Quantum Monte Carlo simulations of ultracold 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: SCES, cold atoms on lattices

Methods: DMFT, QMC, RDMFT, slab approximation, LDA

[N. Blümer and E. V. Gorelik, CPC, in press, doi:10.1016/j.cpc.2010.07.011]

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Effect of nonlocal correlations? Comparisons with direct QMC

[ongoing collaboration with T. Paiva and R. Scalettar]

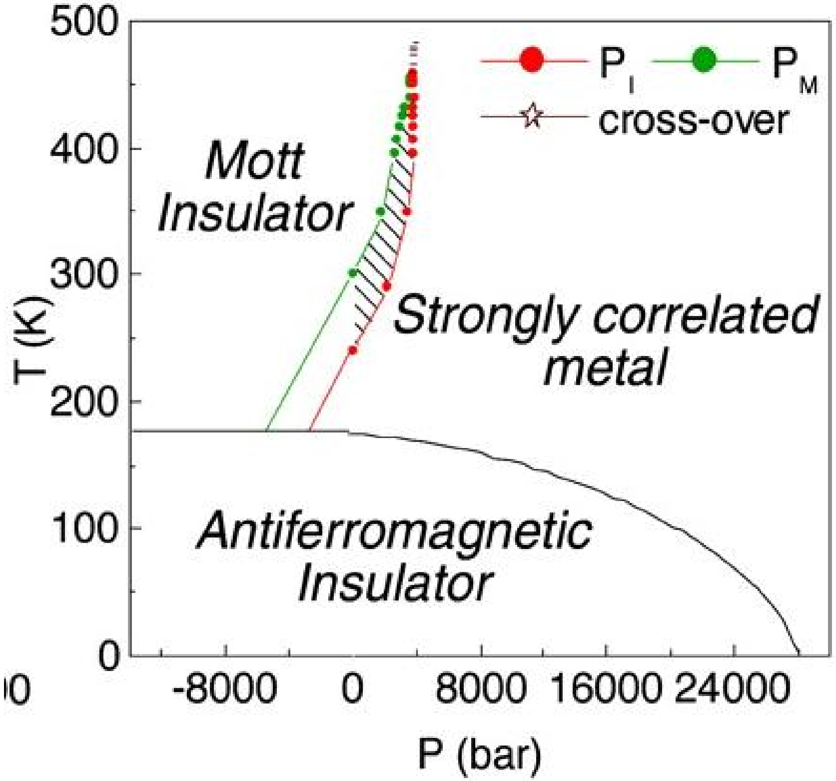
Impact of frustration, triangular lattice

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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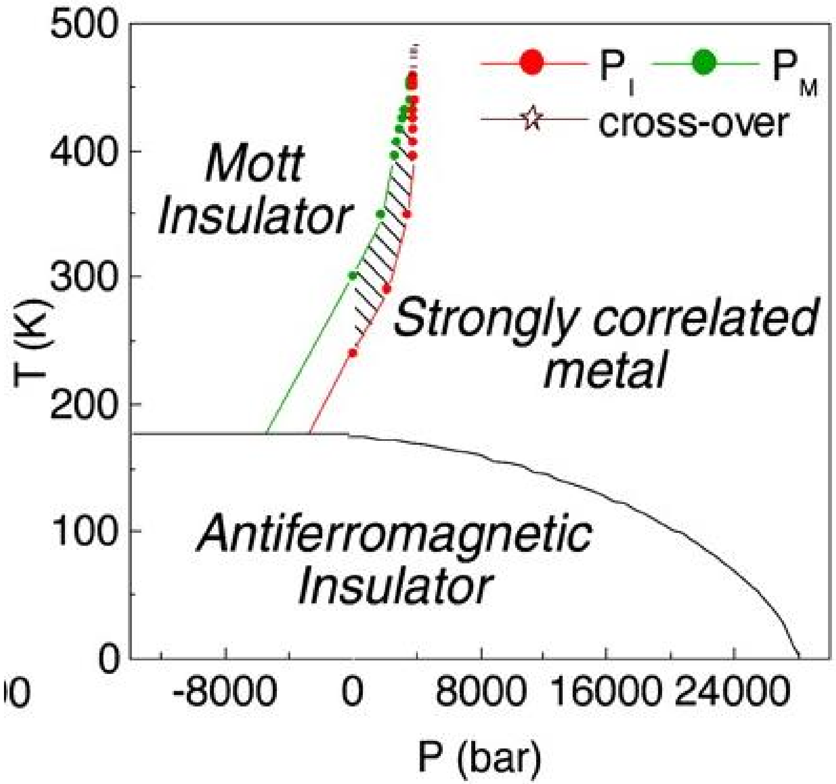

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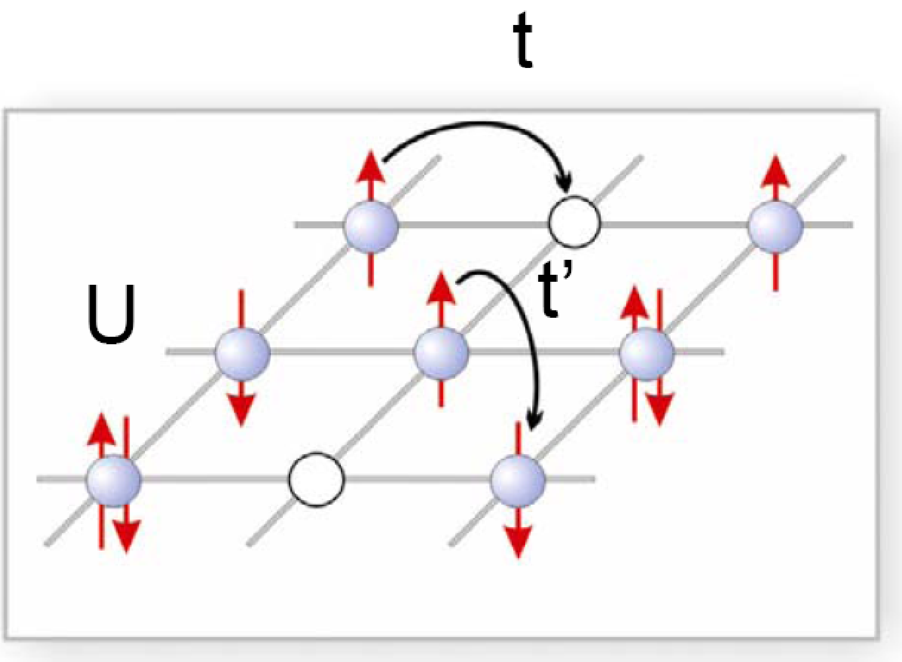
Mott metal-insulator transition and AF: generic physics of 1-band Hubbard model



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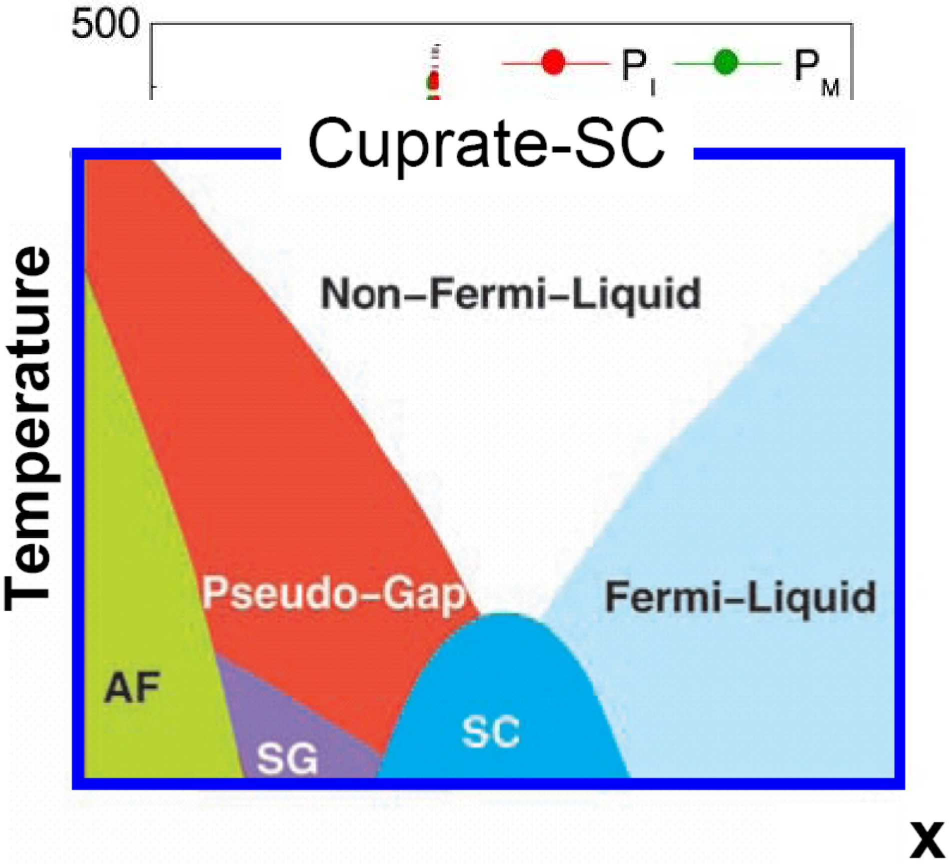

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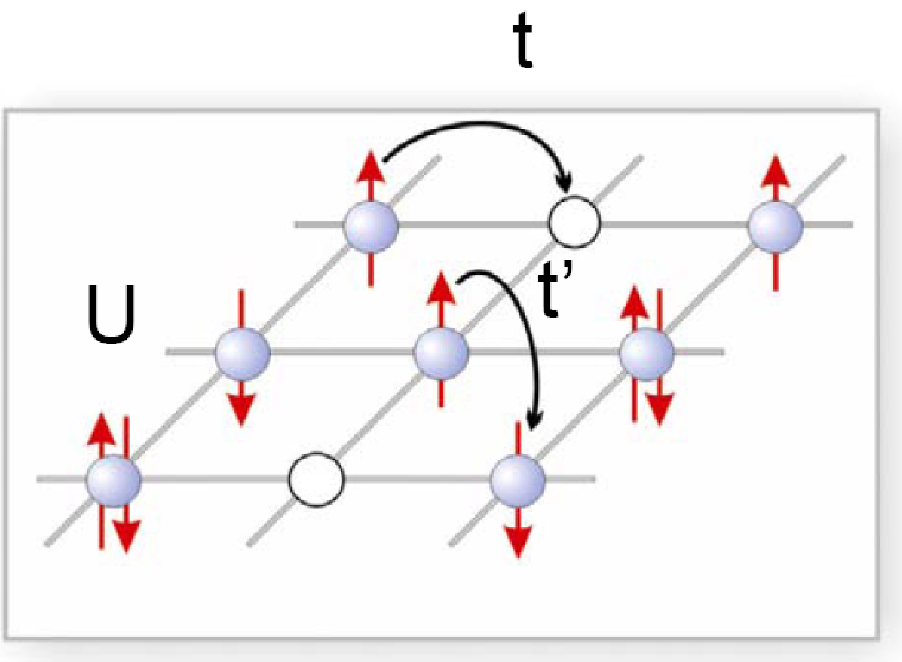

Are AF and Mott phases essential for superconductivity?

