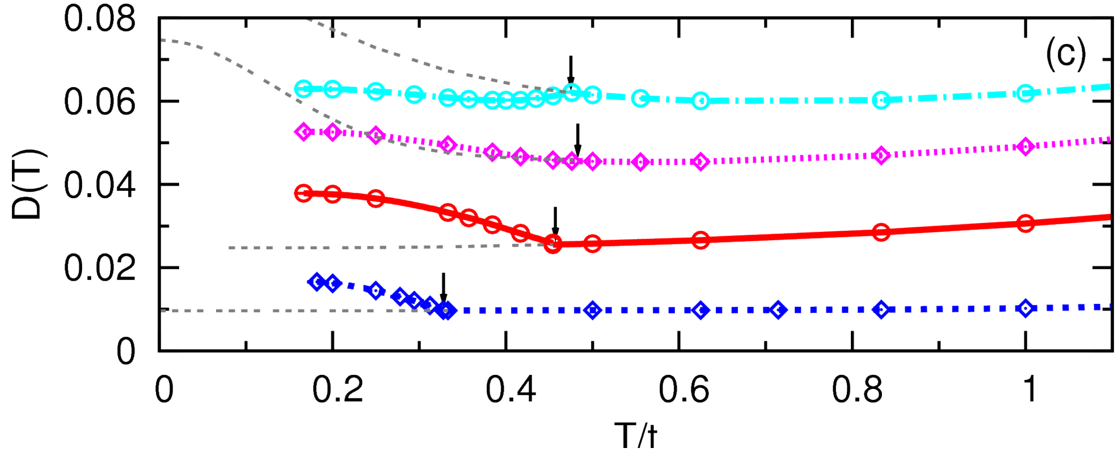

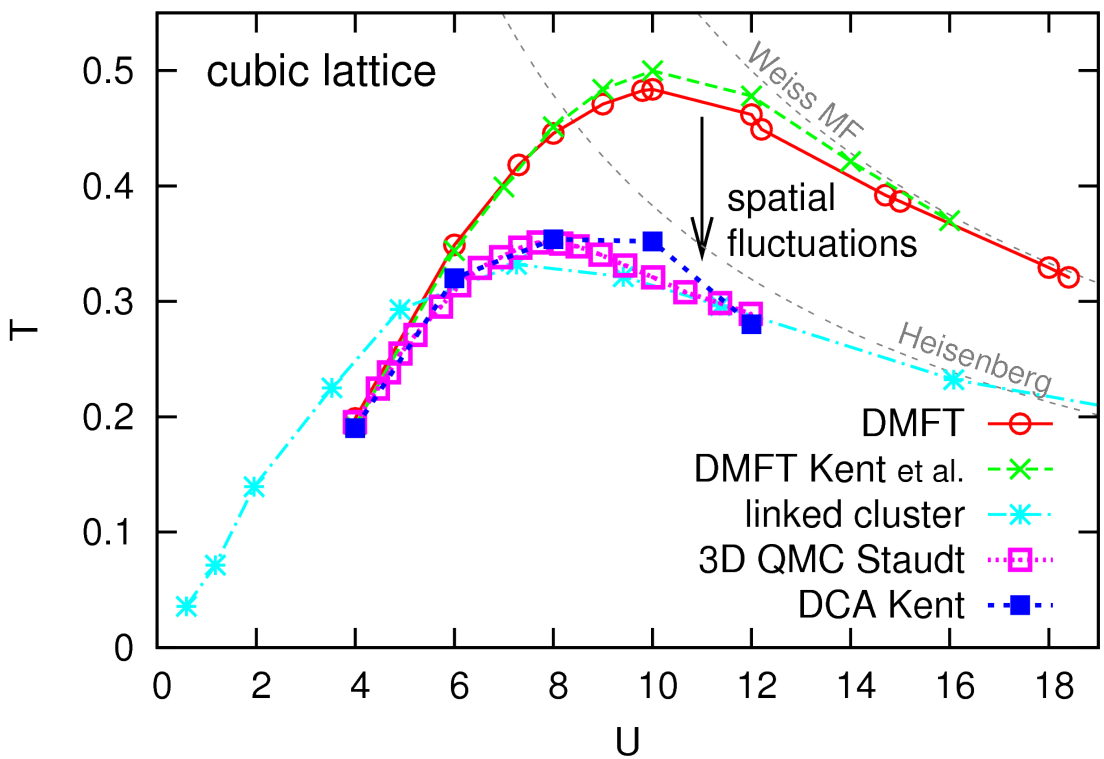

Unavoidable change: kinks cannot remain at $T = T_N^{DMFT} > T_N$!

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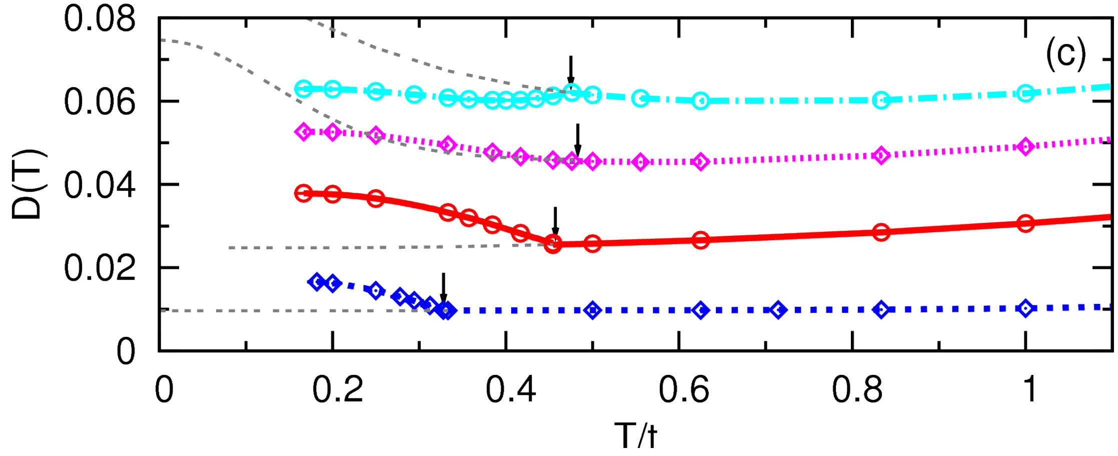

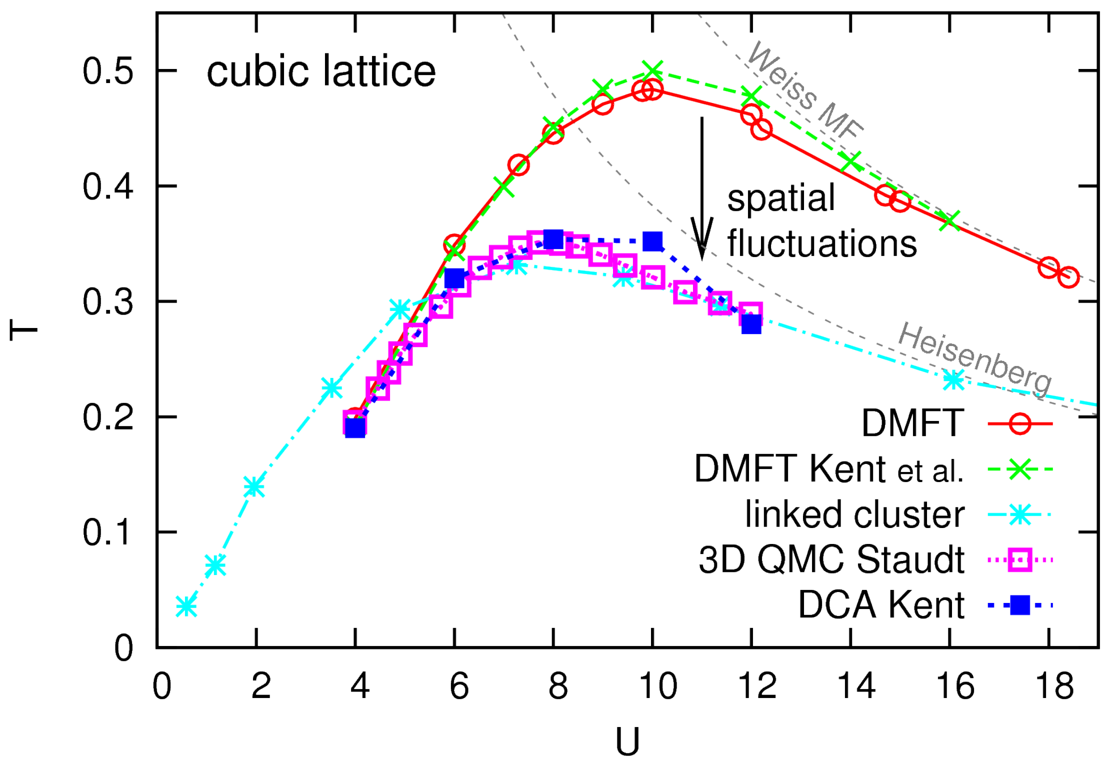

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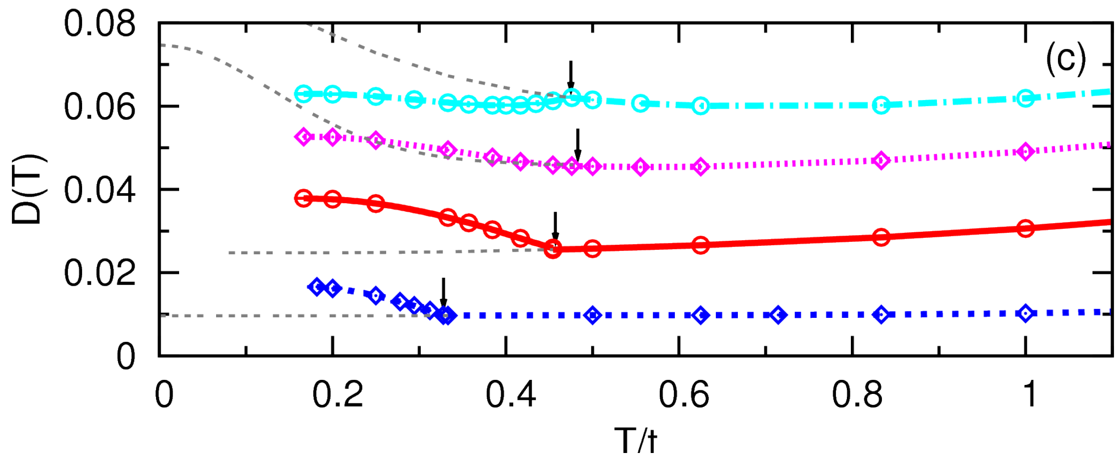

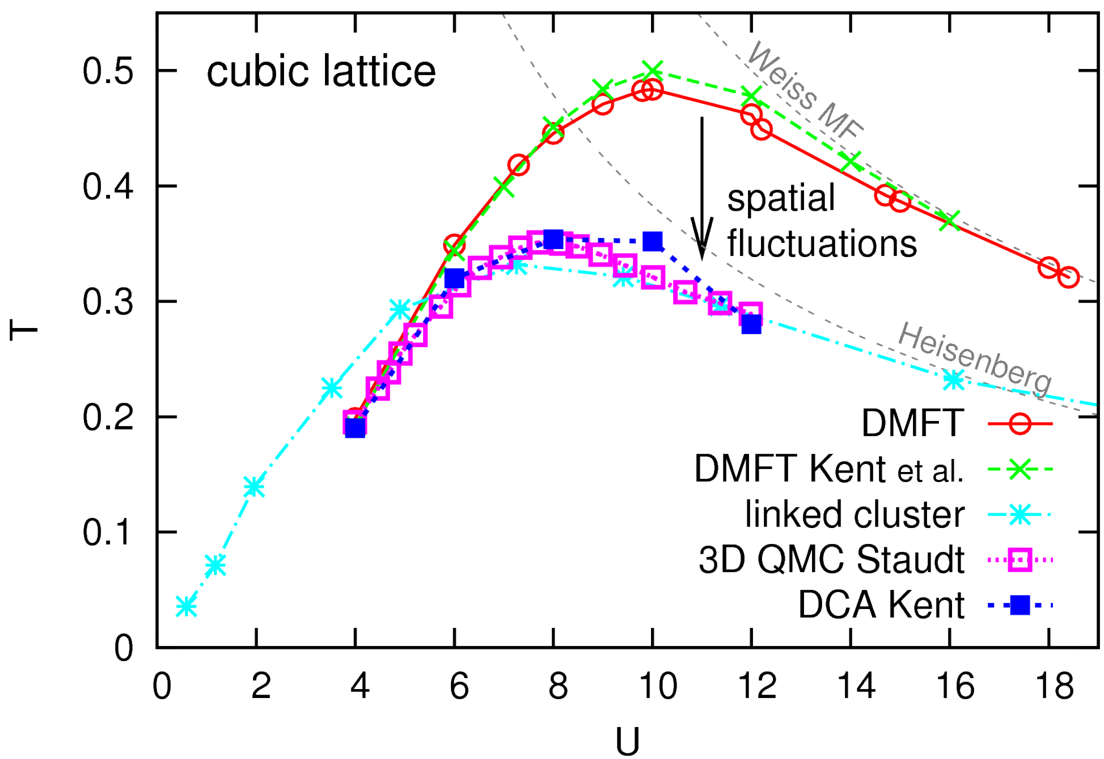

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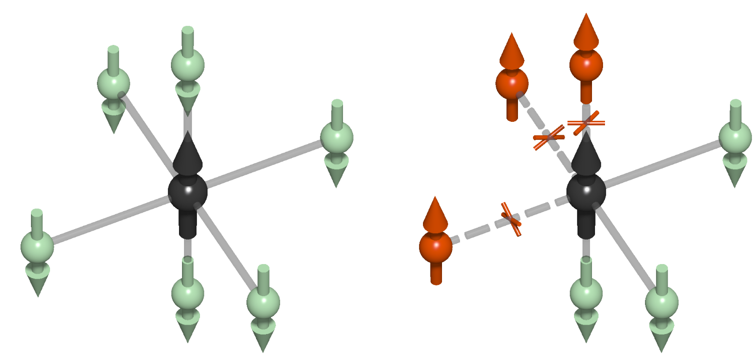