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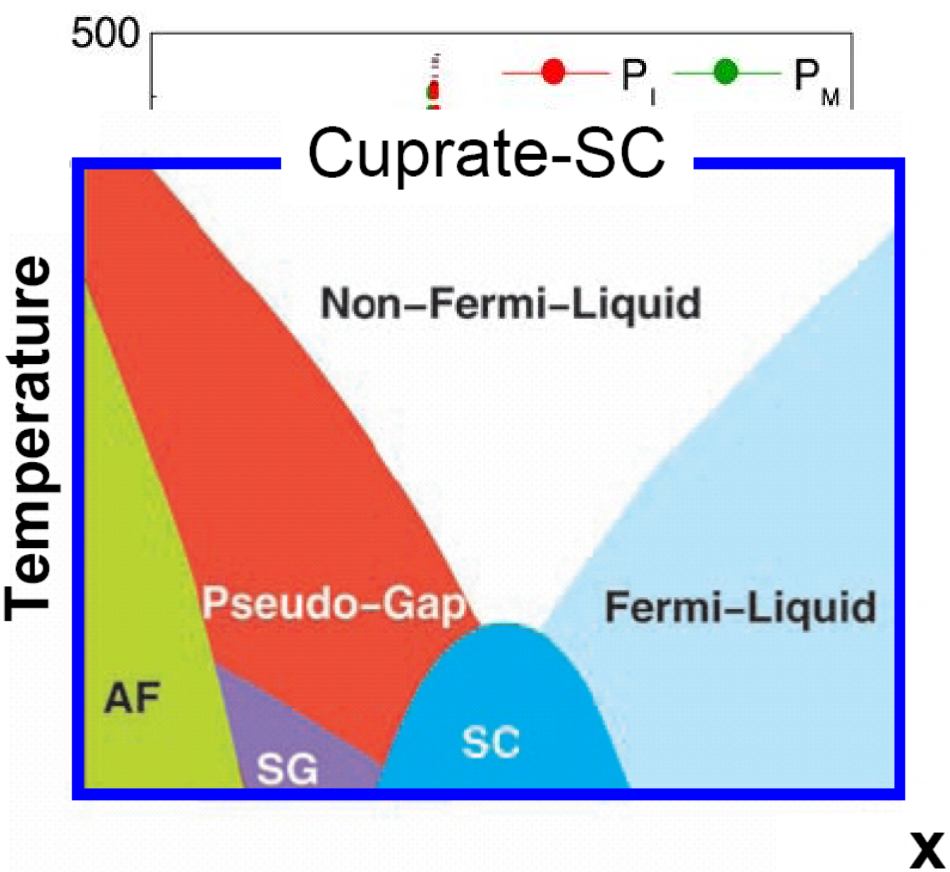

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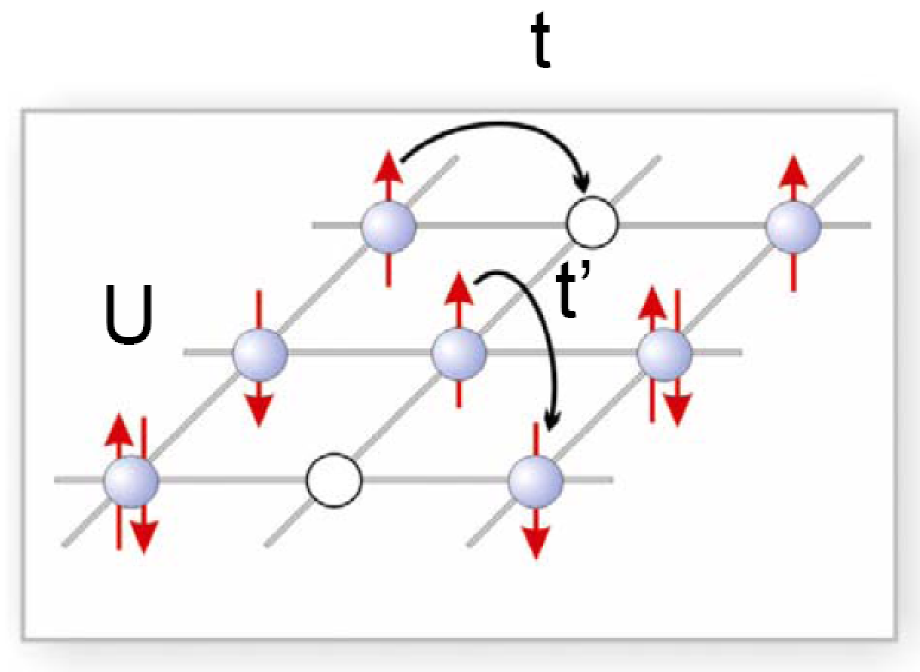


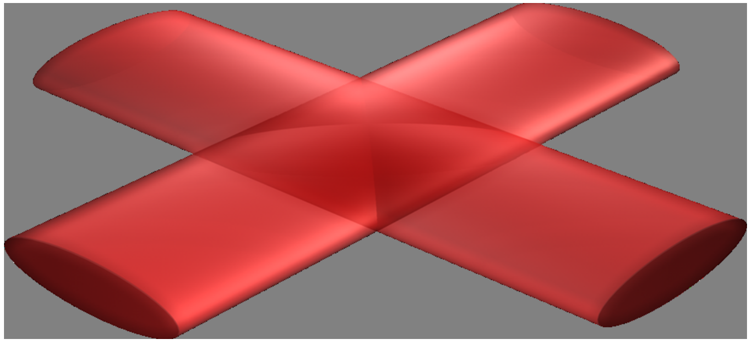
Are AF and Mott phases essential for superconductivity?

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)



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

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

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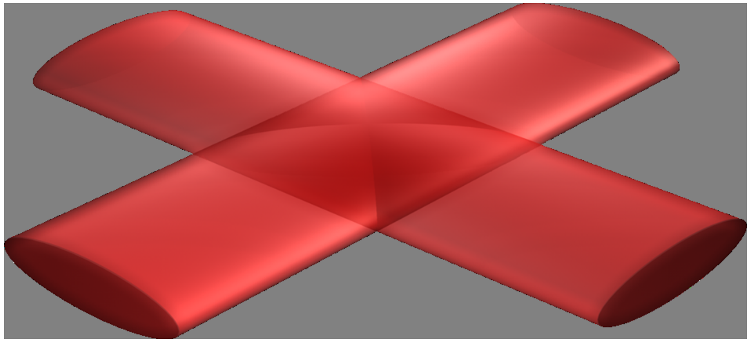

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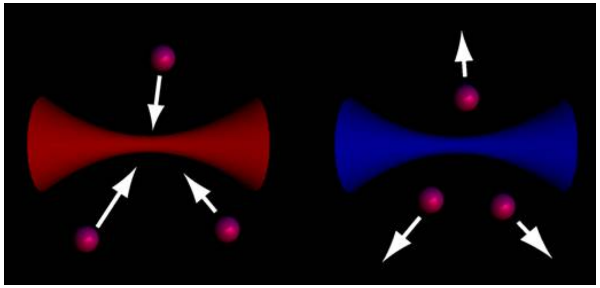

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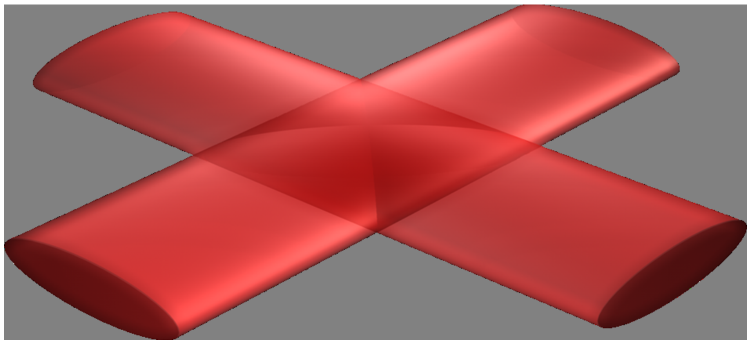

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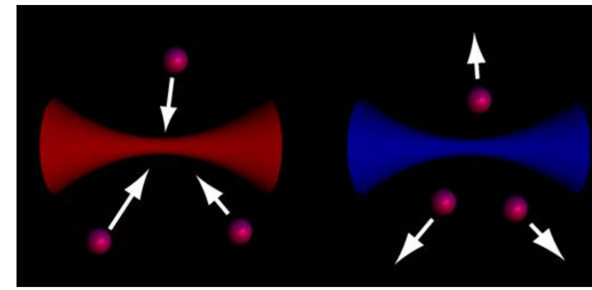
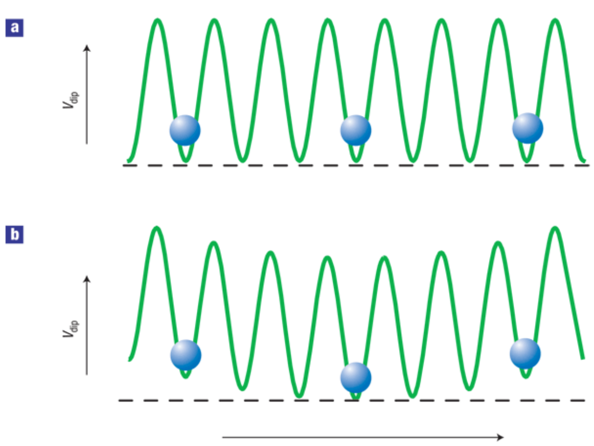


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



Beam profile: (anti) trapping

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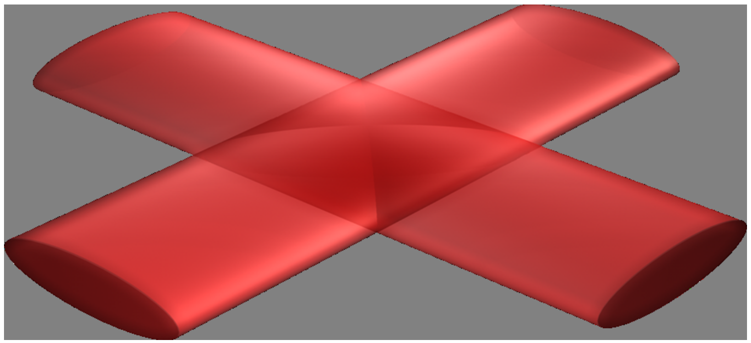

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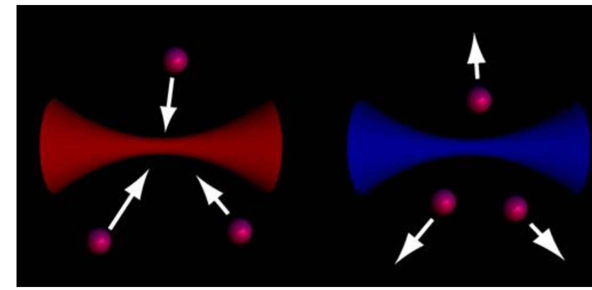

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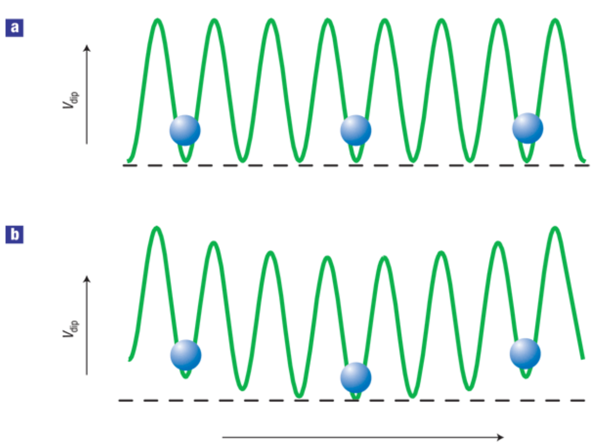


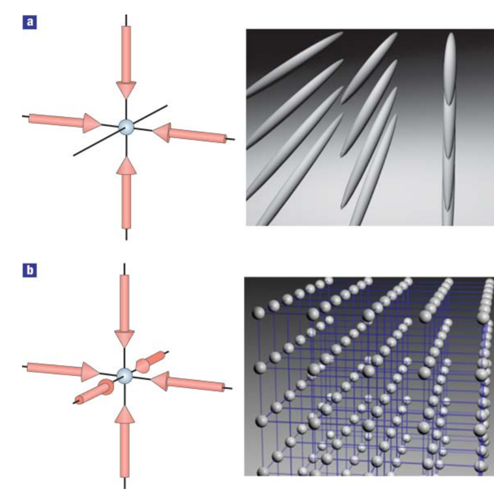
Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