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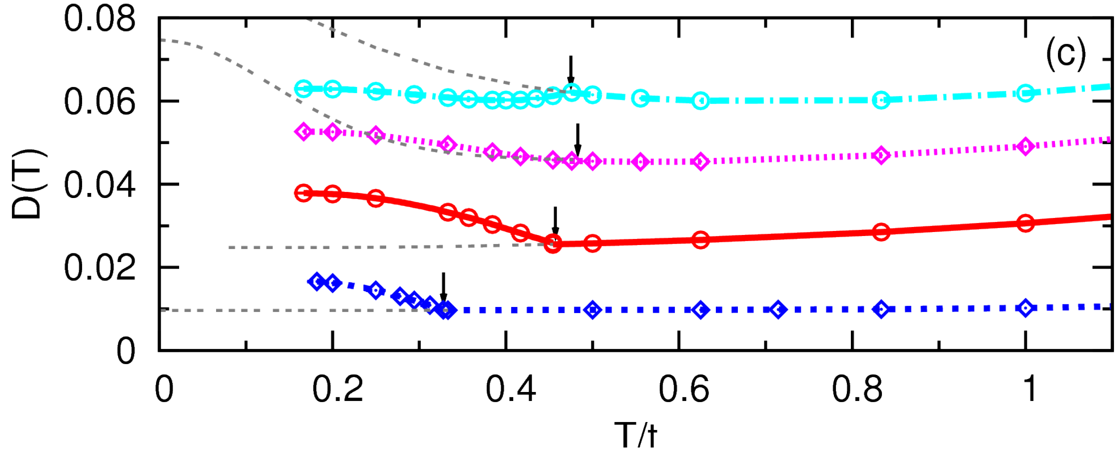

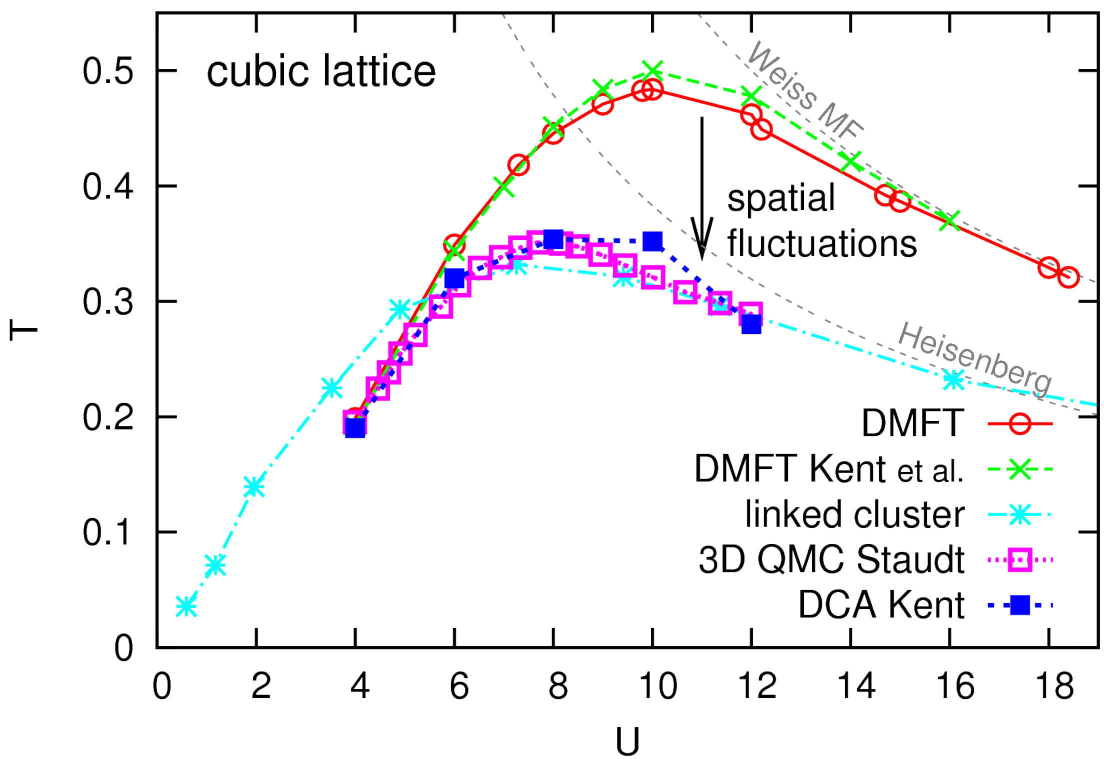

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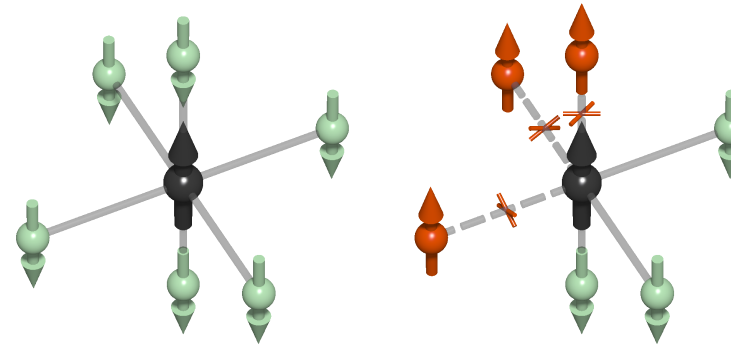
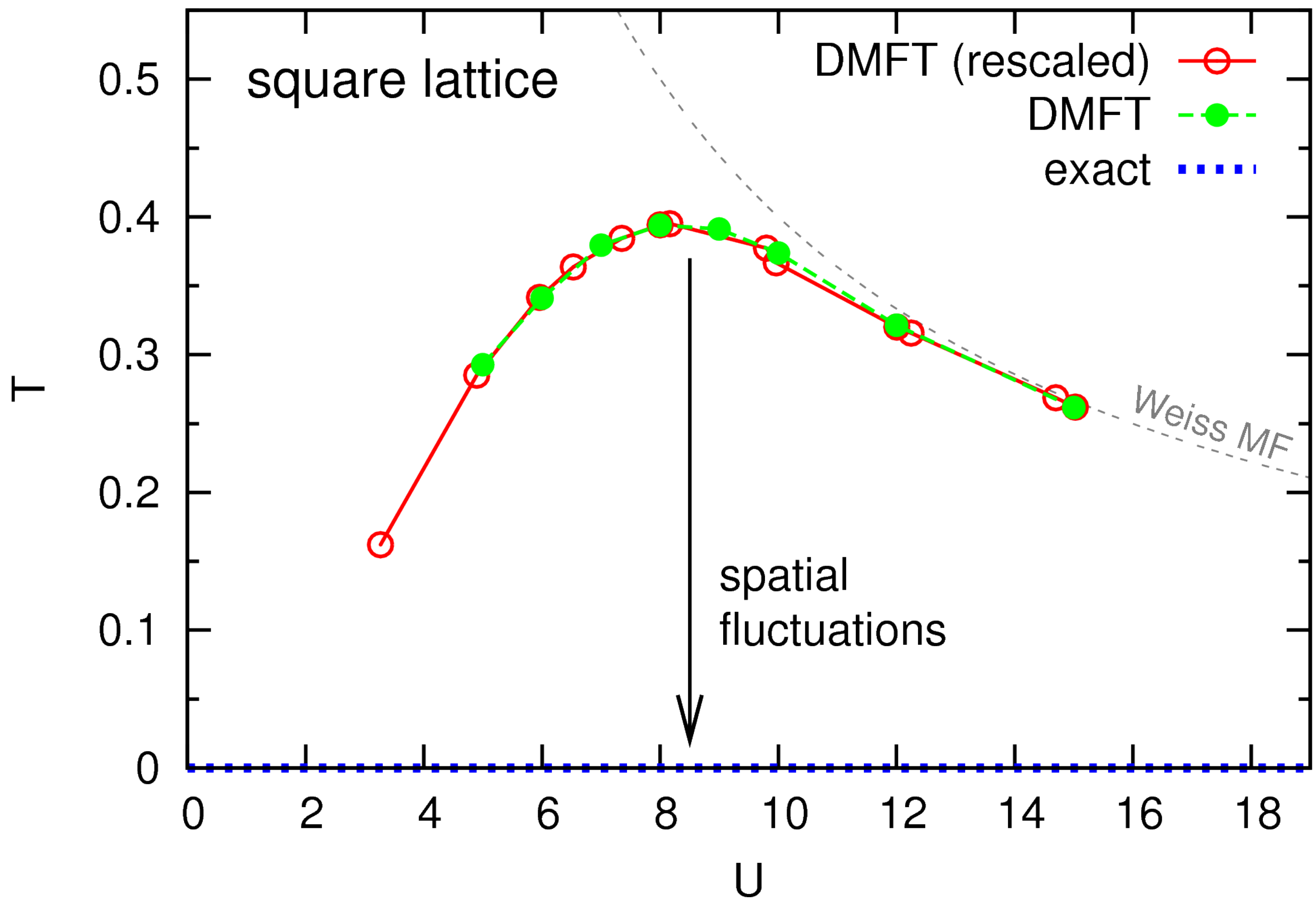


and independ. of long-range order

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



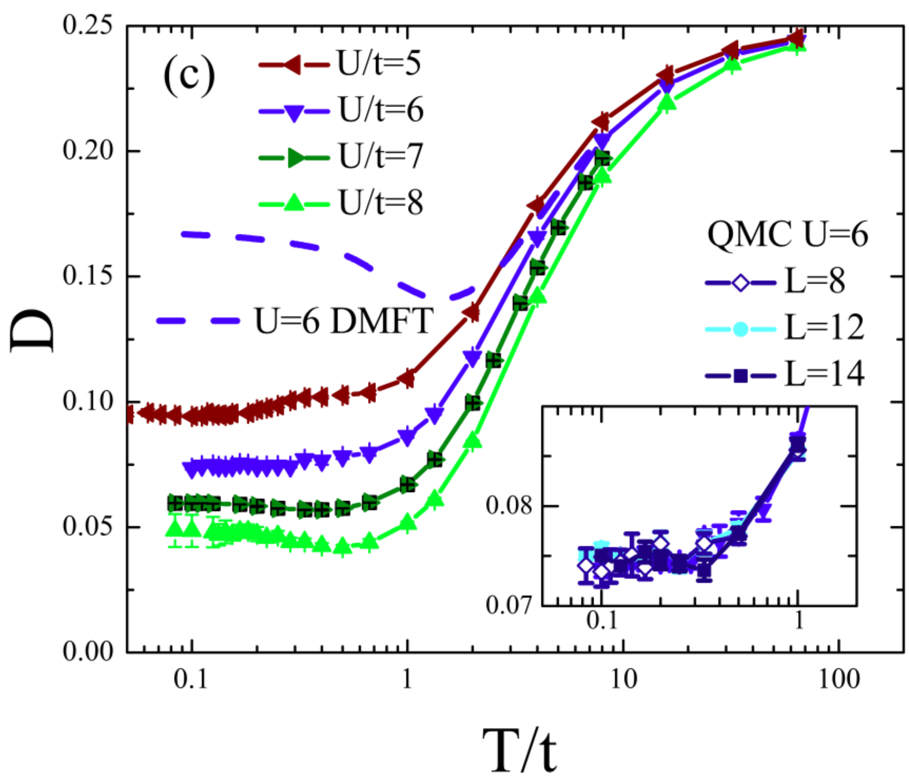
Will any enhancement of D at low T remain? At which temperature scale?

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]
[1]*Instituto de Fisica, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[2]*Department of Physics, University of California, Davis, California 95616, USA*
[3]*Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA*
(Received 18 June 2009; published 11 February 2010)