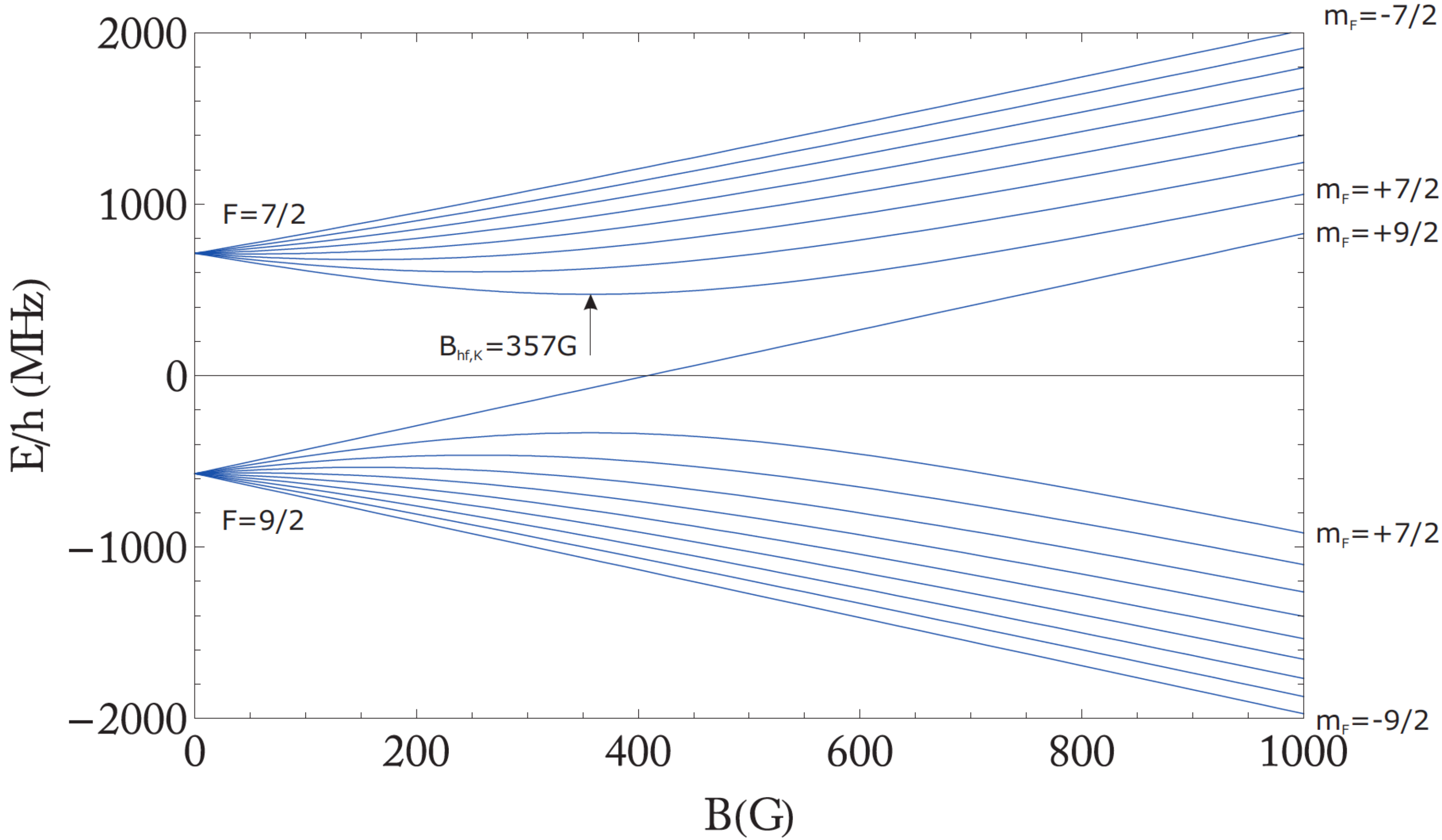
2 pairs of lasers $\rightsquigarrow$ tubes

3 pairs of lasers $\rightsquigarrow$ 3D lattice

hopping t tunable by laser



Large multiplets: reservoir of "flavors"

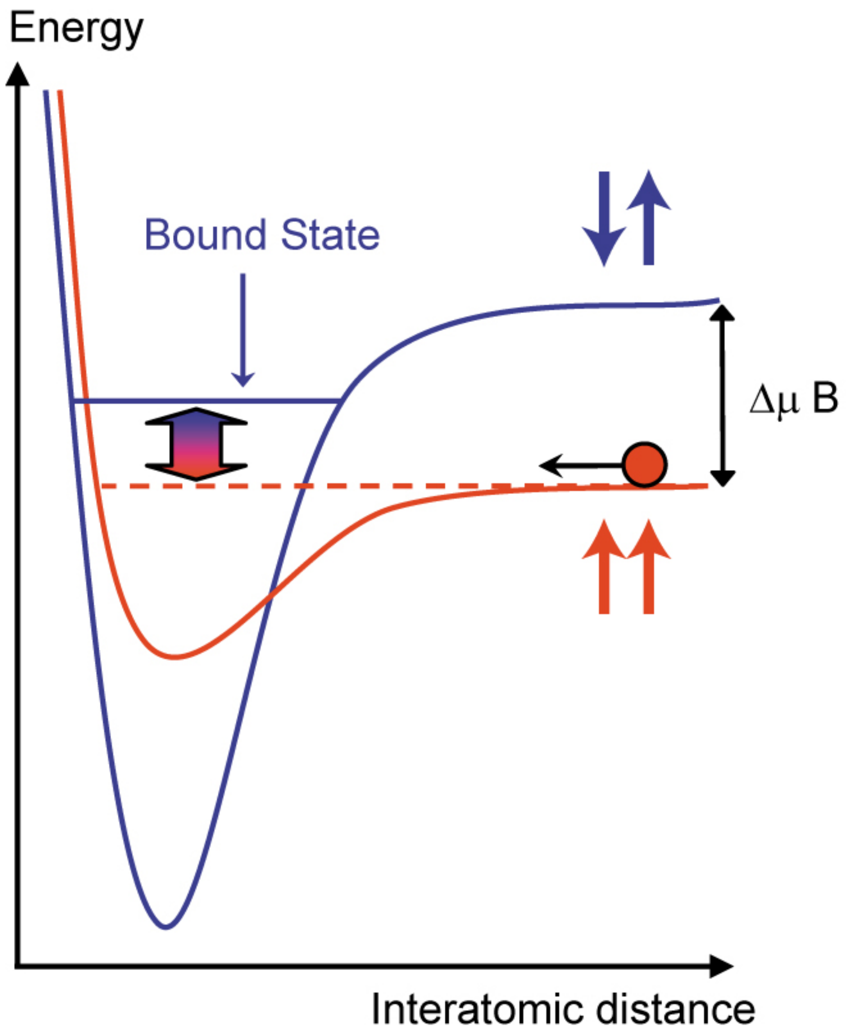


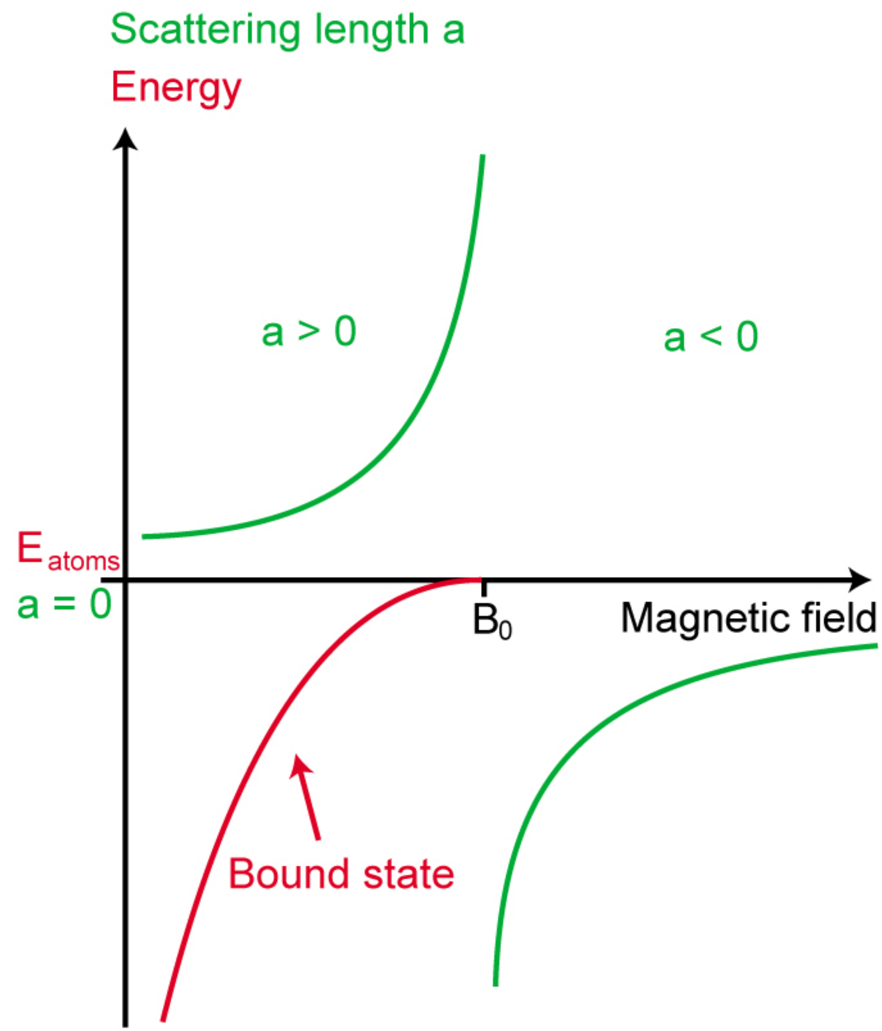
Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

[Tiecke, unpublished]

Interactions can be tuned via Feshbach resonances (here in magnetic field $\boldsymbol{B}$)

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





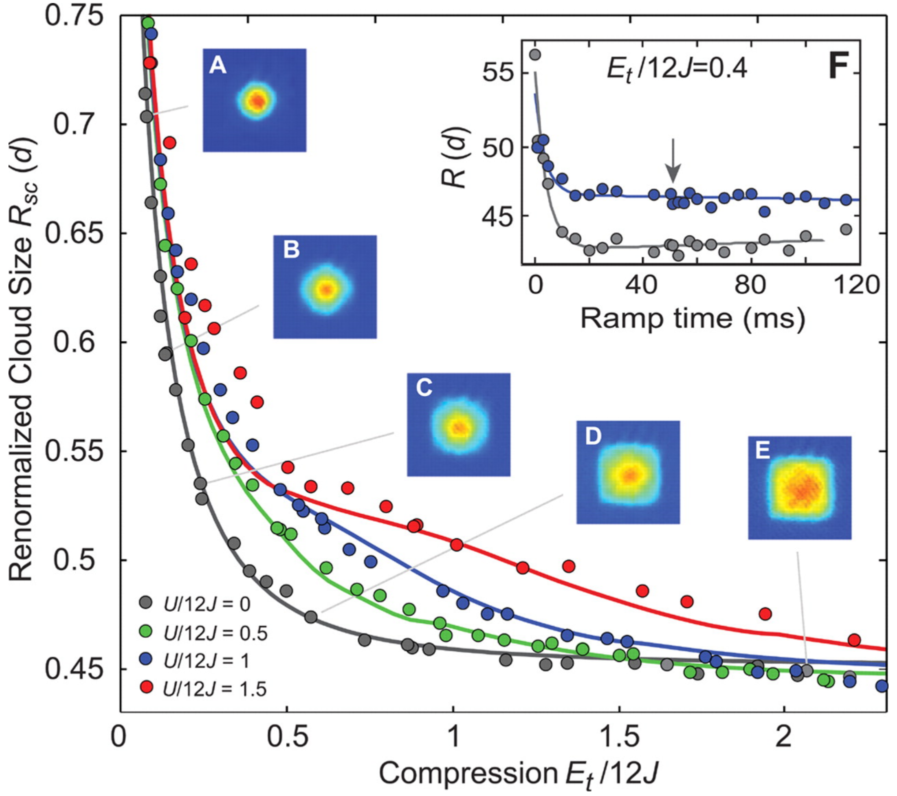
Correlations in ultracold fermions on optical lattices

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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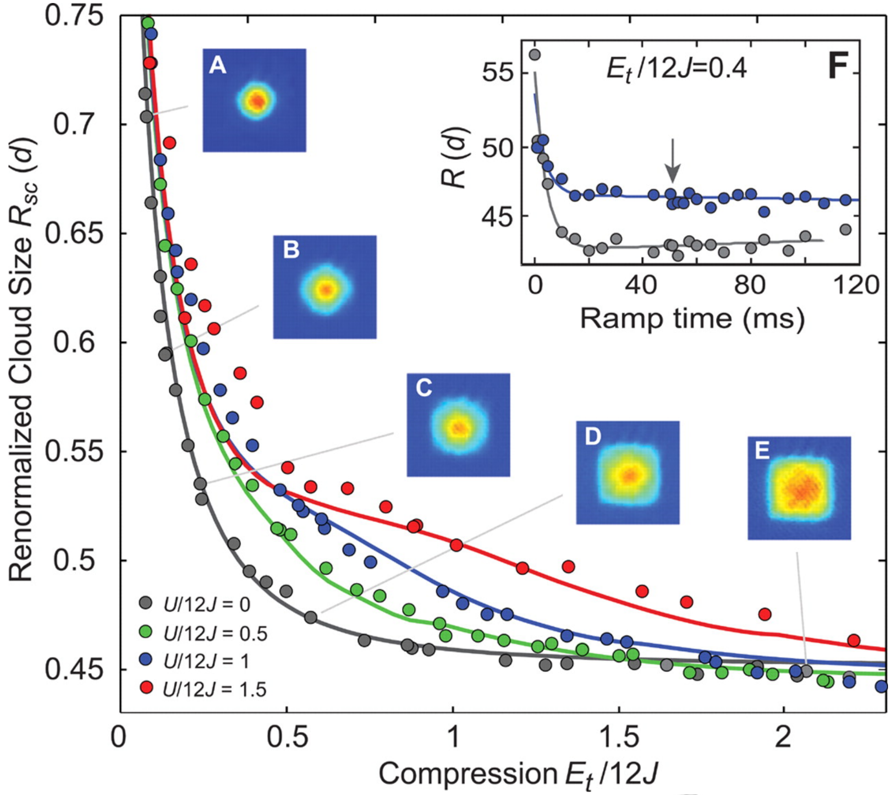
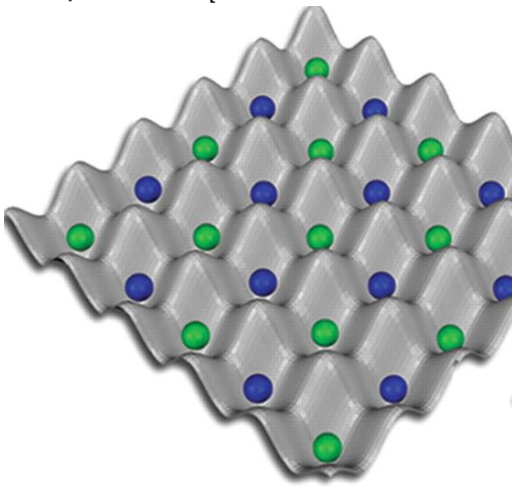


Next grand challenge: AF

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



Problems:

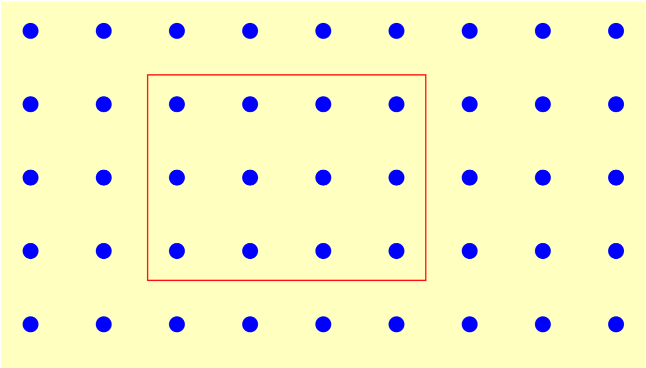
(i) difficult to reach sufficiently low temperatures/entropies

(ii) detection of order parameter is not straightforward

Methods: approaches for Hubbard model

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

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



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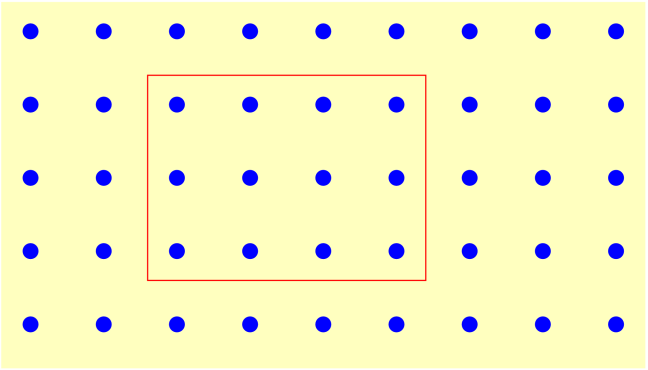
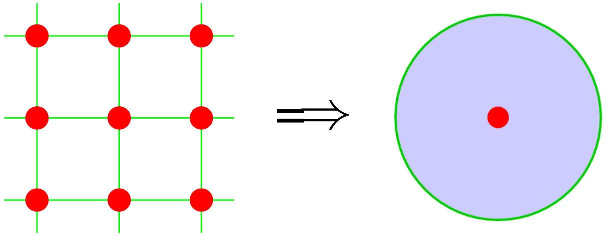


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

[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 $Z \to \infty$



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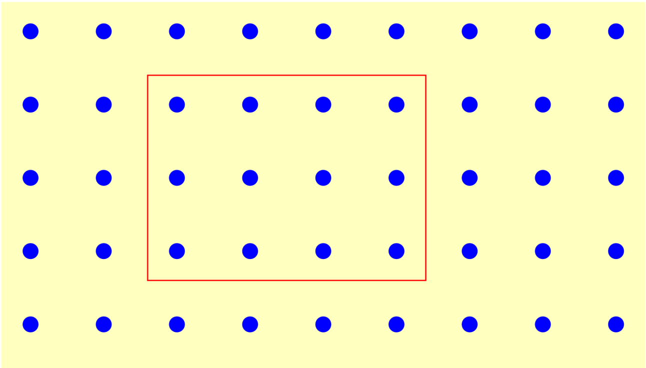

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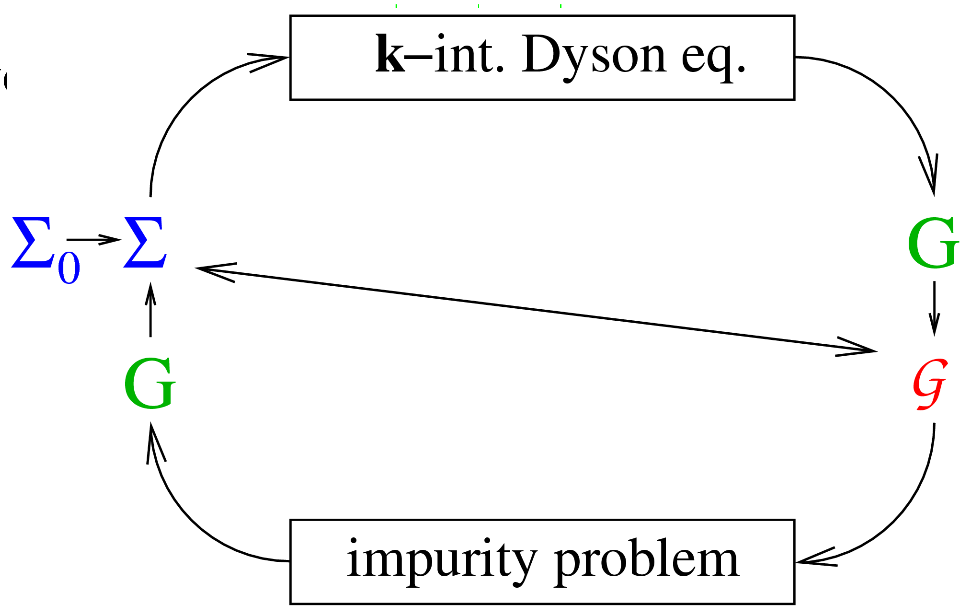
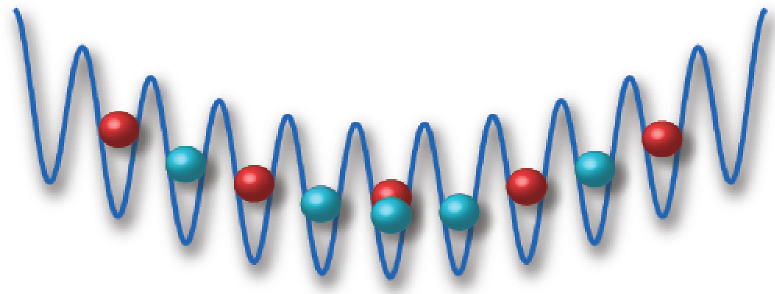
DMFT solution approached iteratively

- usually trivial: lattice Dyson equation
- difficult: impurity problem (IPT, ED, QMC, NRG, . . .)



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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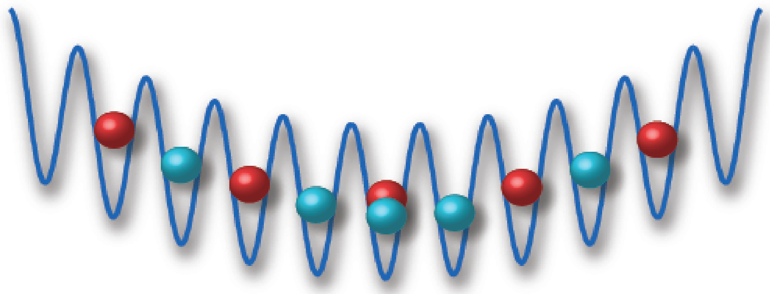

Real-space DMFT: use local, but site-dependent, self-energy

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

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

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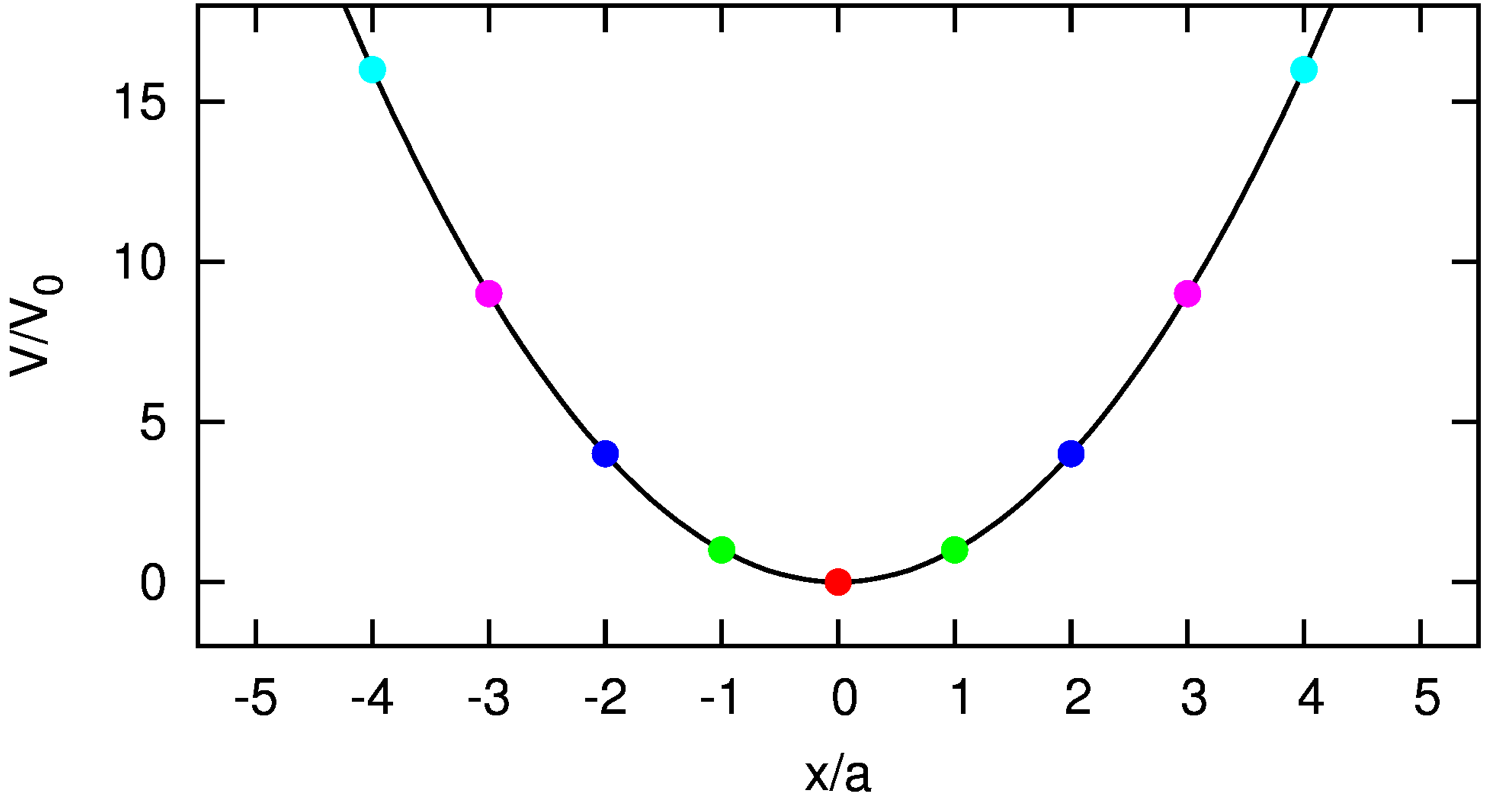
Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