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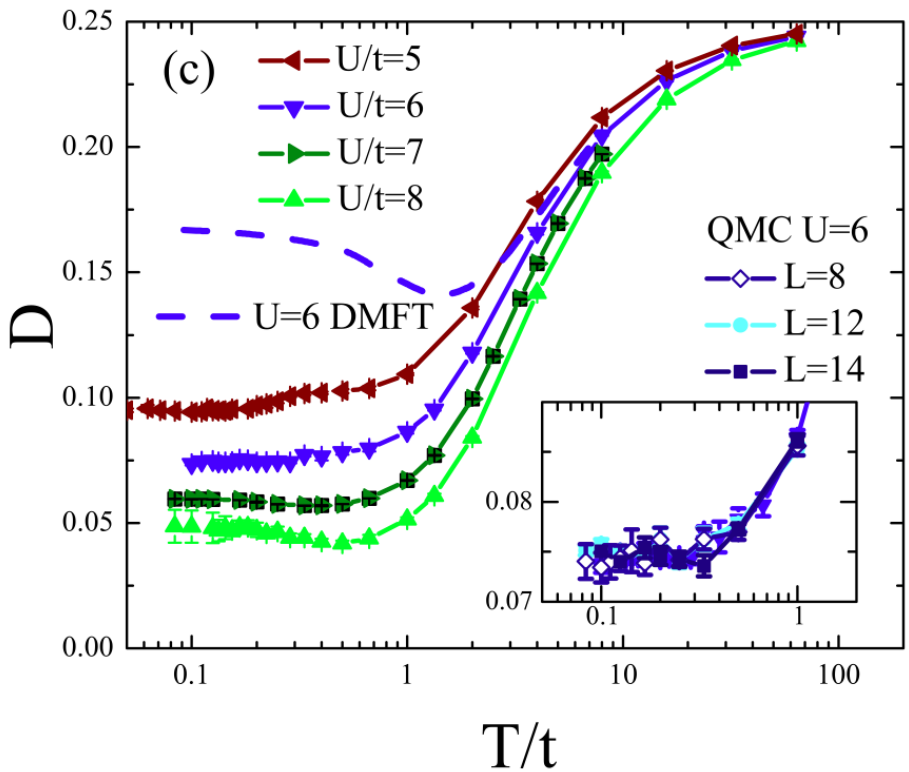
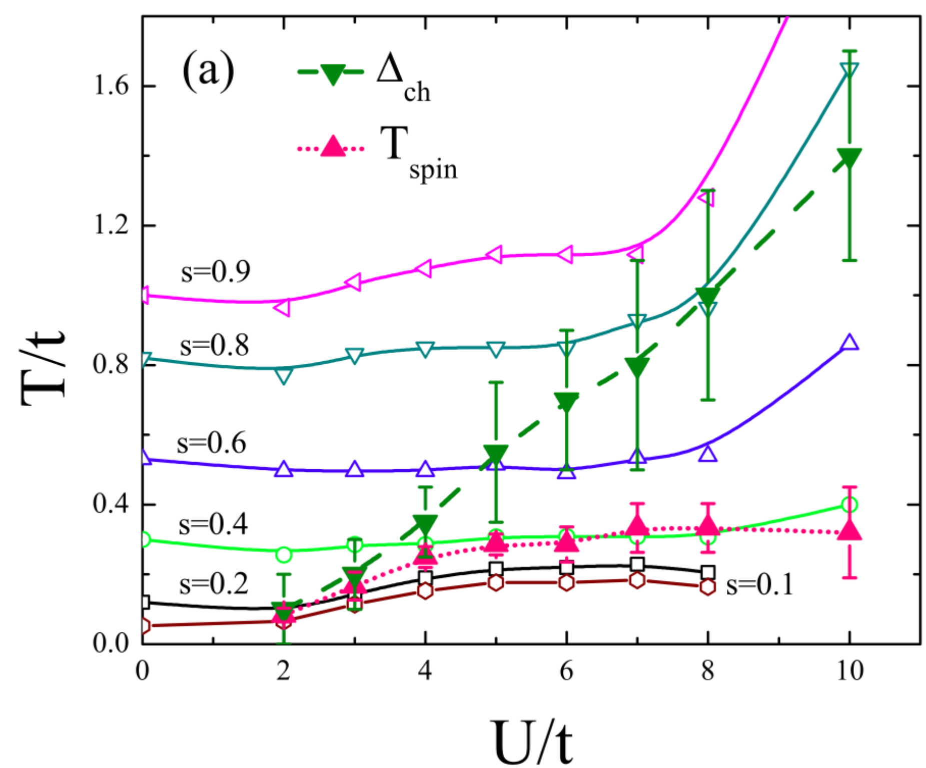
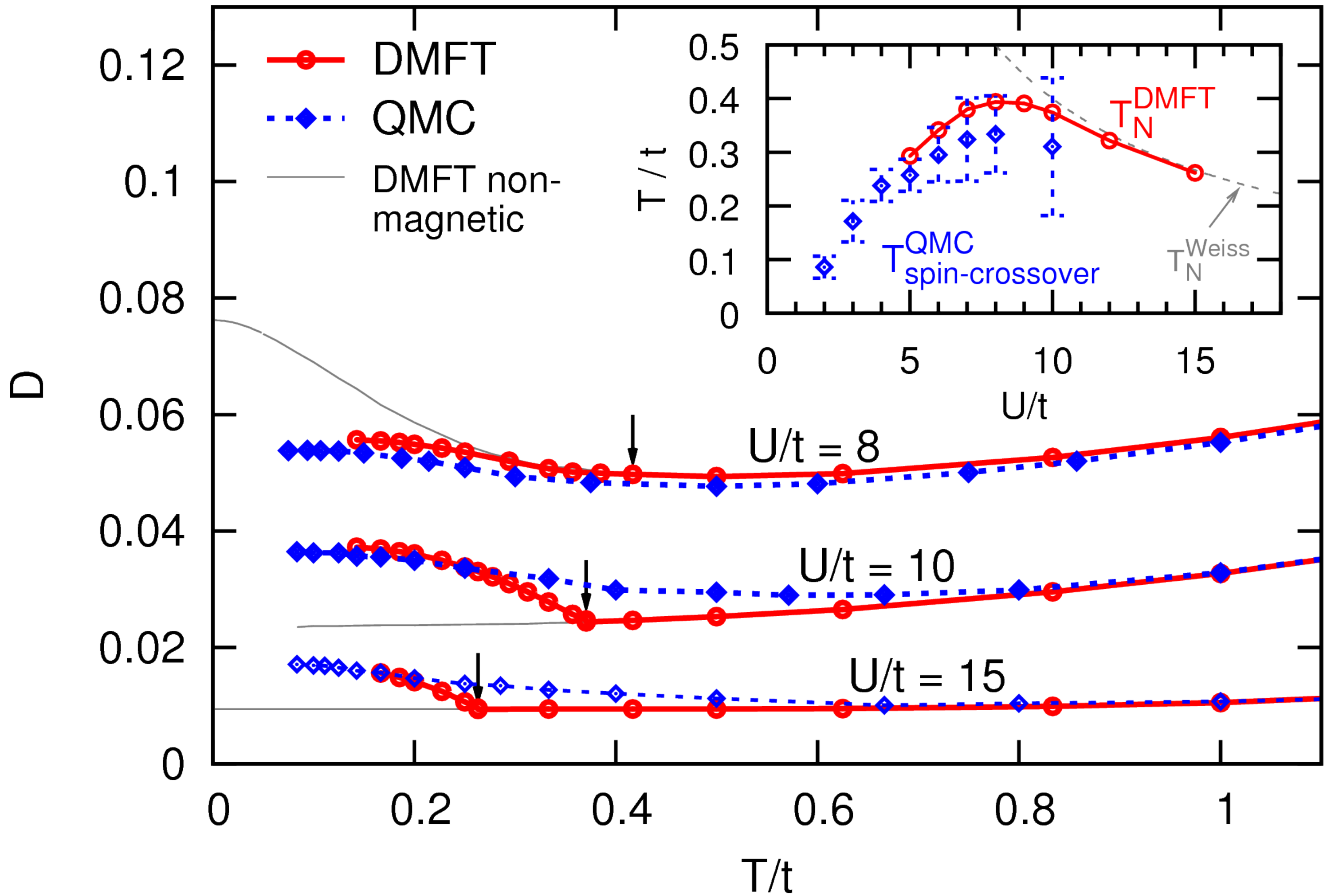




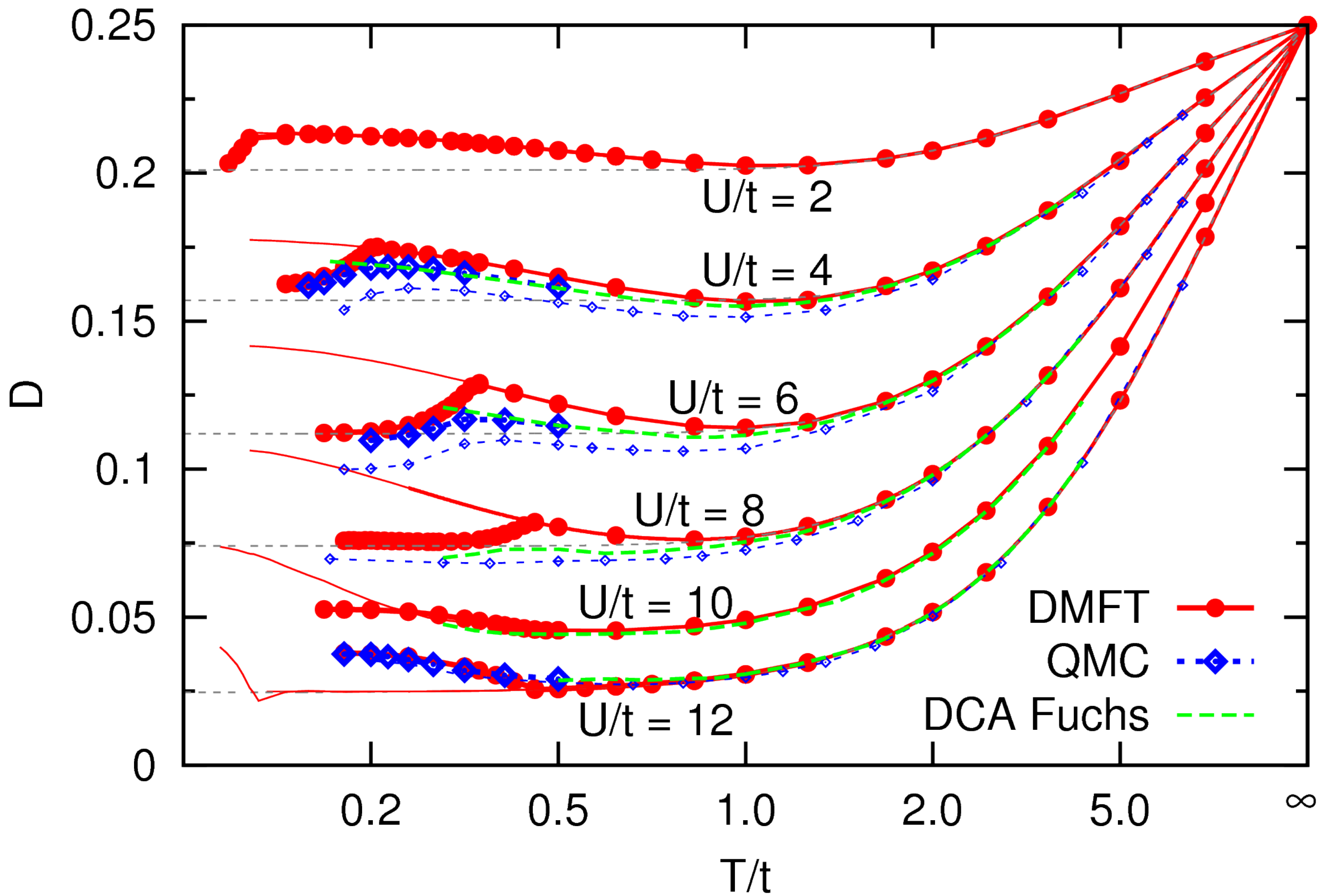
Comparison DMFT – direct QMC for the 2d square lattice ($n = 1$)



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

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

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

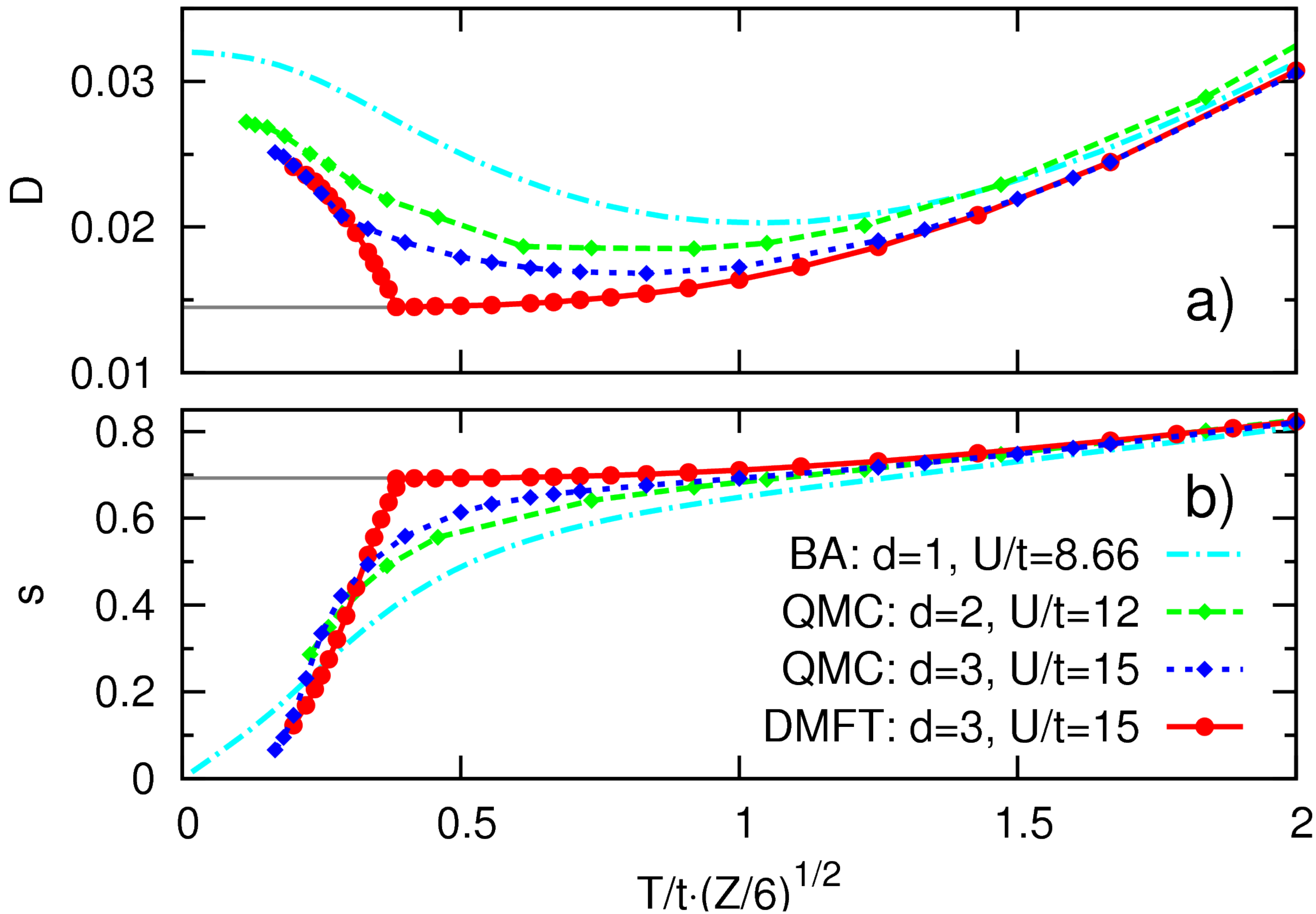


Excellent general agreement, even at small U (reduction of D by AF)

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]
[1]*Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France*
[2]*Département de Physique Théorique, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genéve 4, Switzerland*
[3]*Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France*
[4]*Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA*
(Received 15 September 2010; published 10 February 2011)