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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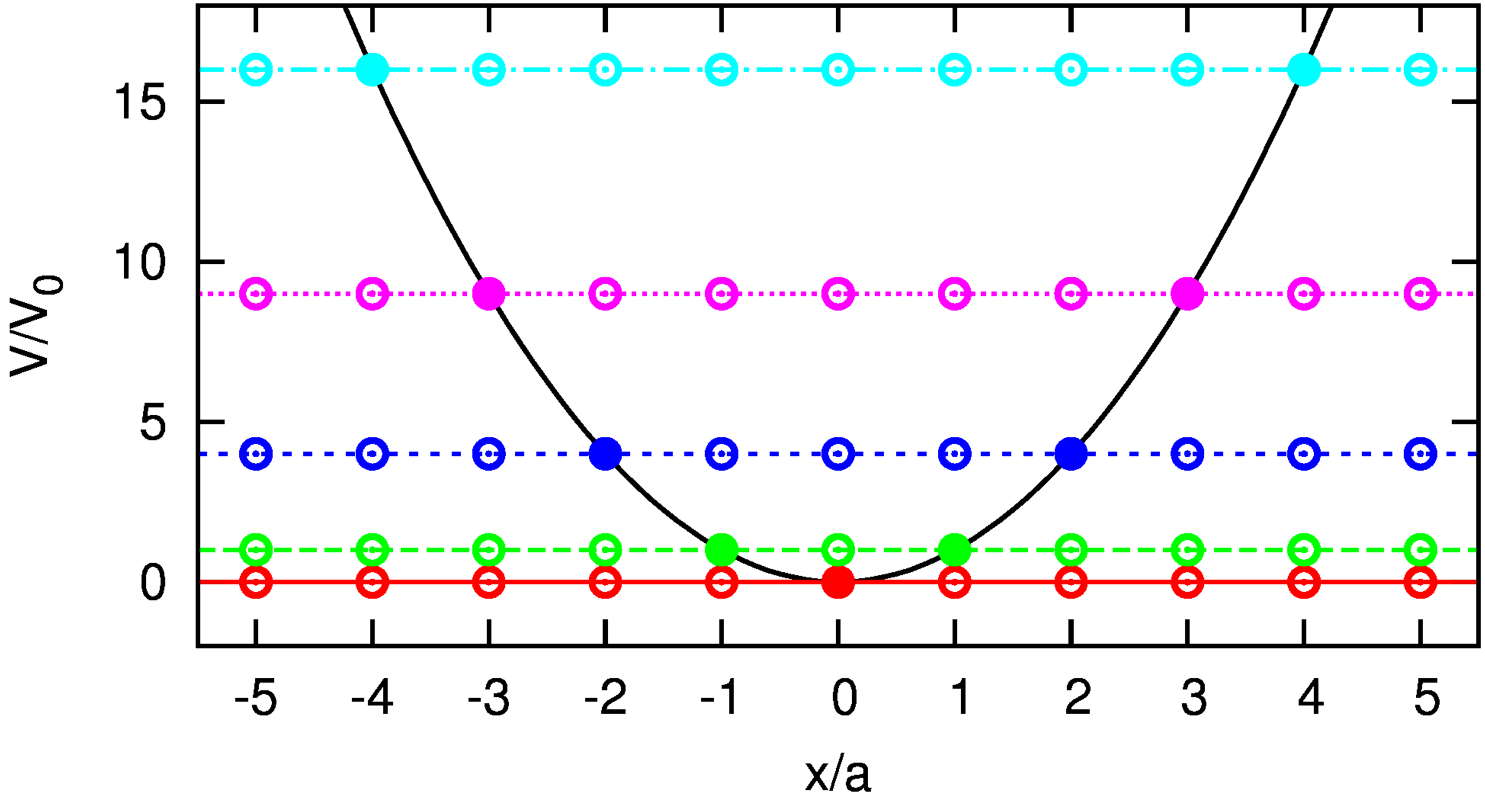


. . . will be used for comparison to RDMFT

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

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

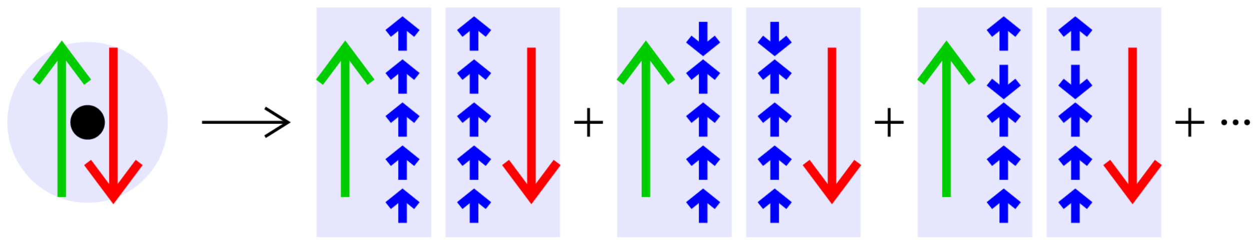
Green function G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

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

(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

+ numerically exact, + no sign problem, (density-type interactions) − effort scales as T^{-3}

Antiferromagnetic order at finite T in an optical trap

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

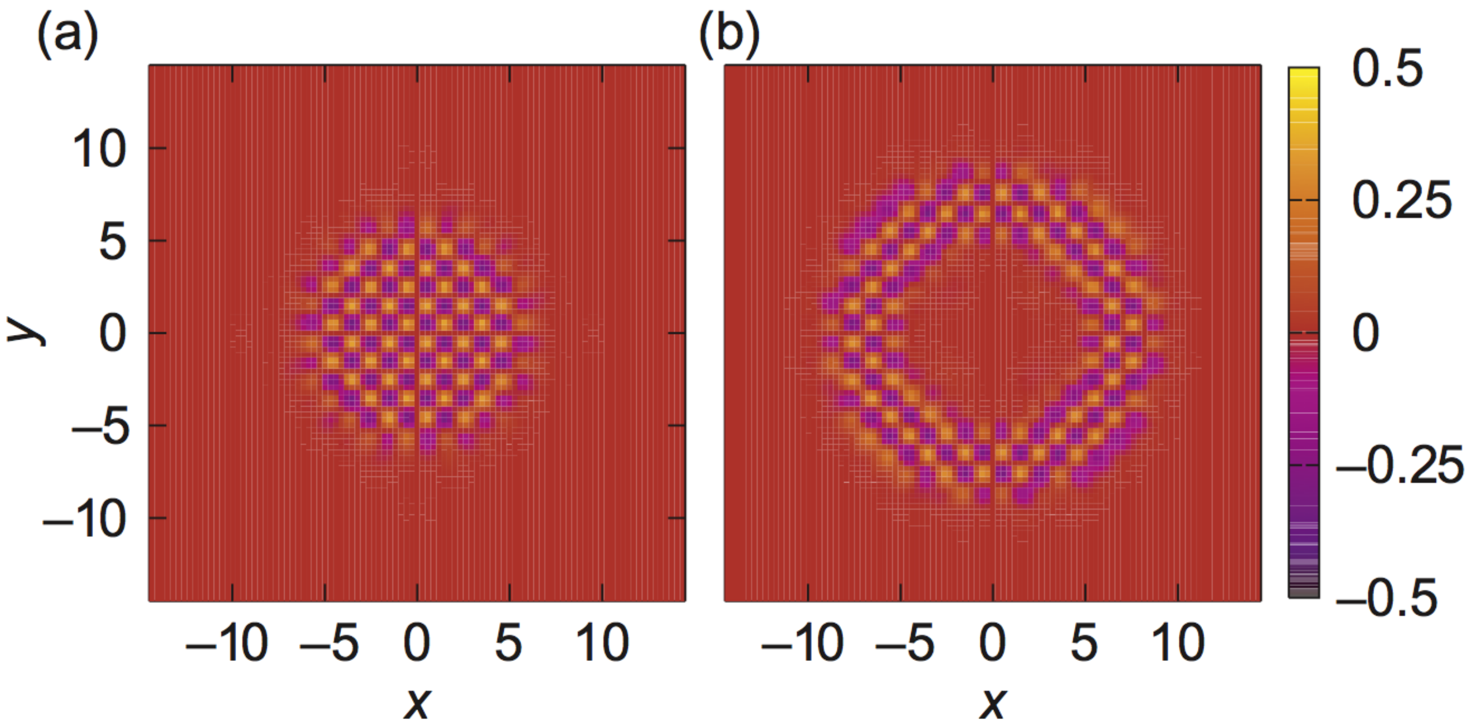
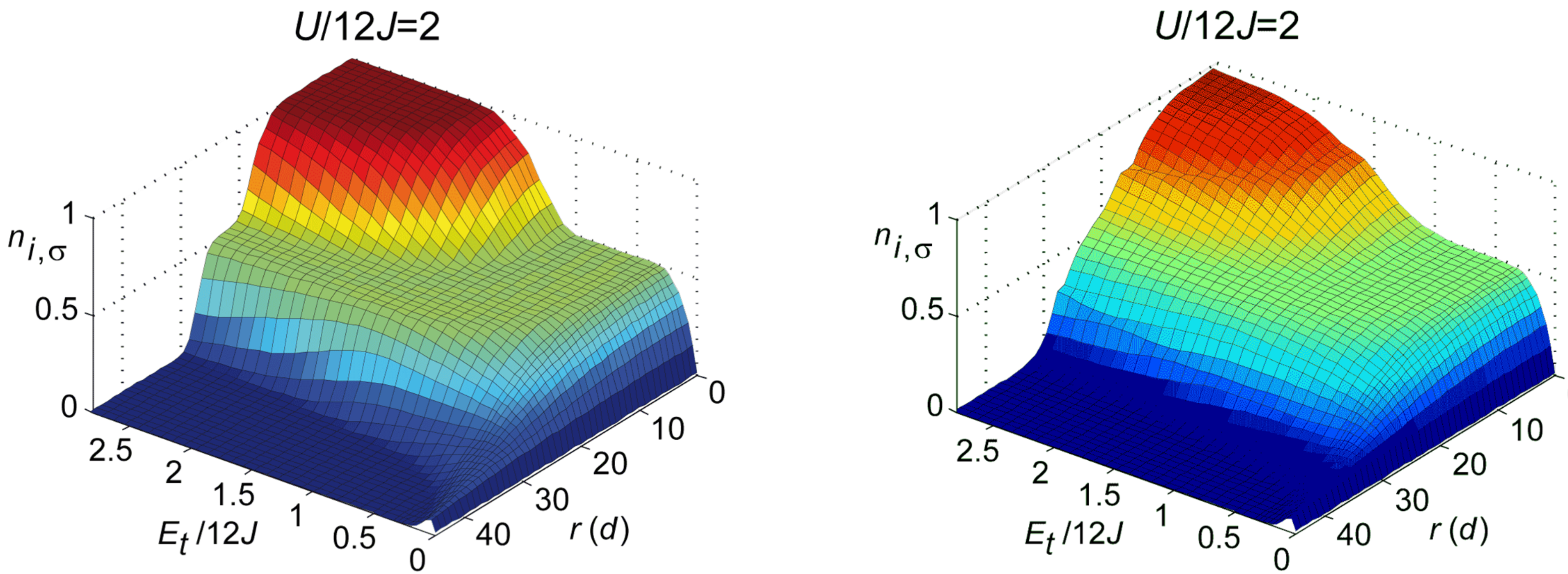


Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_\uparrow = \mu_\downarrow = 5$; (b) $V = 0.2$ and $\mu_\uparrow = \mu_\downarrow = 15$. Energies are expressed in units of the hopping parameter J.