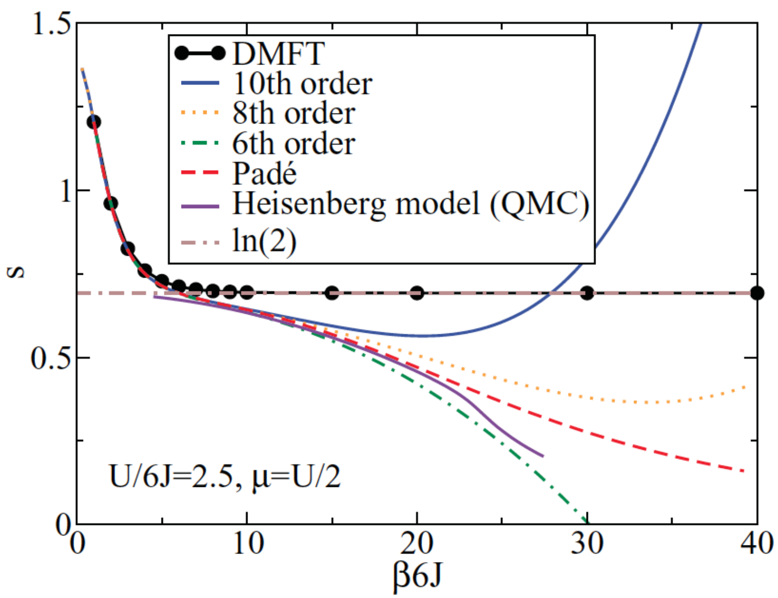
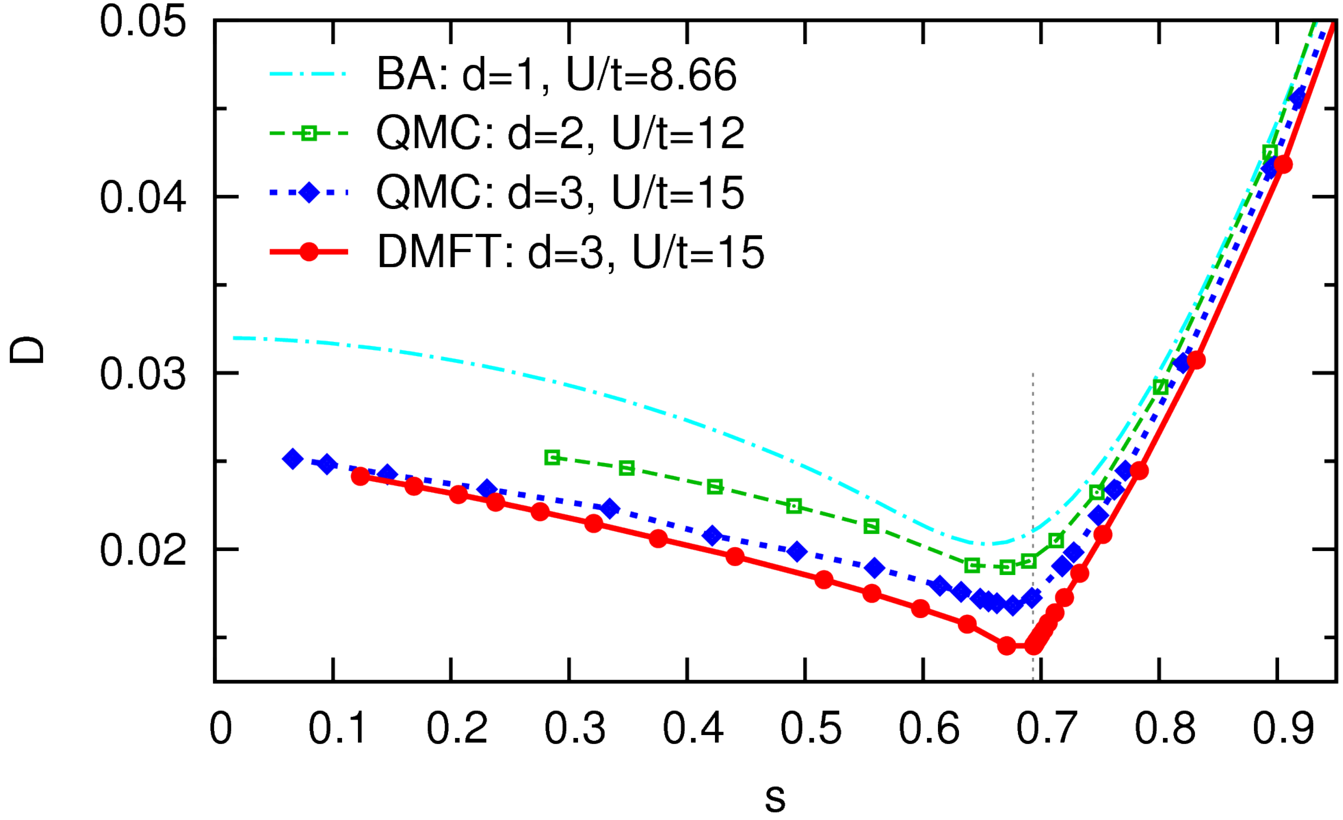


FIG. 14. (Color online) Entropy per particle in a system at half filling and intermediate interaction strength $U/6J = 2.5$ obtained by series expansion, DMFT, and QMC (for the Heisenberg model) [26].

Double occupancy as a universal measure of AF correlations + entropy



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

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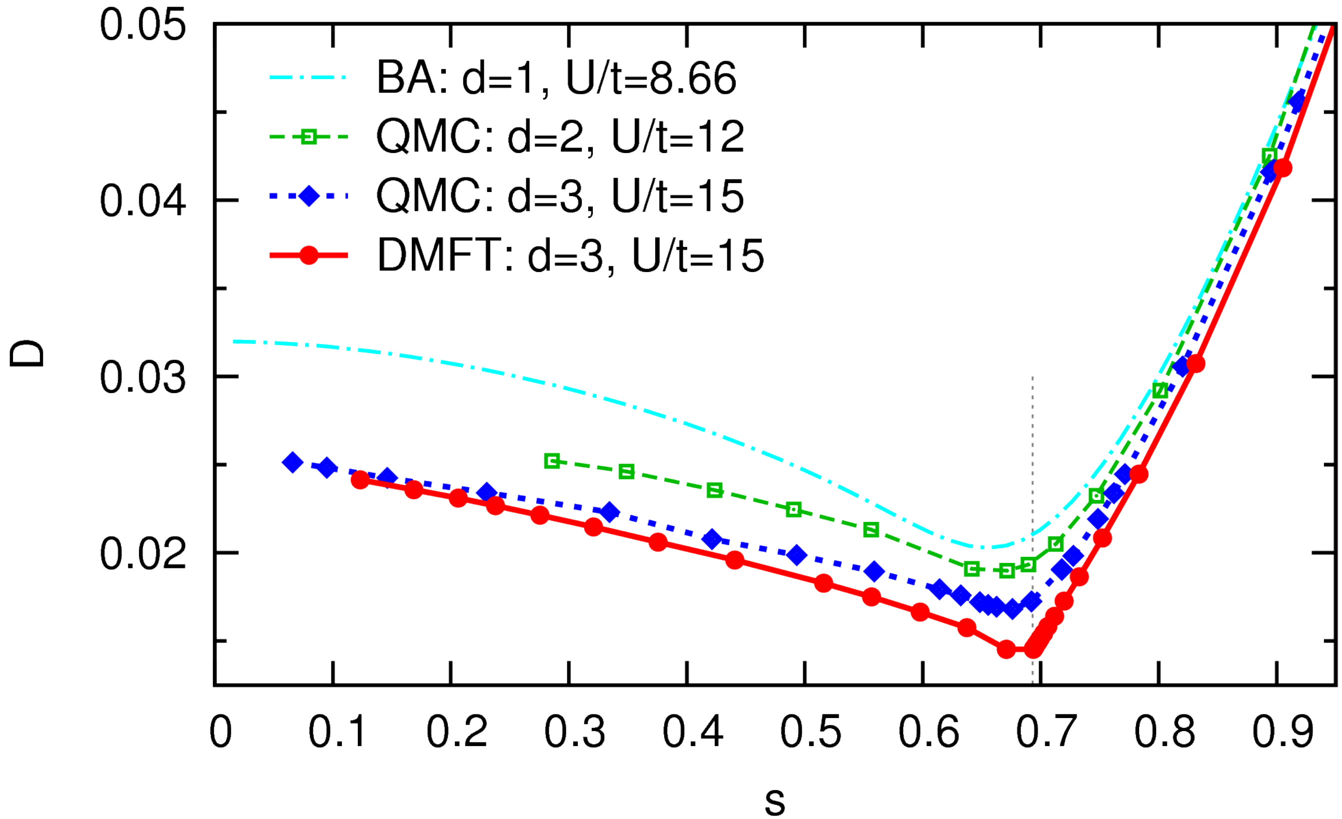

For all dimensions: $\min\{D(s)\}$ at $s \approx \log 2$

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

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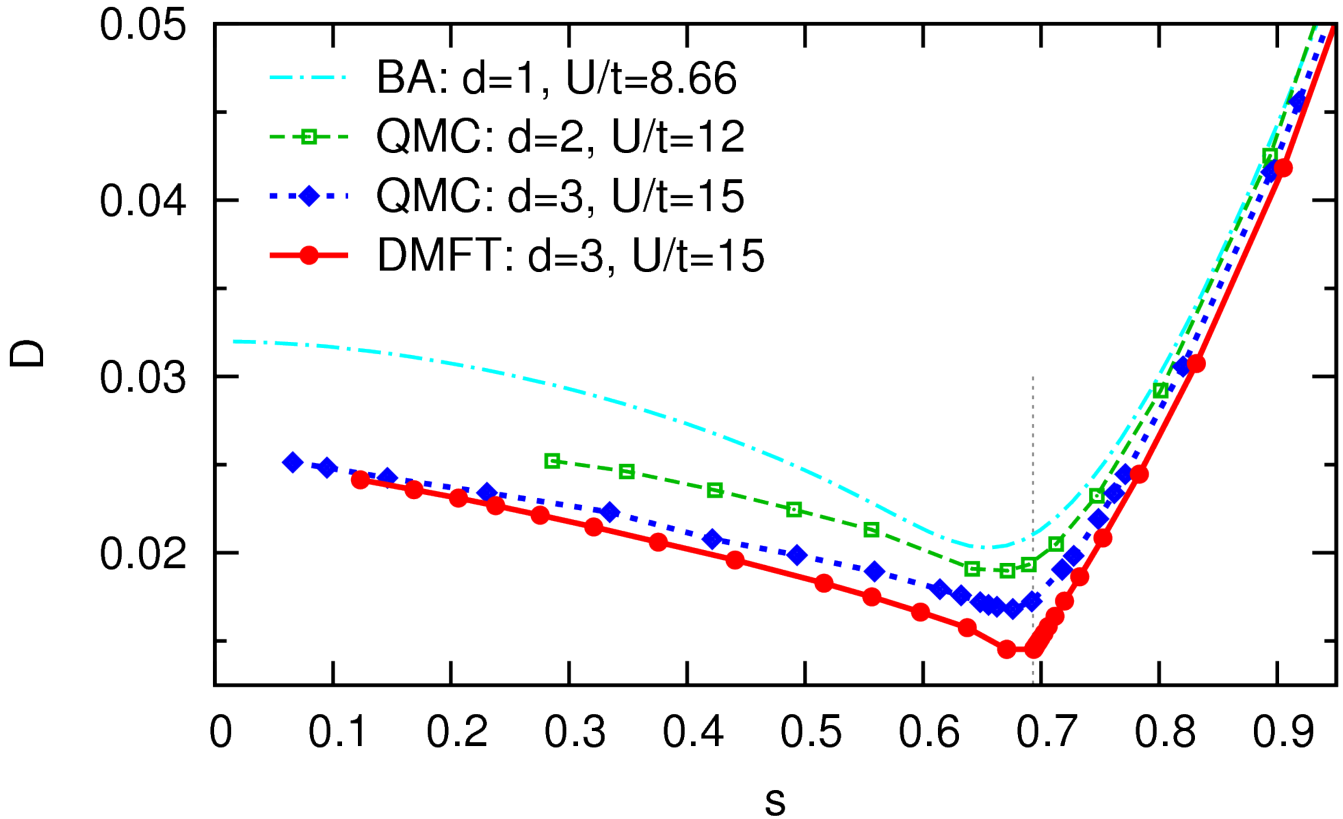

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Effect is larger for lower dimensions:

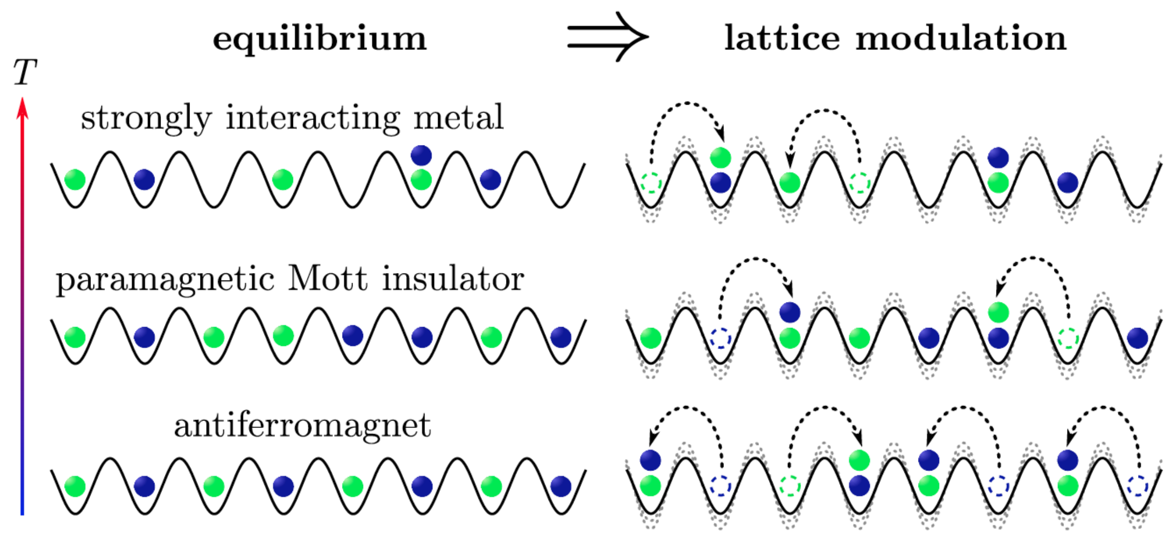
$$\langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle_0 = \begin{cases} -1.00 & DMFT \\ -1.20 & (d = 3) \\ -1.34 & (d = 2) \\ -1.77 & (d = 1) \end{cases}$$

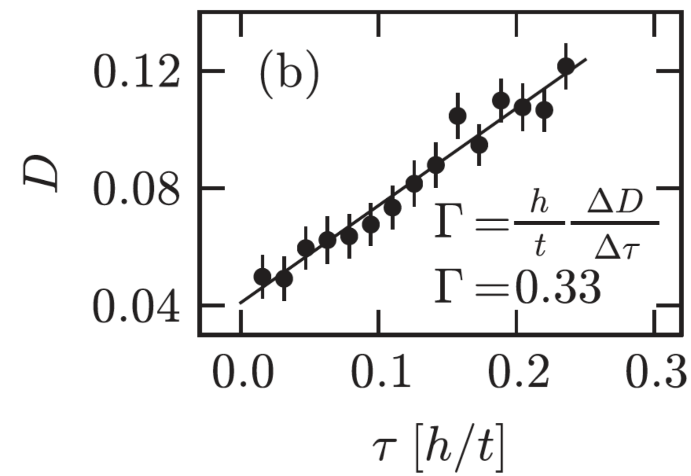
PRL **106,** 145302 (2011) PHYSICAL REVIEW LETTERS week ending 8 APRIL 2011

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

Daniel Greif, Leticia Tarruell,* Thomas Uehlinger, Robert Jördens, and Tilman Esslinger
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.

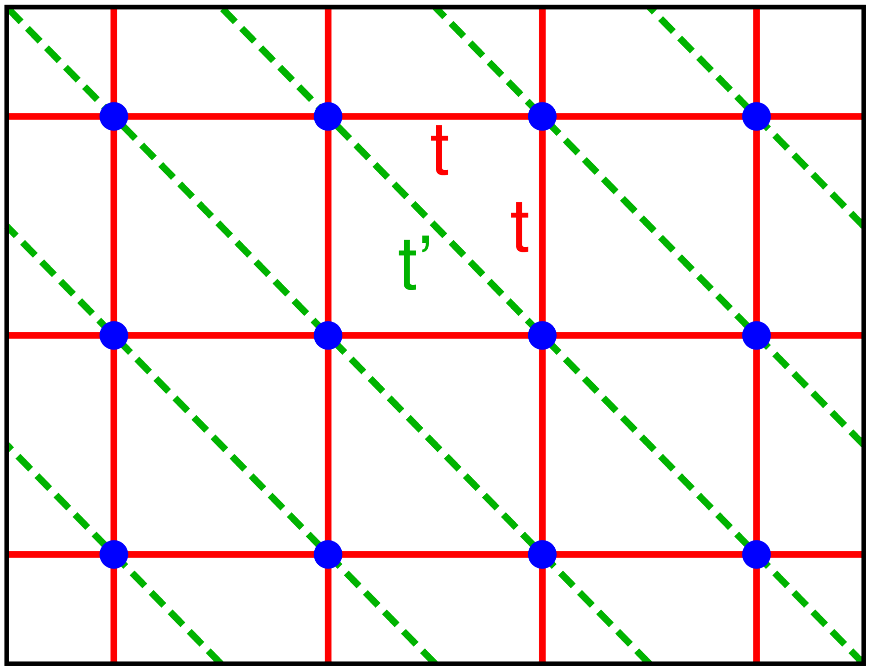




Correlator $\mathcal{P}_{i,i+1} = \sum_\sigma \langle n_{i,\sigma}(1 - n_{i,\bar\sigma})\, n_{i+1,\bar\sigma}(1 - n_{i+1,\sigma})\rangle \xrightarrow{n\to 1} (1 - \langle \sigma_i^z \sigma_{i+1}^z \rangle)/2$ MF?

Impact of frustration: towards the triangular lattice

Introduce frustration in controlled way
as diagonal hopping in square lattice:



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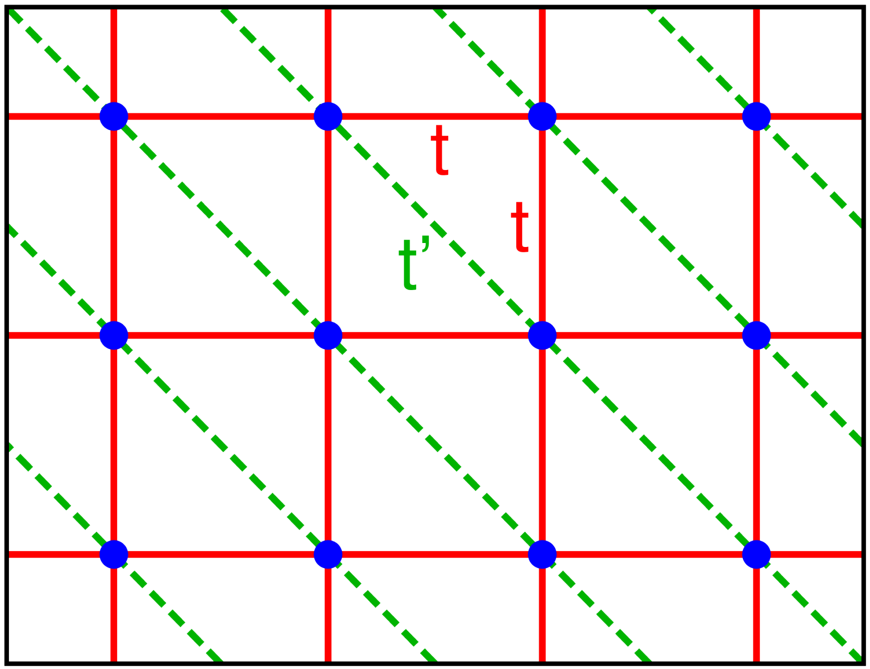

Imai, Kawakami, PRB **65**, 233103 (2002)
Merino, Powell, McKenzie, PRB (2006)
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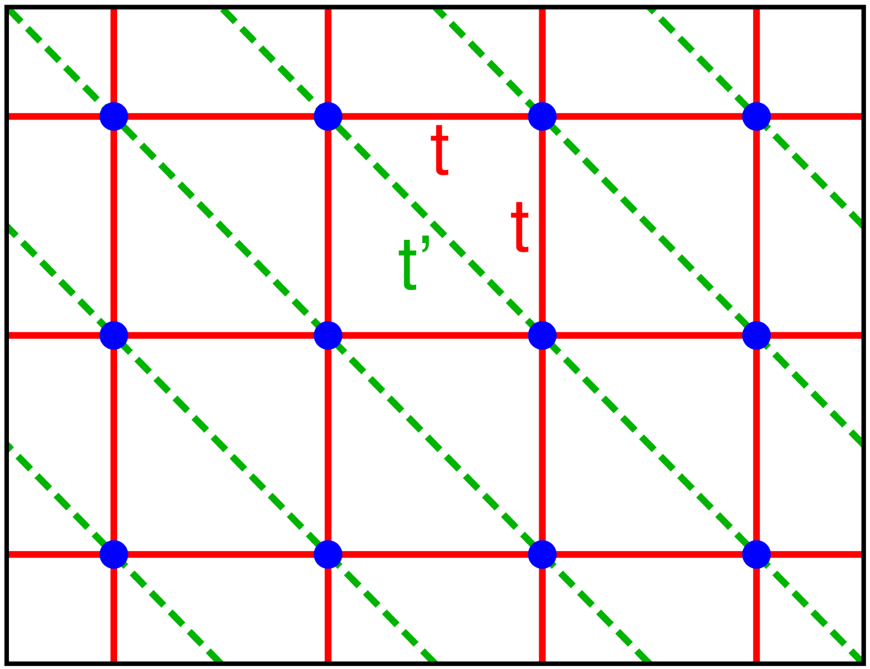

Problem: t' also changes bandwidth

$$\langle\epsilon^2\rangle \equiv \int_{-\infty}^{\infty} d\epsilon\, \epsilon^2 \rho_0(\epsilon) = 4t^2 + 2t'^2$$

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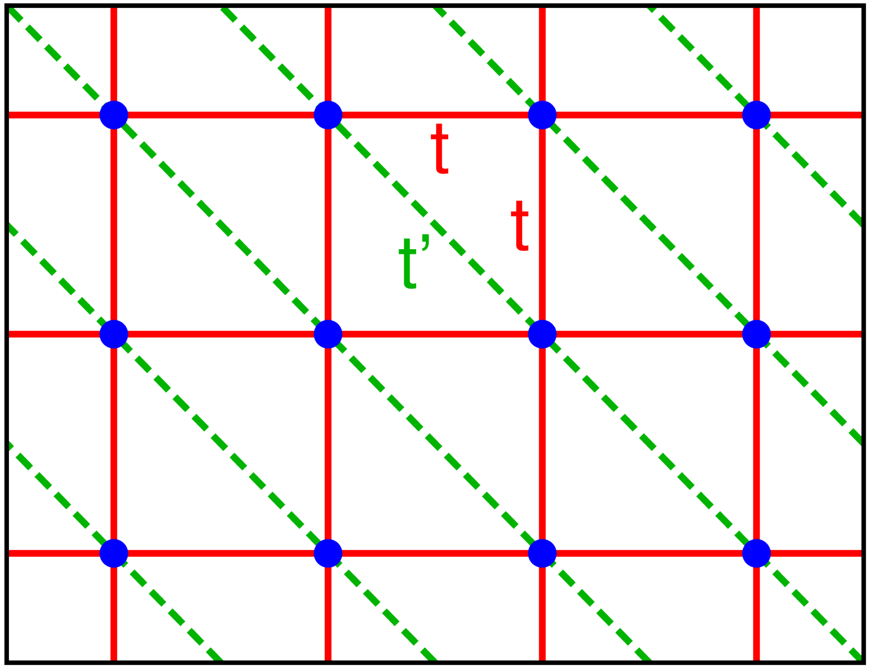

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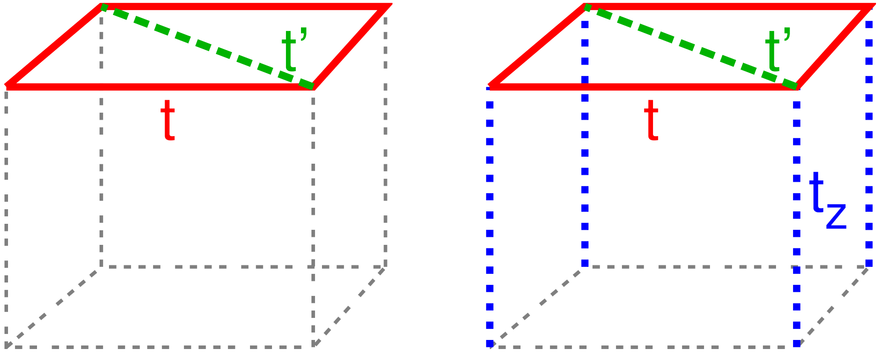
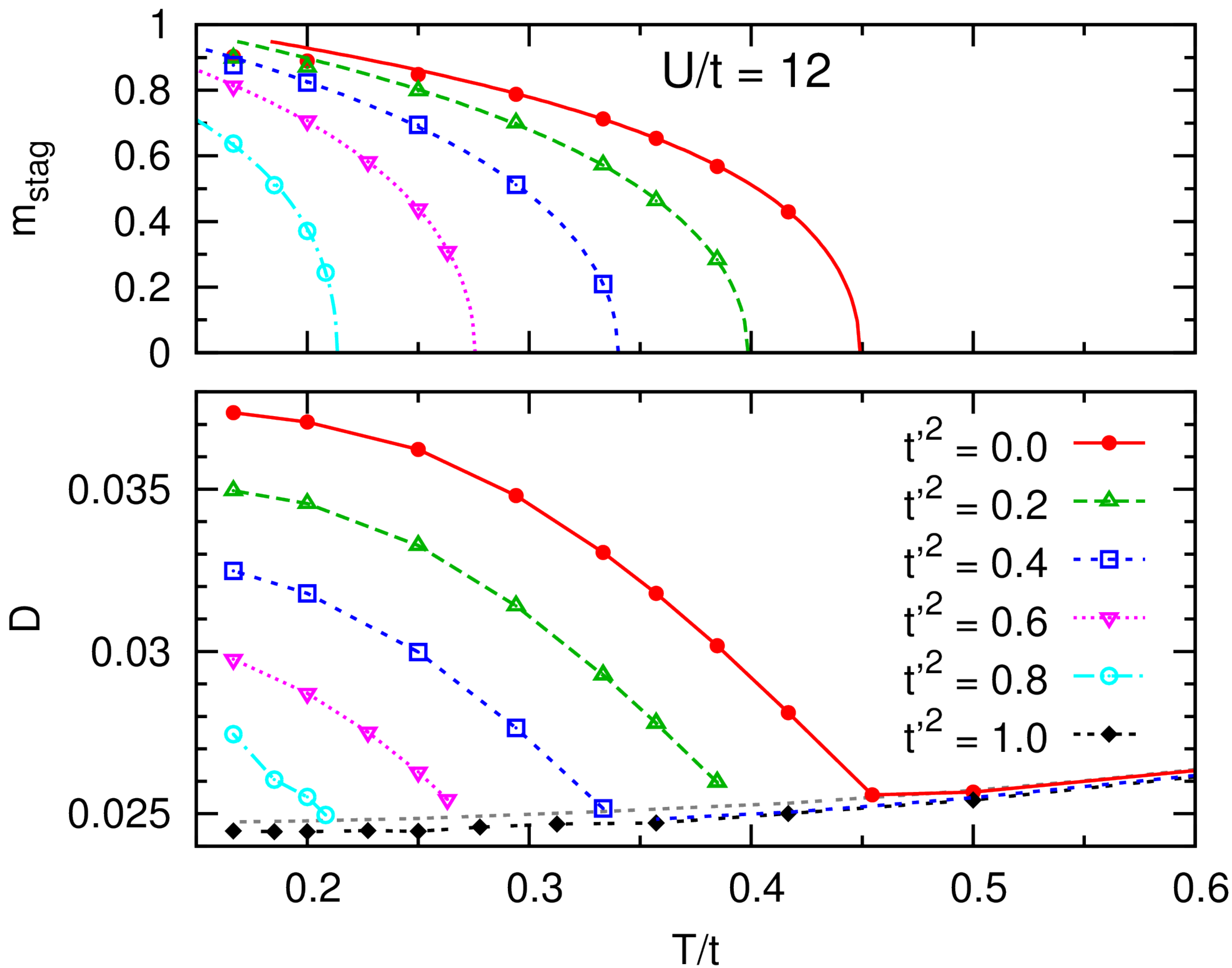
$$\langle \epsilon^2 \rangle \equiv \int_{-\infty}^{\infty} d\epsilon\, \epsilon^2 \rho_0(\epsilon) = 4t^2 + 2t'^2$$