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

But: NRG problematic at elevated temperatures

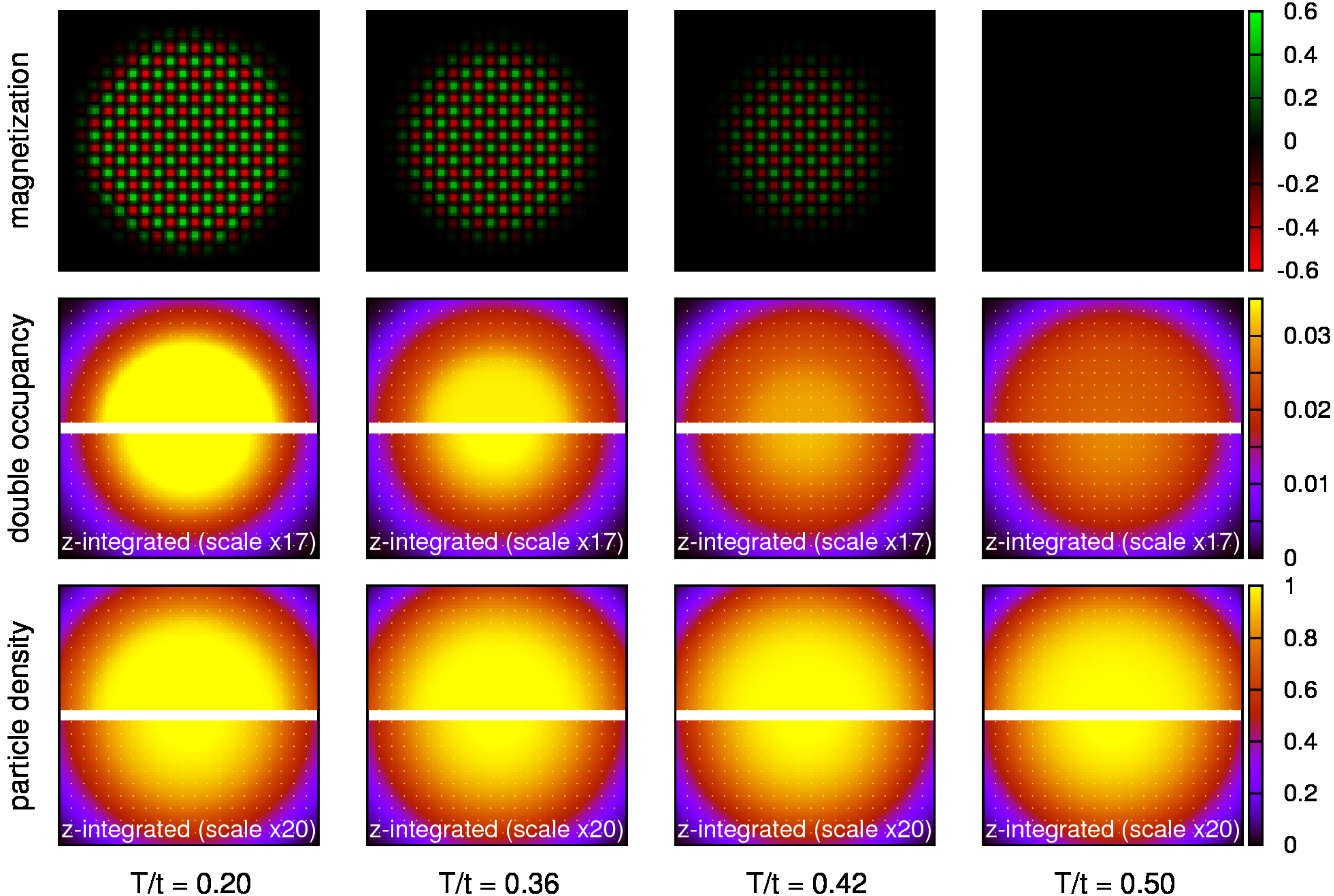


$T = 0.07t$ $T = 0.15t$

Additional plateau/kinks at $n_\sigma \approx 0.8$ for $T = 0.15t$ [Rosch group, courtesy of U. Schneider]

However: experimental temperatures are high ⇝ advantage for QMC!

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



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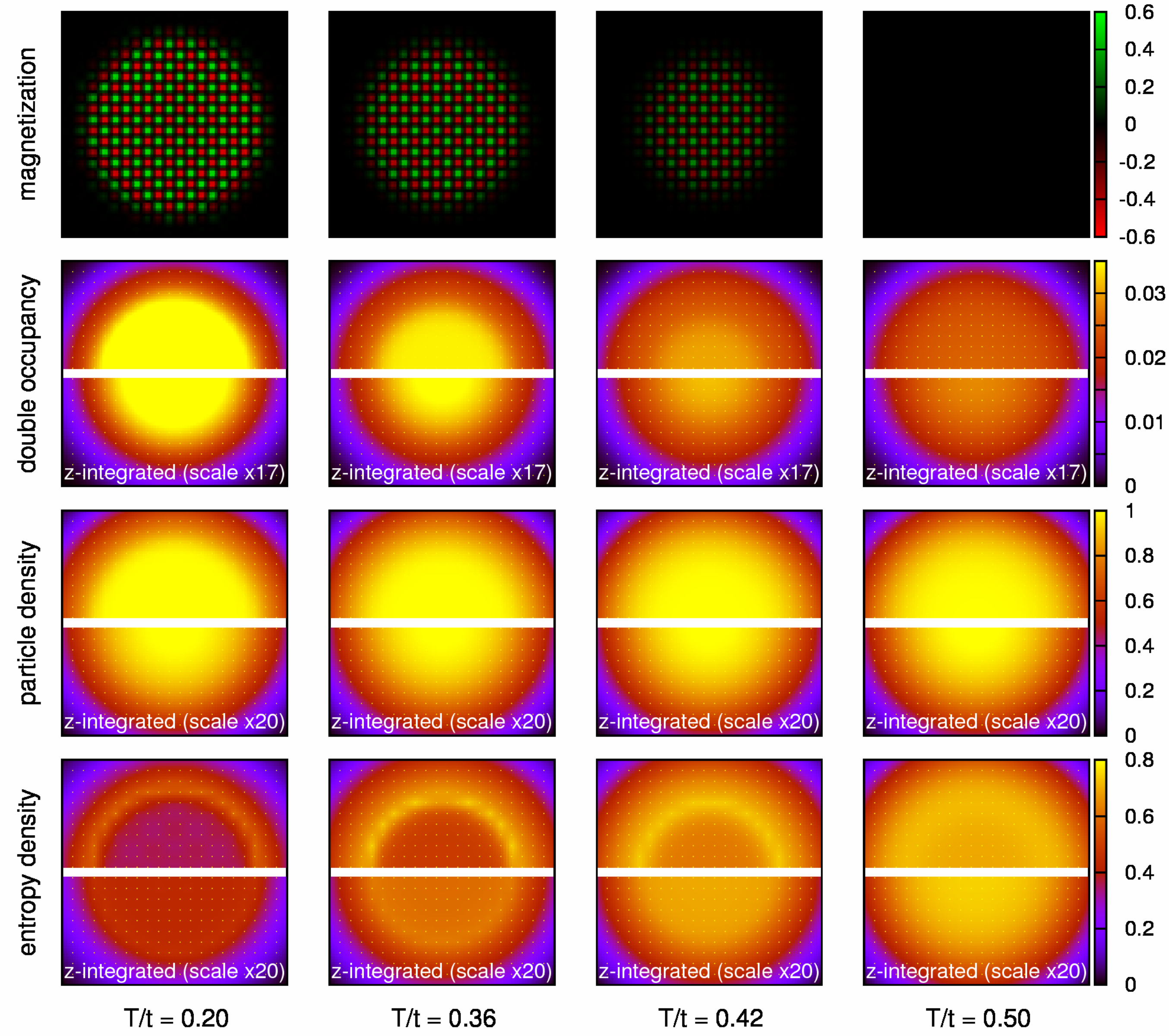


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

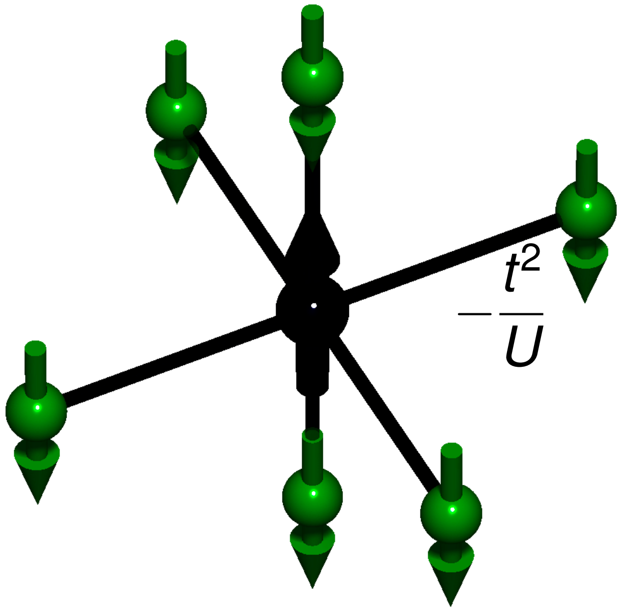
$\sim$ 6000 atoms (naively $\sim 30^3 = 27000$ sites needed)

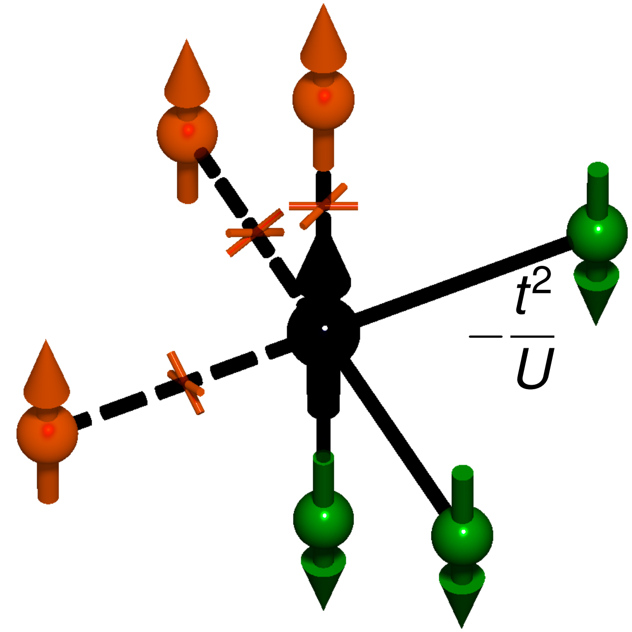
Entropy

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

Enhanced double occupancy: a signature of AF order

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





AF state:

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

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

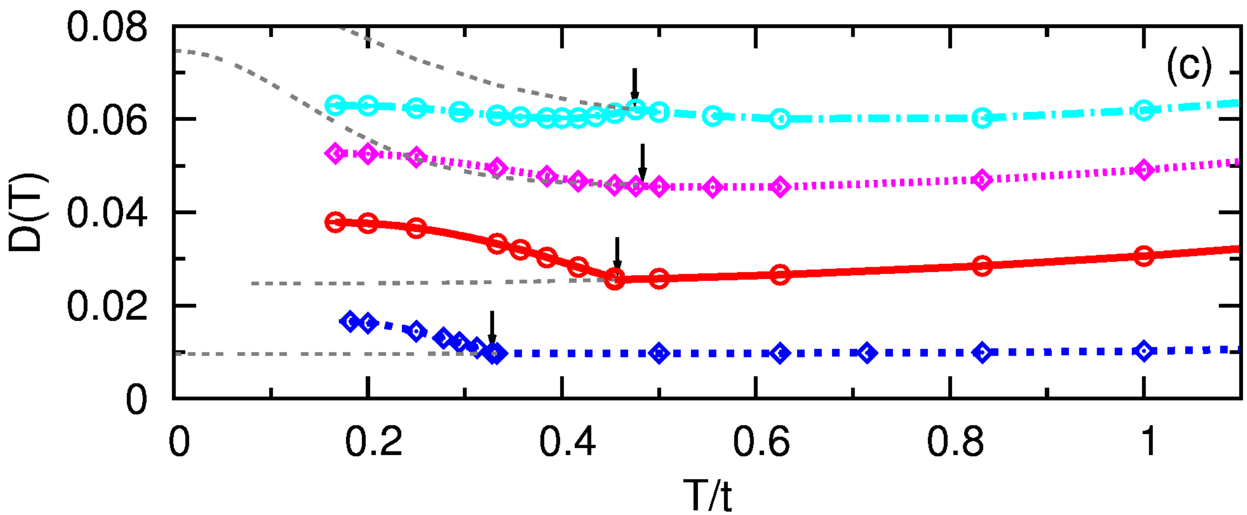
Paramagnetic state:

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 $D_{\mathbf{AF}}/D_{\mathbf{p}} \stackrel{U\to\infty}{\longrightarrow} 2$.

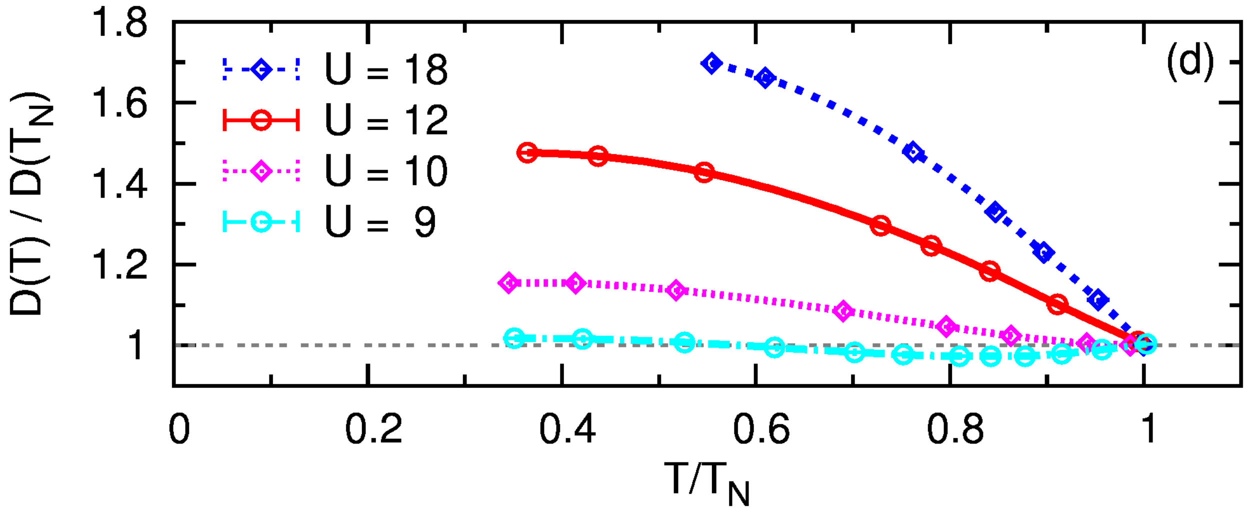
DMFT-QMC estimates of D at half filling



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

arrows: Néel temperatures

thin lines: metastable paramagnetic phase.

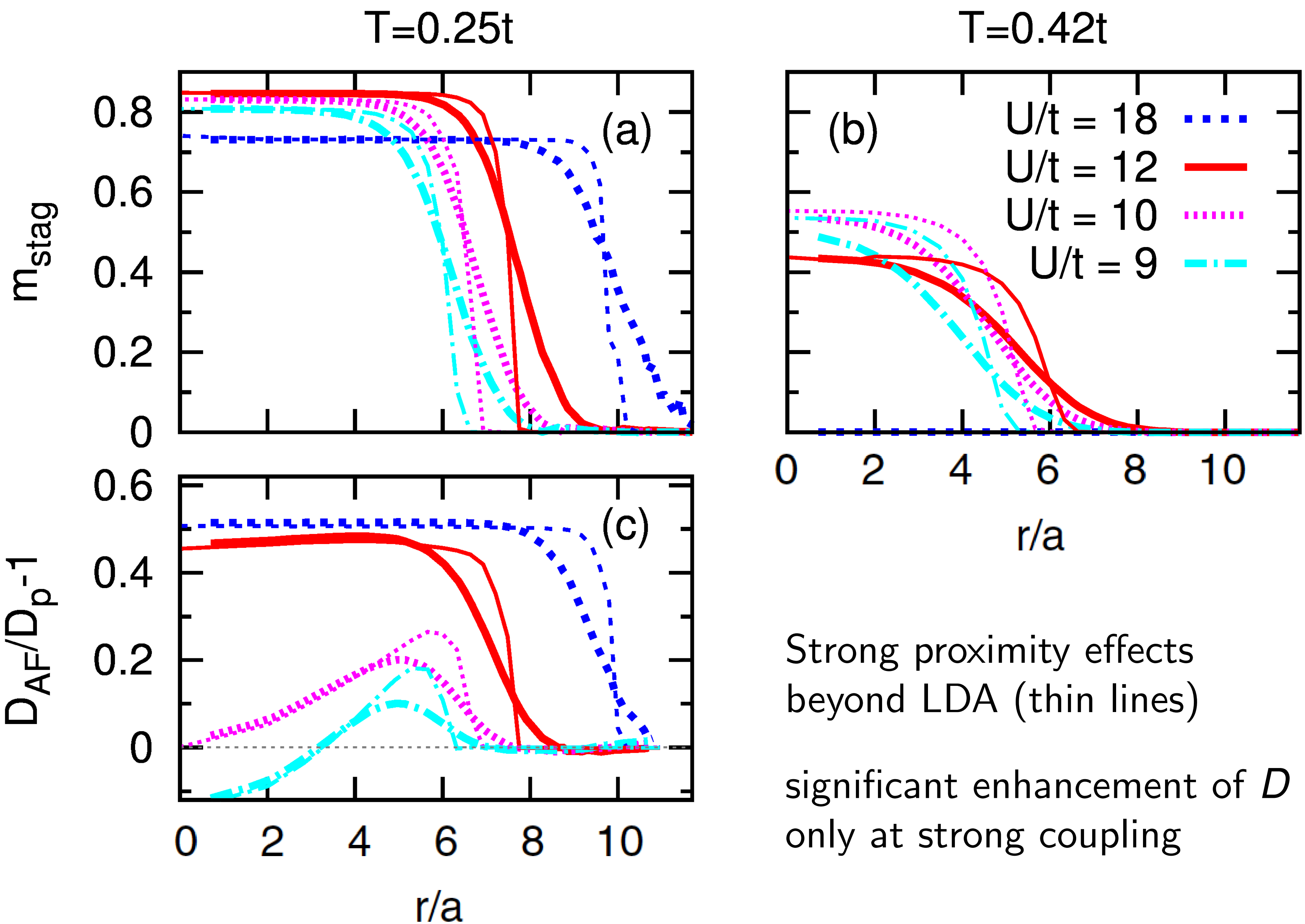


Data scaled to values of critical point:

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

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

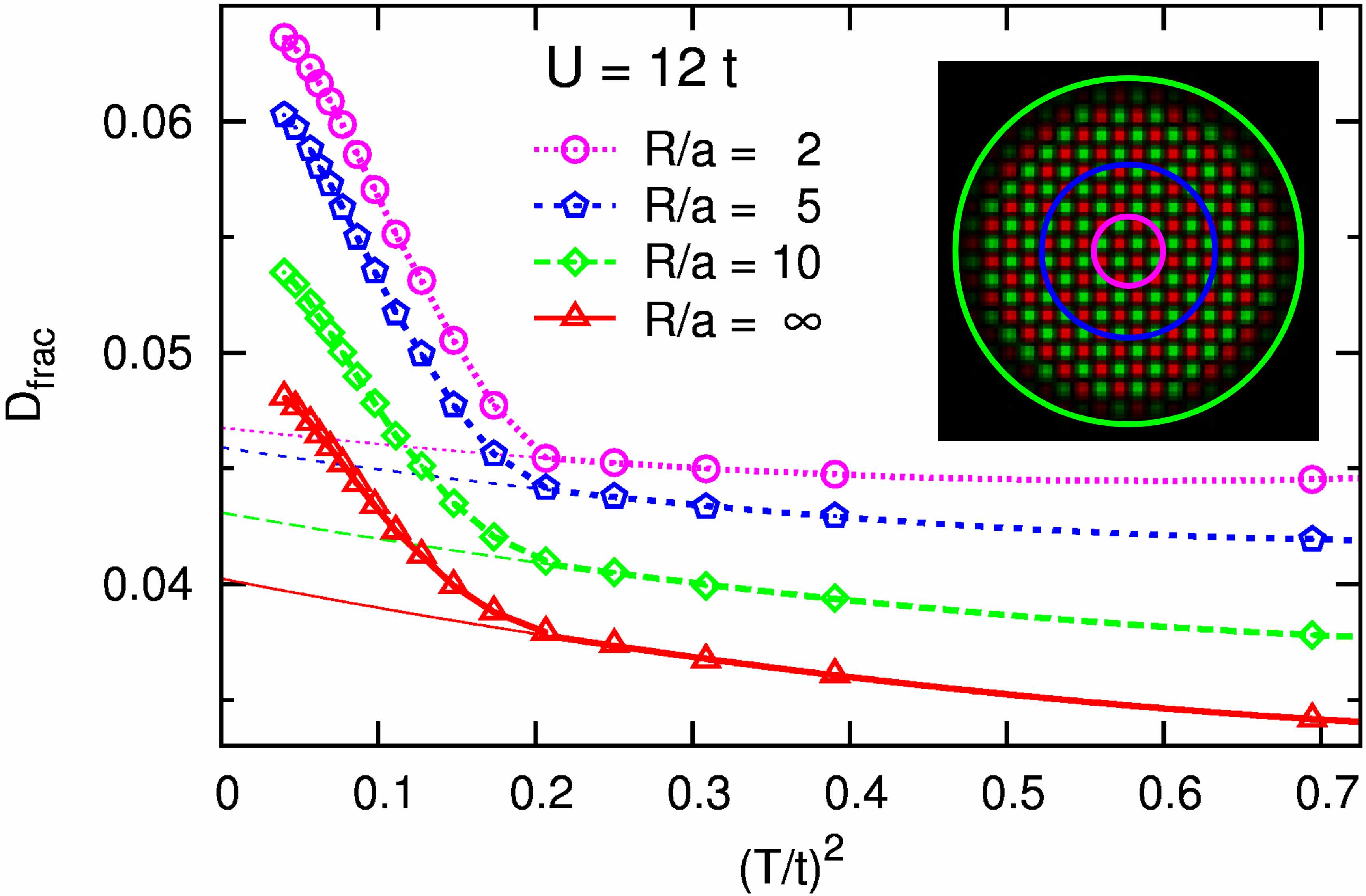
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



Strong proximity effects beyond LDA (thin lines)

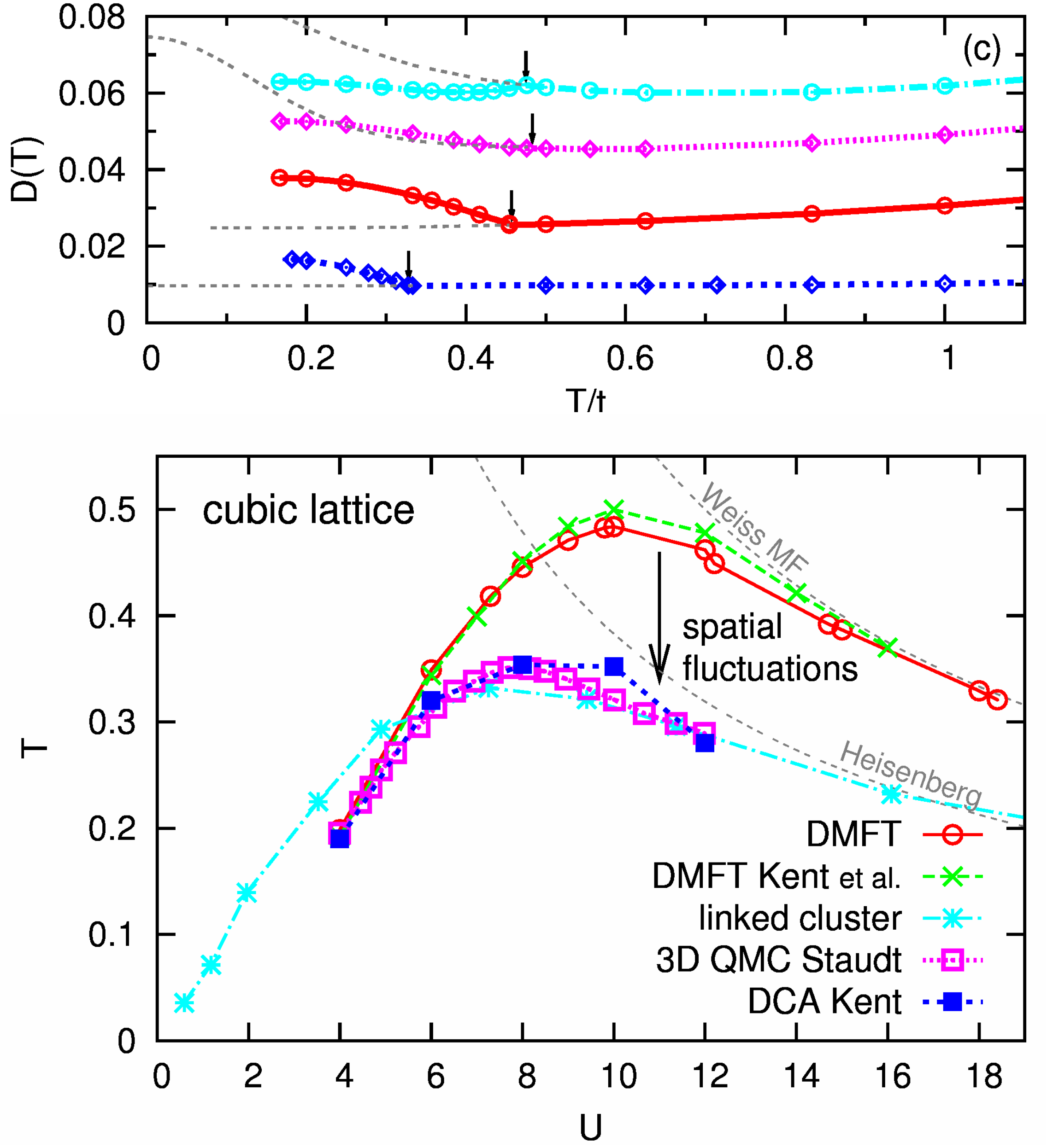
significant enhancement of D only at strong coupling