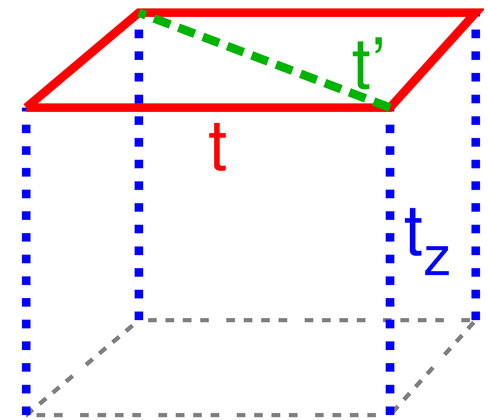
Solution: add third dimension
and hopping t_z between planes



with $t_z^2 = t^2 - t'^2$

Tuning the frustration from the cubic to the triangular lattice

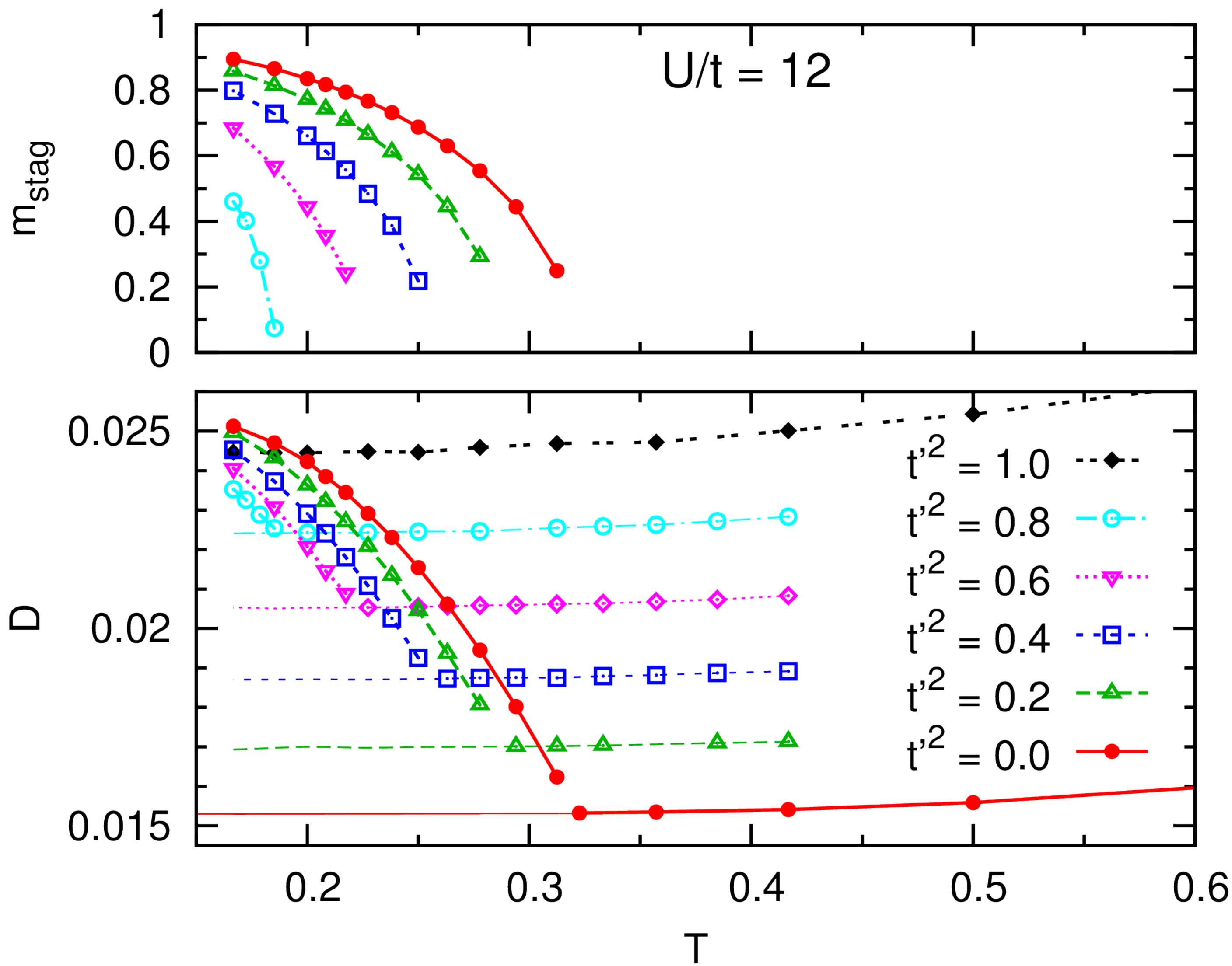


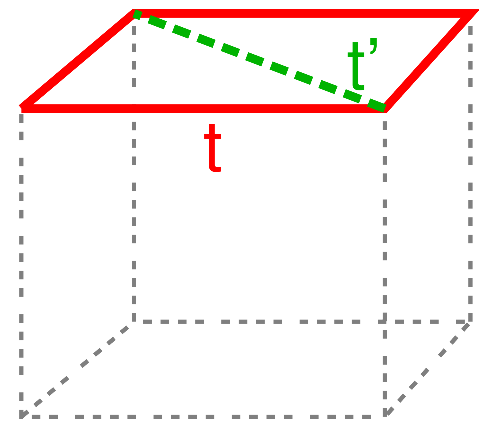


D suppressed before AF breaks down

paramagnetic phase hardly affected by t'

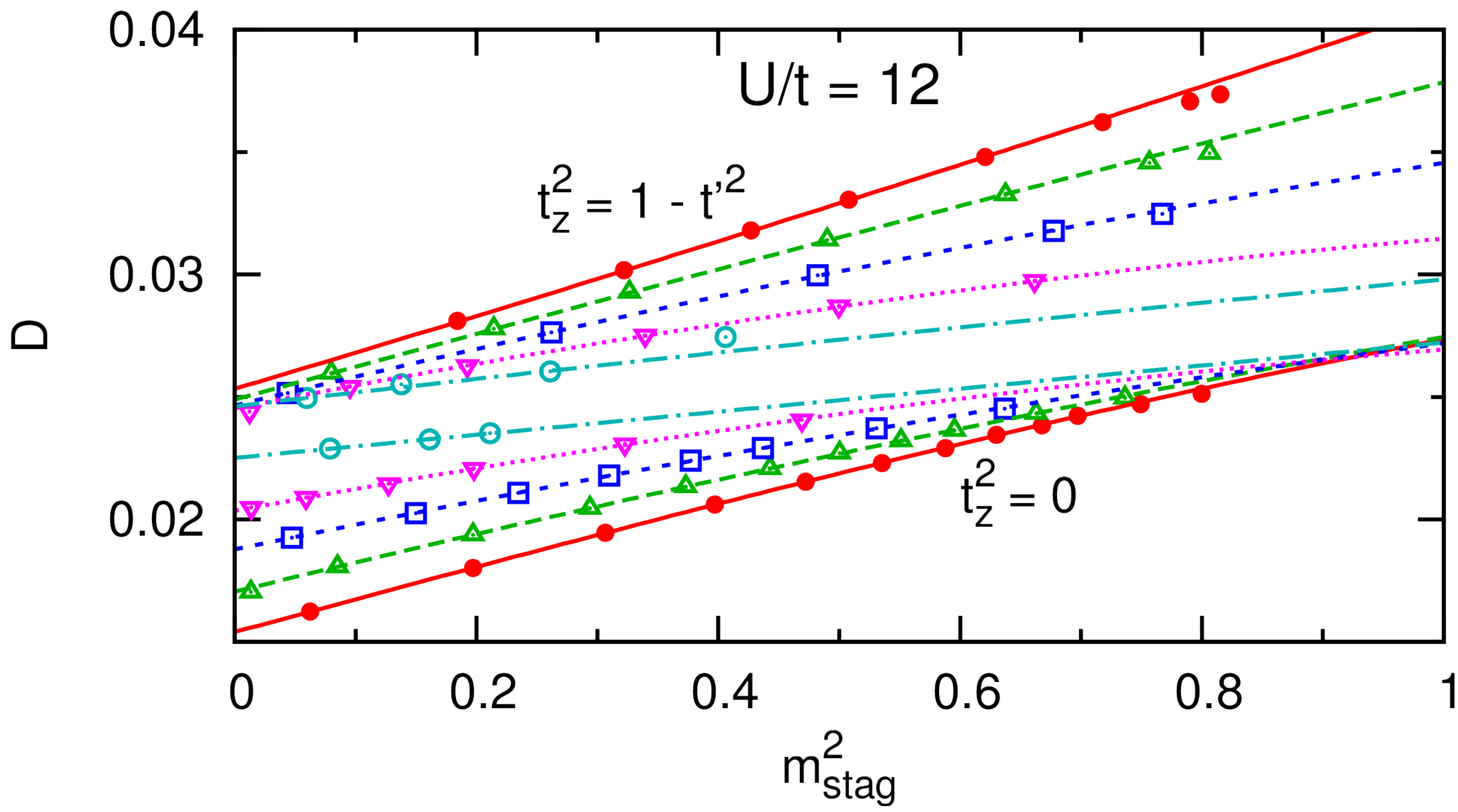
Tuning the frustration from the square to the triangular lattice





Now situation reversed: strong t'^2 dependence only in paramagnetic phase

Double occupancy: a quantitative measure of AF correlations? Yes!



Quantitative confirmation of strong coupling picture: results collaps in

- paramagnetic limit for $t_z^2 = 1 - t'^2$
- AF limit for $t_z^2 = 0$

Summary

QMC based implementation of real-space DMFT

Accurate, efficient for cold-atom temperatures, extremely 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

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

DMFT surprisingly accurate in low dimensions

Double occupancy: universal probe of AF correlations and entropy

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

Outlook

Skipped: Mott transition for 3 degenerate flavors in (U, T, μ) space

[E. V. Gorelik, N. Blümer, Phys. Rev. A **80**, 051602(R) (2009)]

3D calculations for realistic trap parameters and system sizes

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

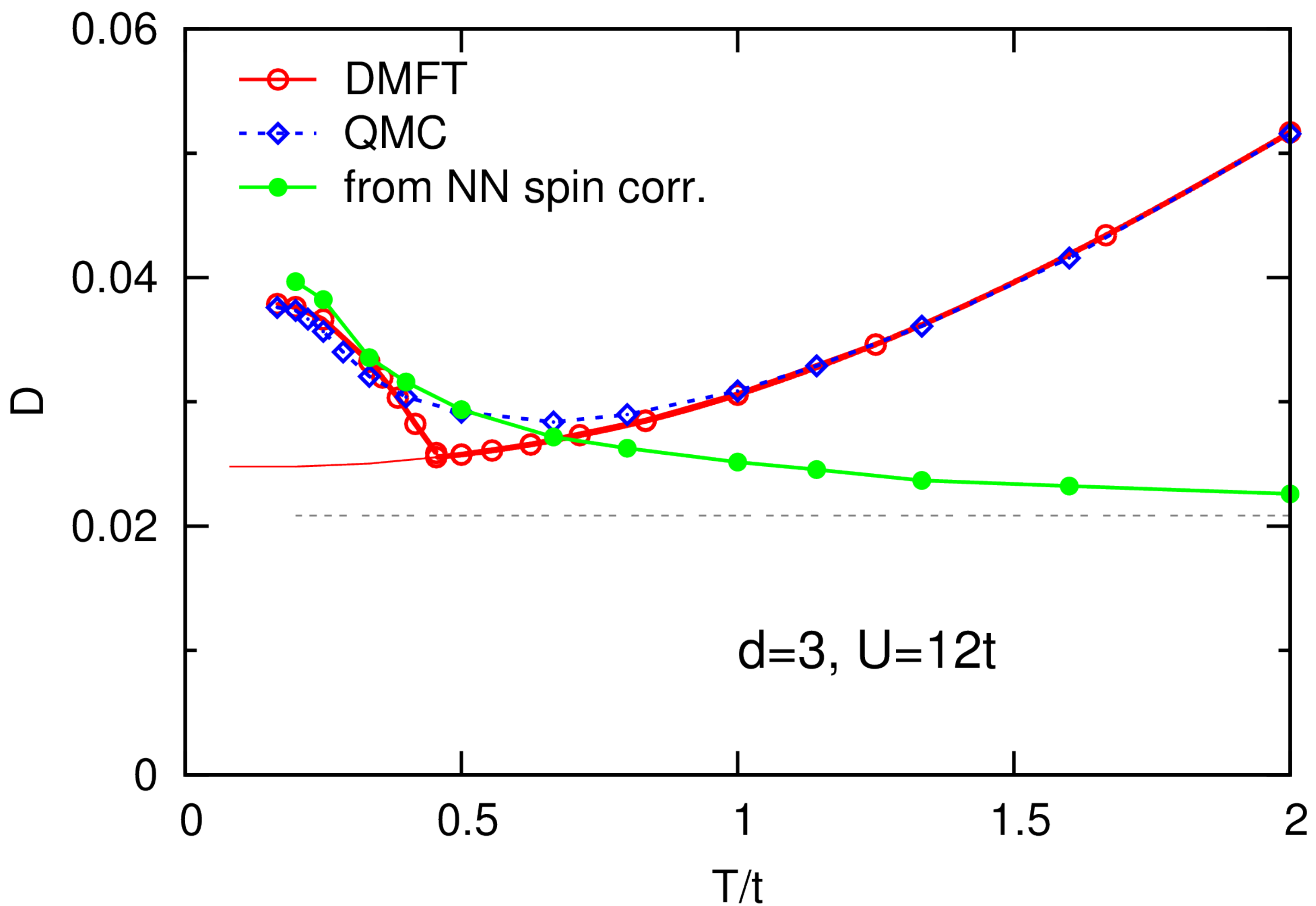
Multigrid HF-QMC for RDMFT; impact of higher Bloch bands

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

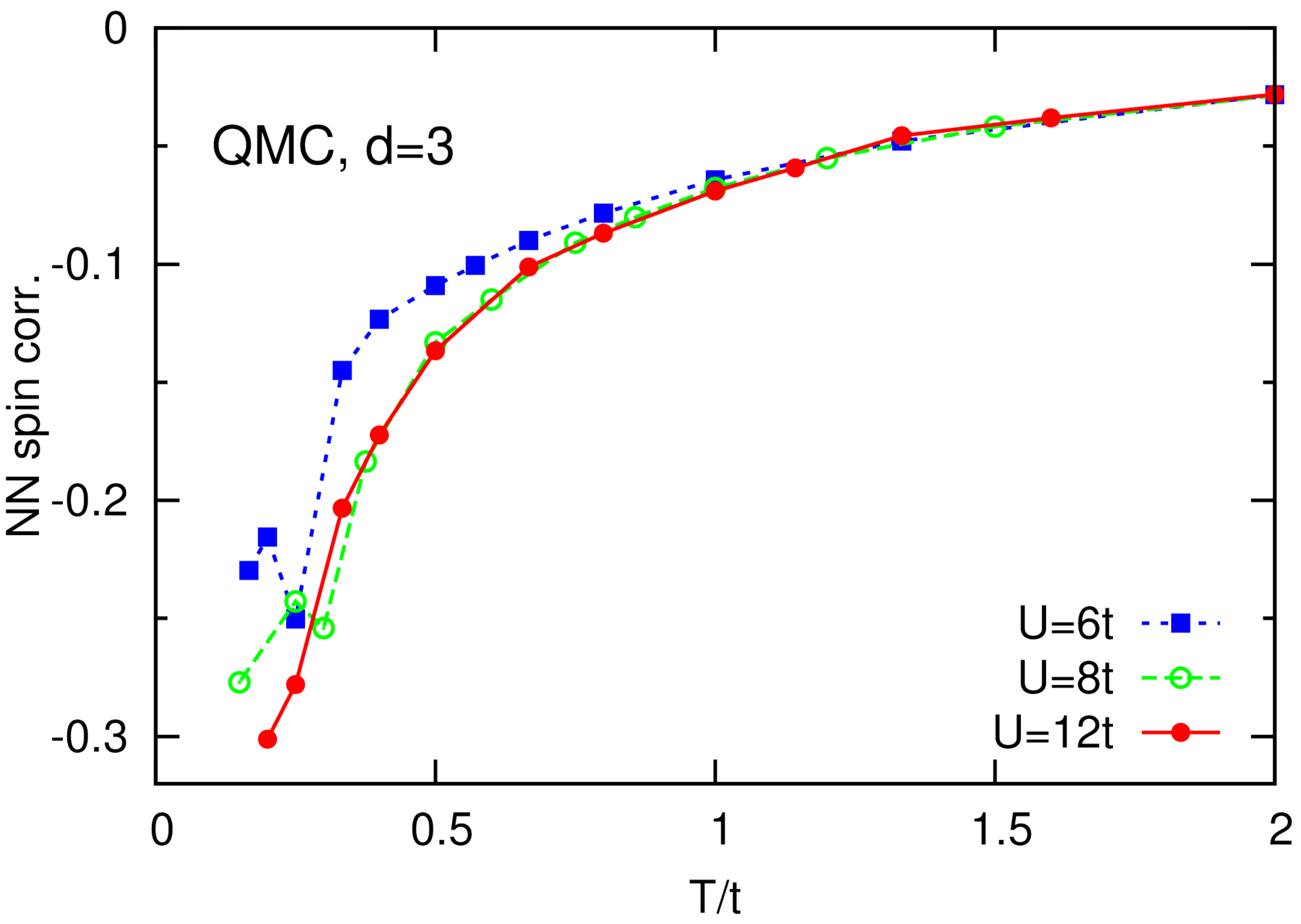
QMC impurity solver development (DFG project with F. Assaad and P. Werner)

Thanks to: E. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek,
U. Schneider, I. Bloch, H. Moritz, L. Tarruell,
R. Scalettar, T. Paiva, A. Rosch, P. van Dongen and DFG (TR49)

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



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



QMC, d=3
NN spin corr.
T/t
0
-0.1
-0.2
-0.3
0
0.5
1
1.5
2
U=6t
U=8t
U=12t

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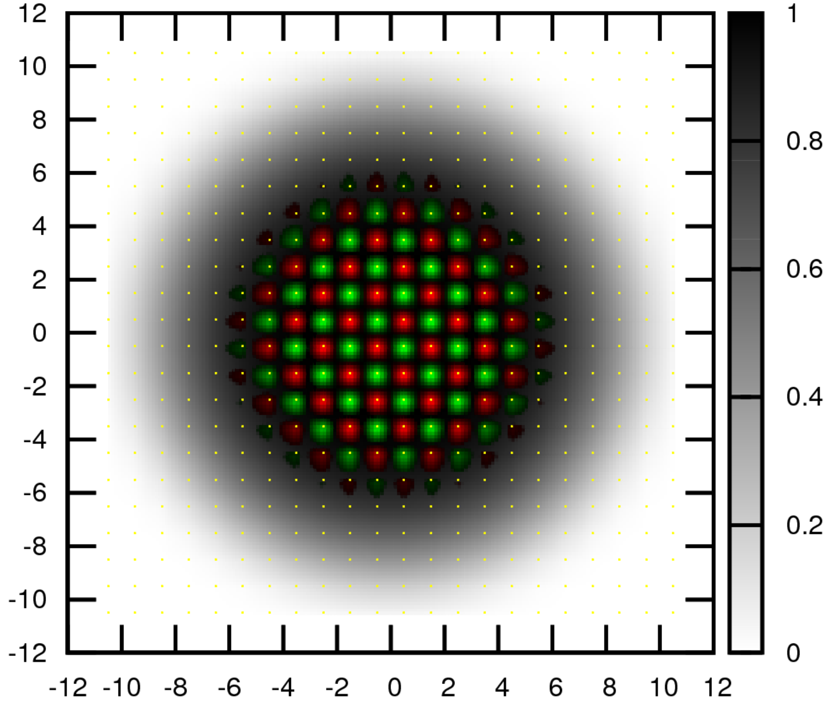
Practical (dense inversion, fully parallel): $\lesssim$ 10000 sites $\rightsquigarrow$ need smart strategies



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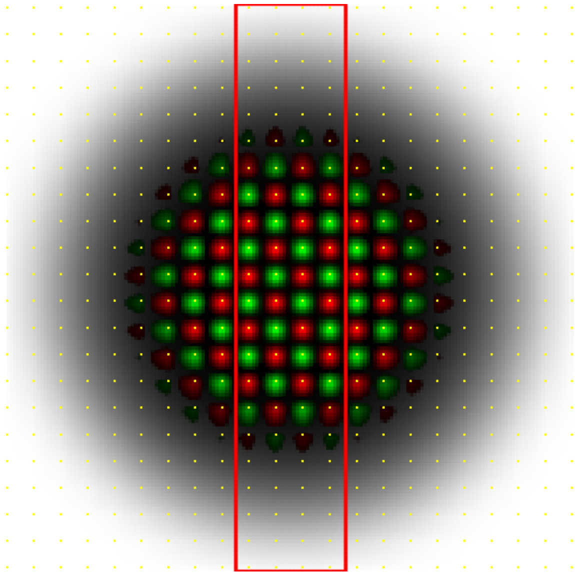

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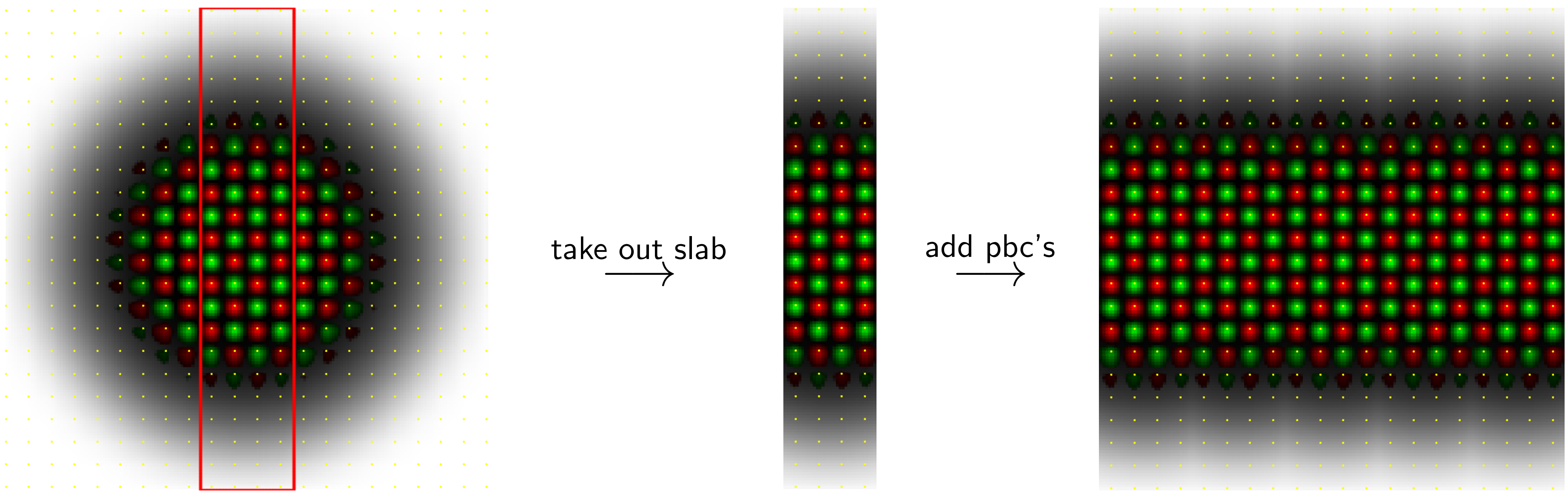
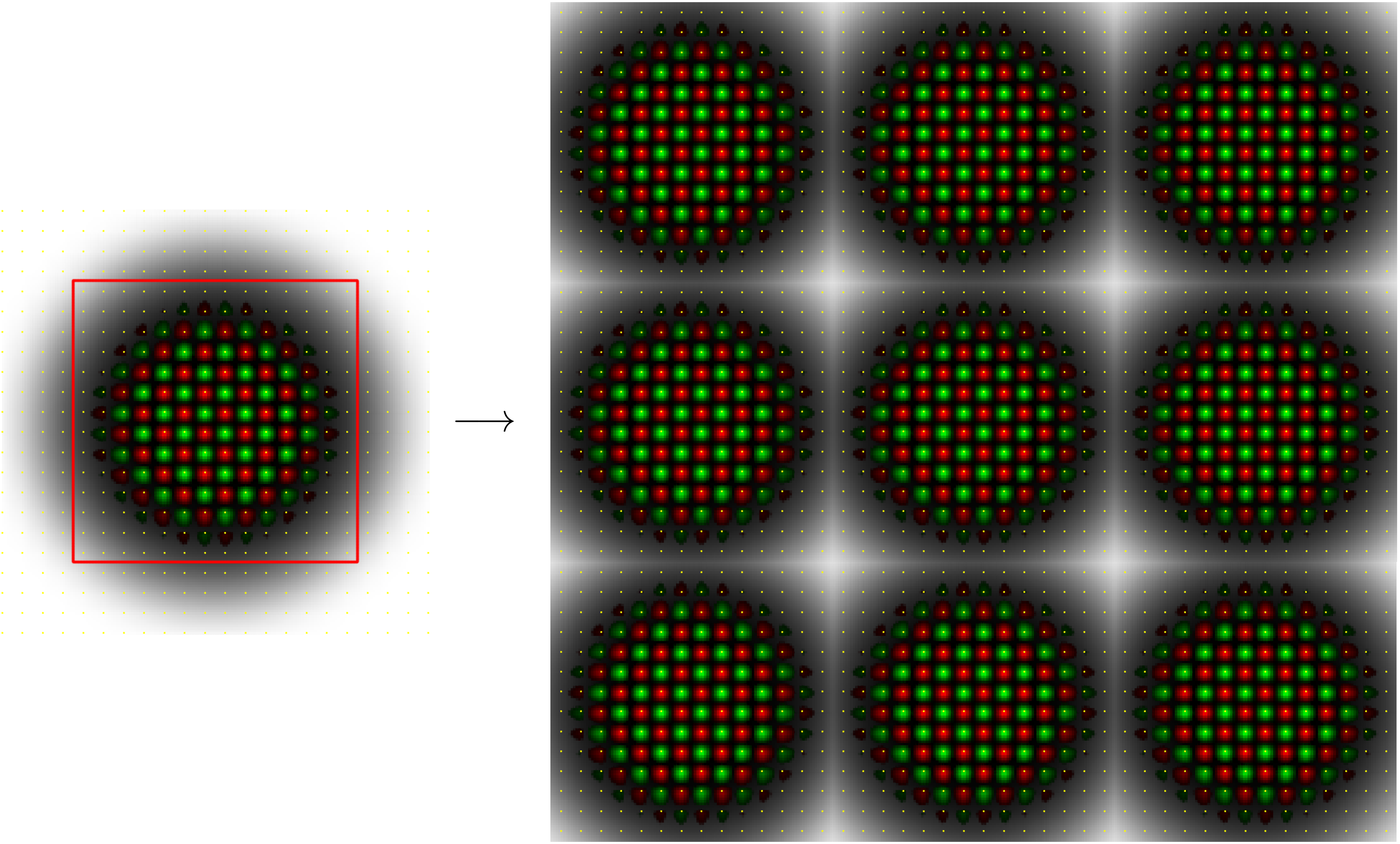


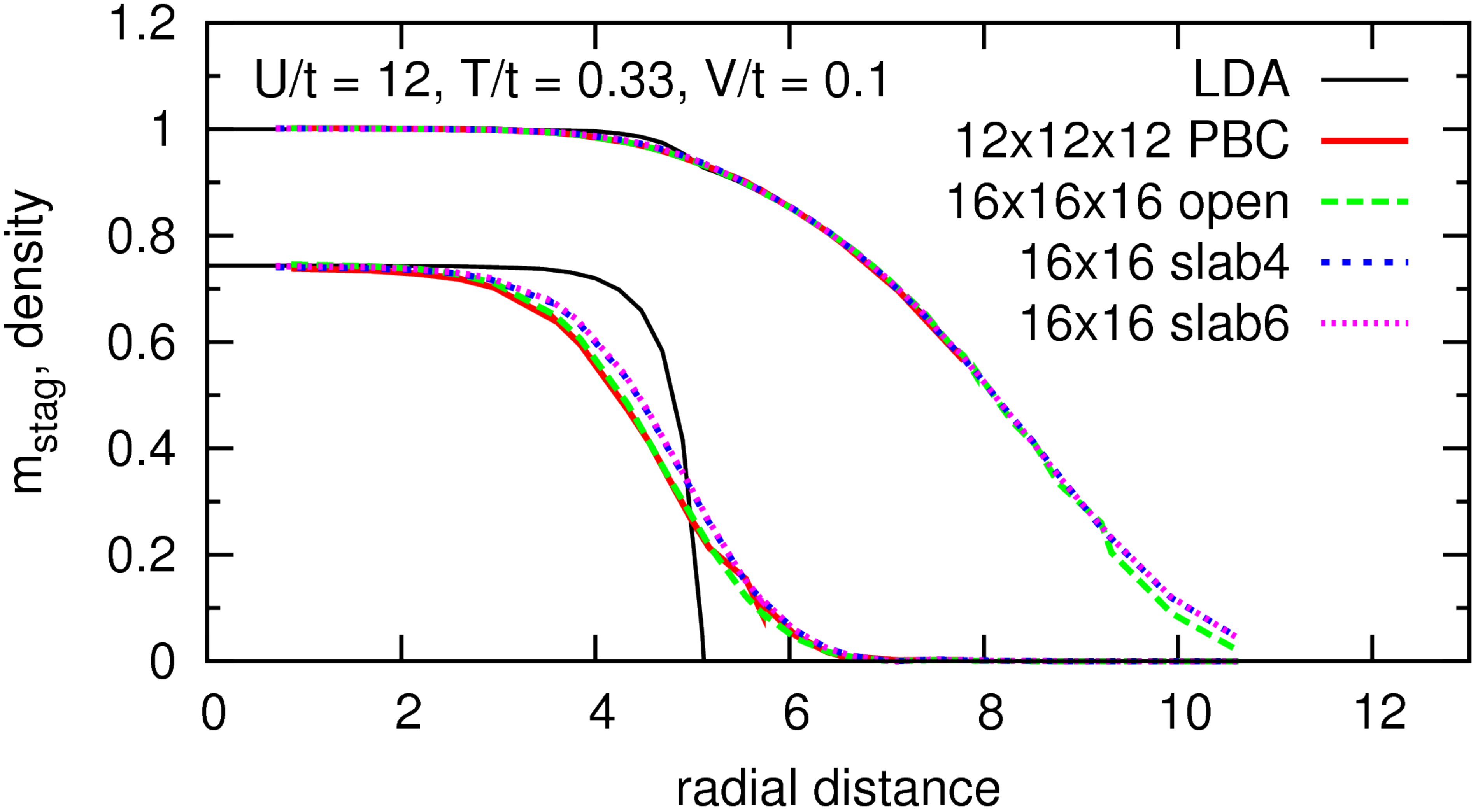
In practice: cylindrical potential (equivalent layers)

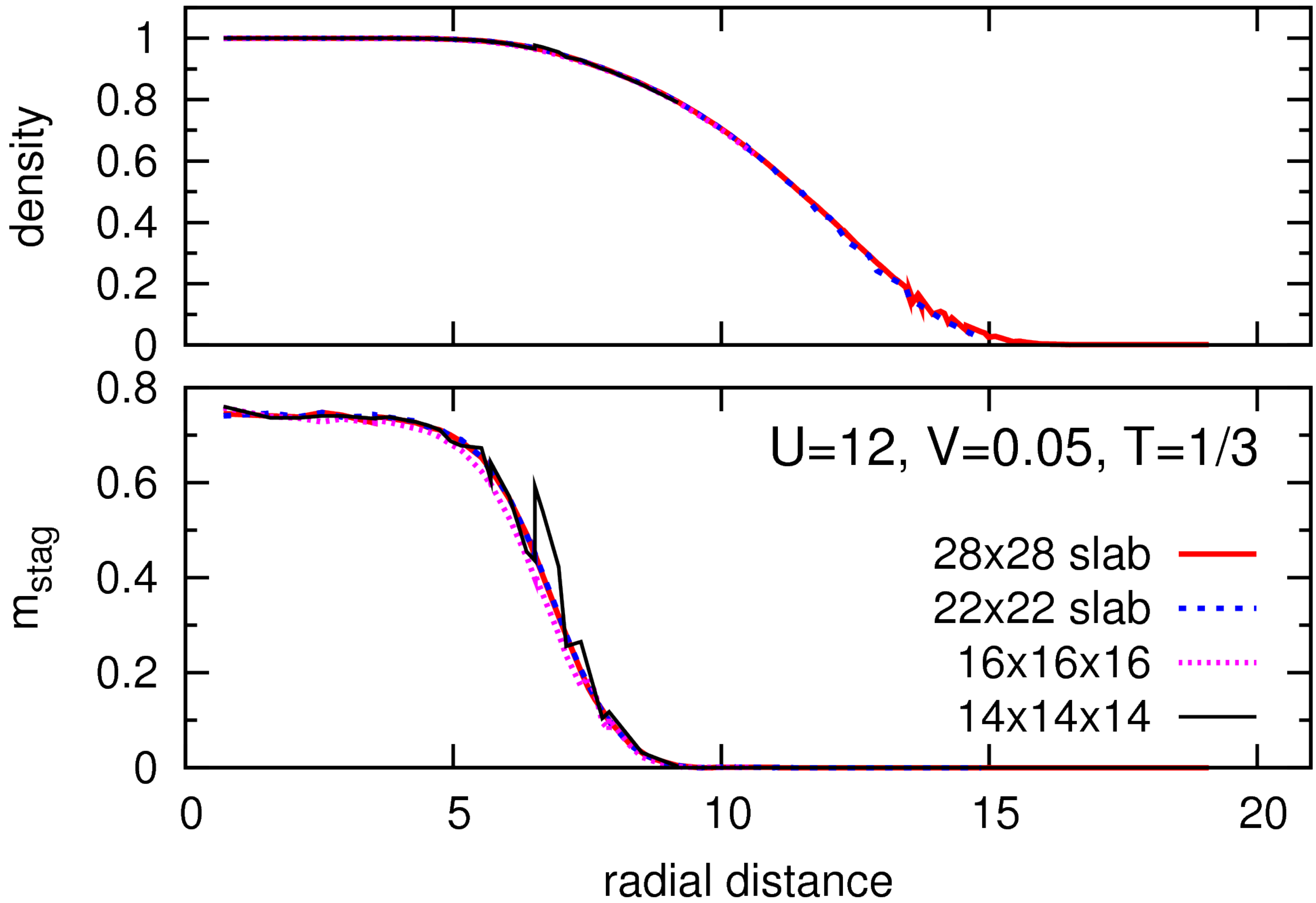
Alternative: 3D calculation, but focus on AF core (pbc's in all 3 directions):



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

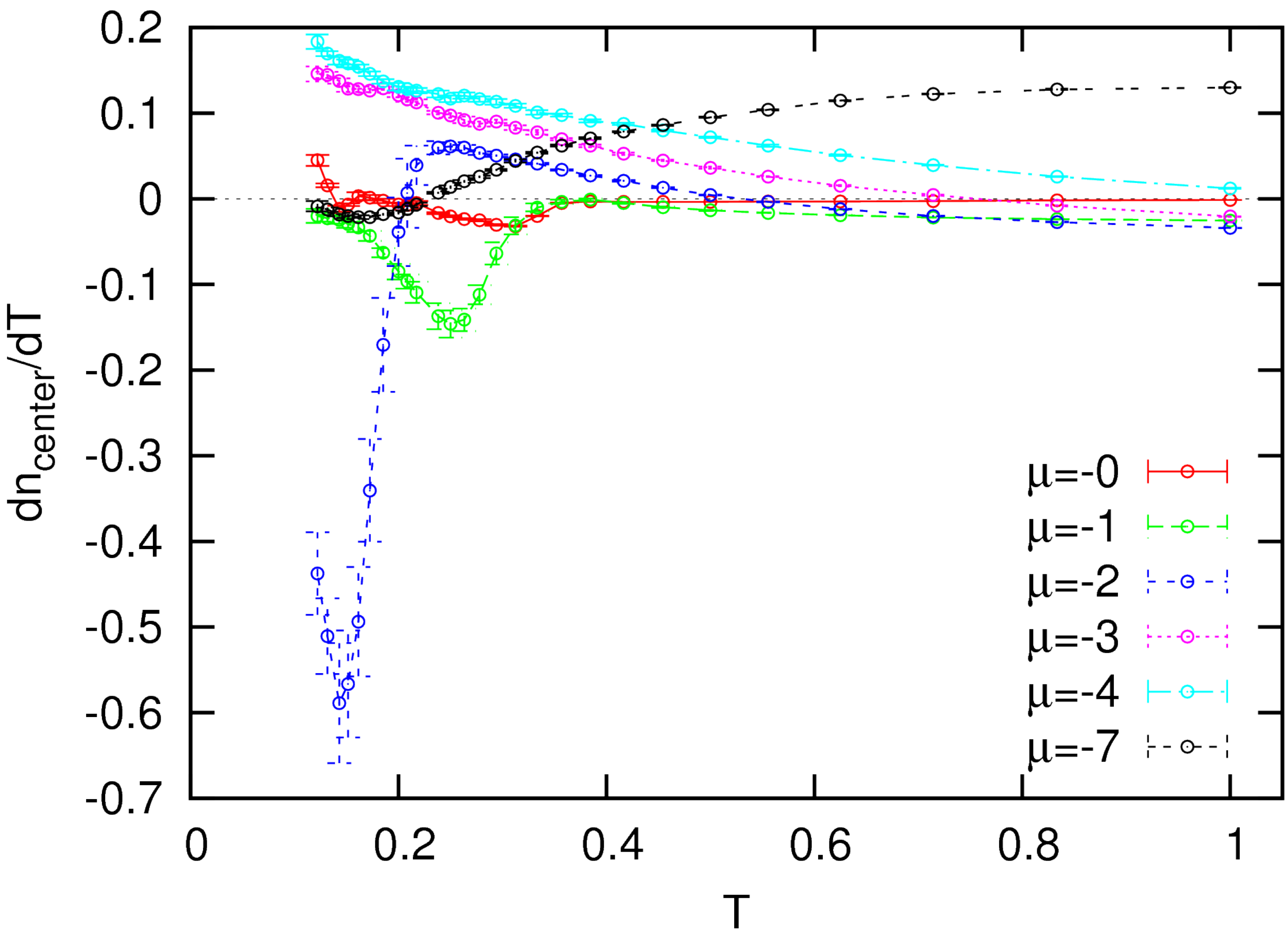
Test: slab versus minimal core 3D calculation (all with pbc)





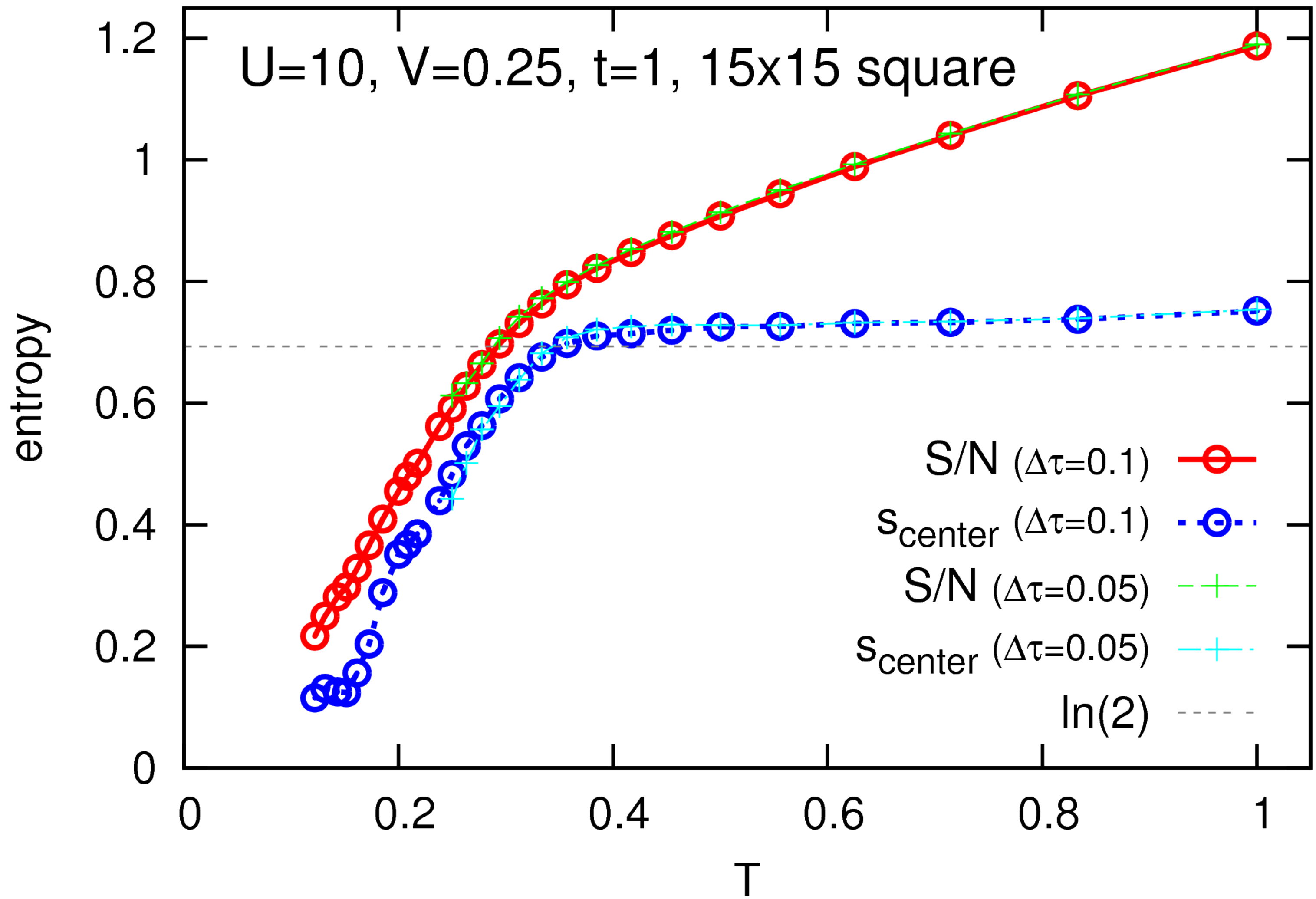
Significant deviations only if core touches boundaries!

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 ($\rightsquigarrow$ need fine integration grid)



very small discretization dependence

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