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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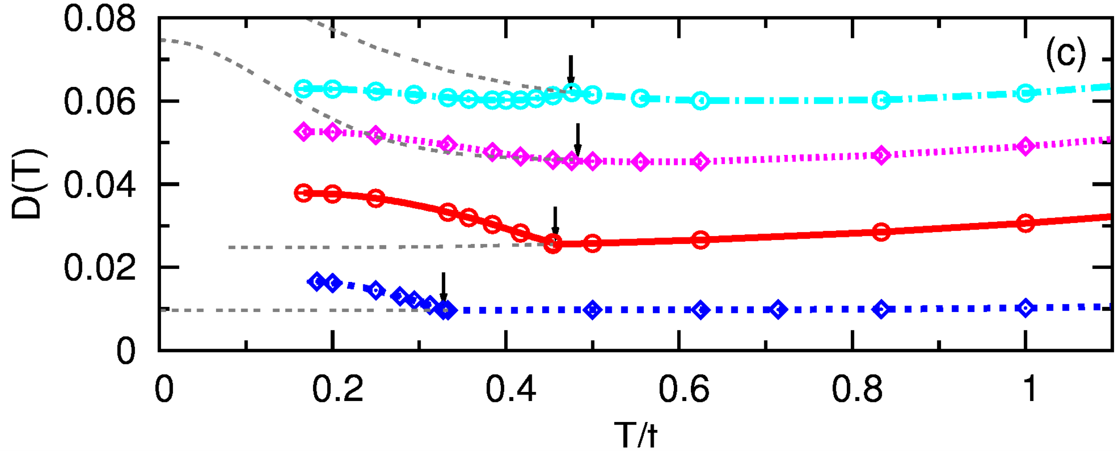
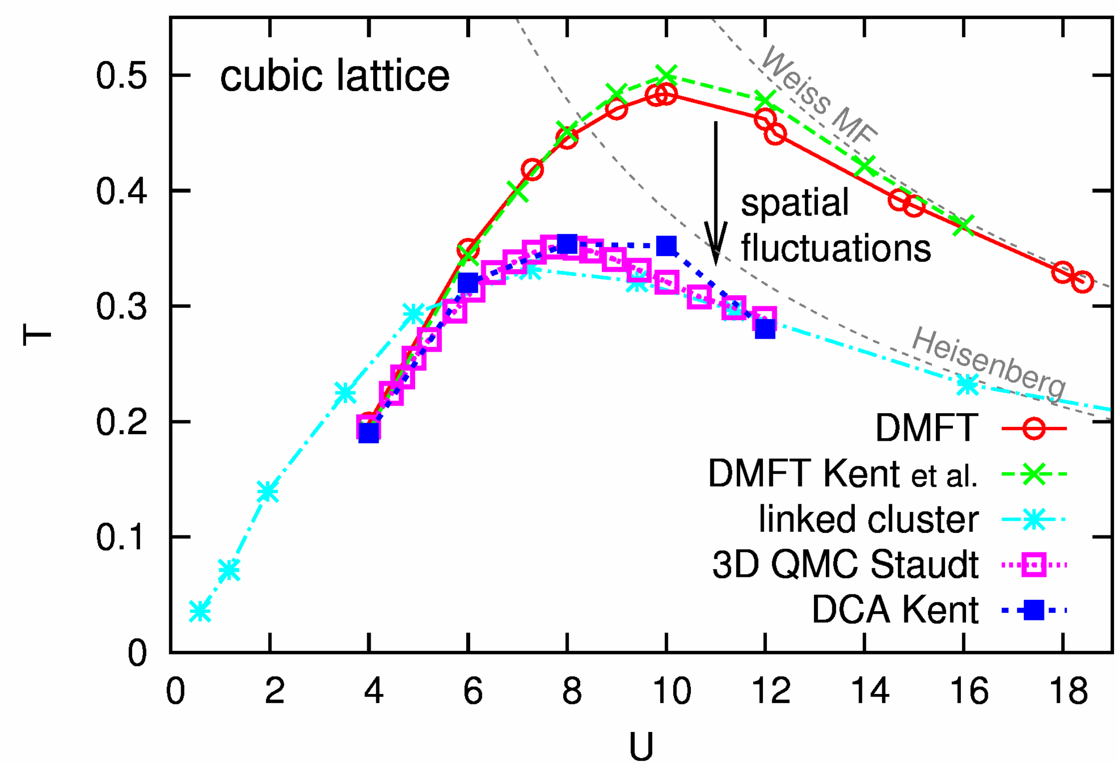


Unavoidable change: kinks cannot remain at $T = T_N^{DMFT} > T_N$!



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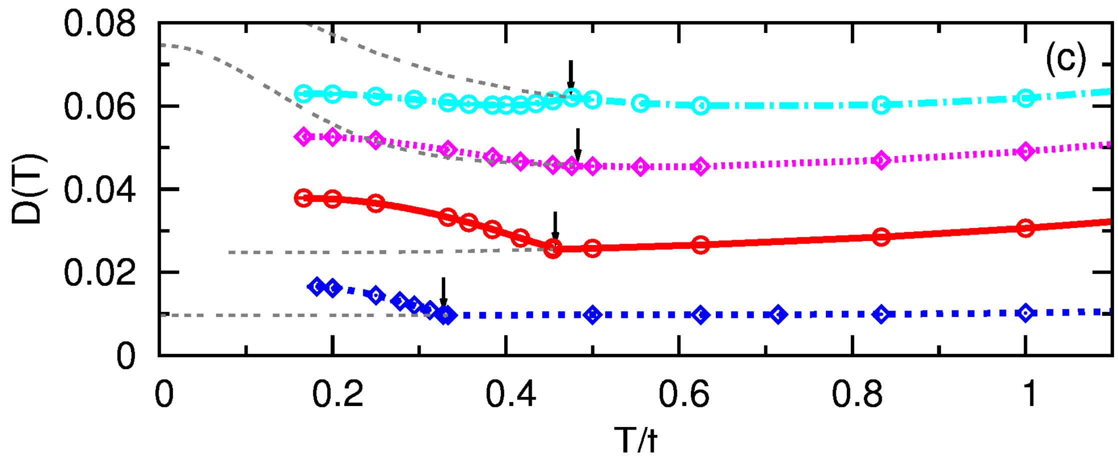

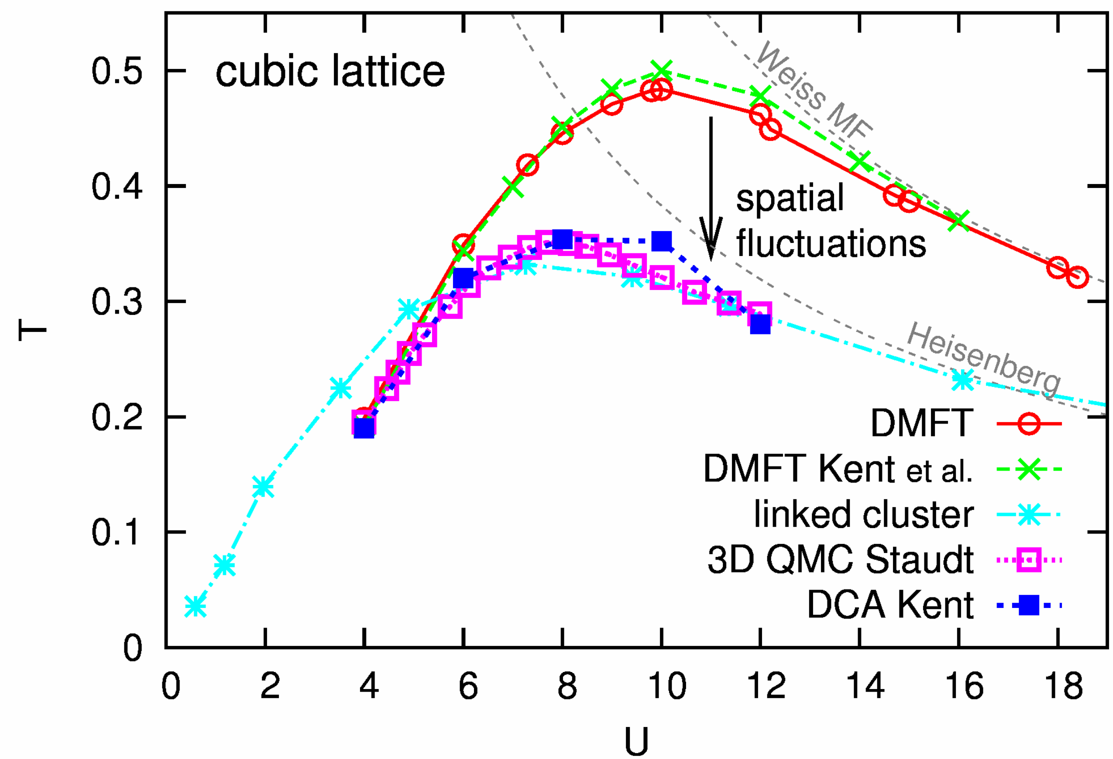

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Constraints:

- DMFT results for D(T) agree with high-T expansion at $T >> T_N$ [Jördens et al., PRL (2010)]

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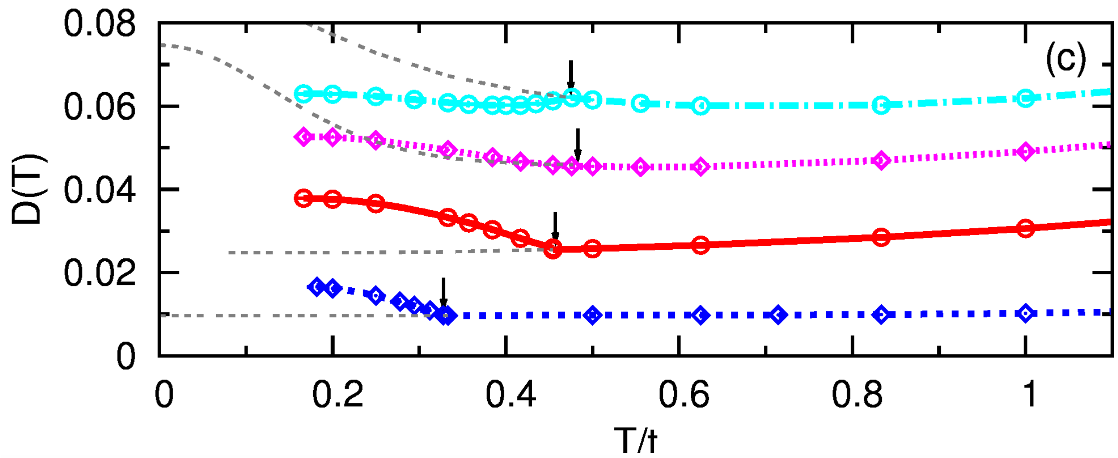

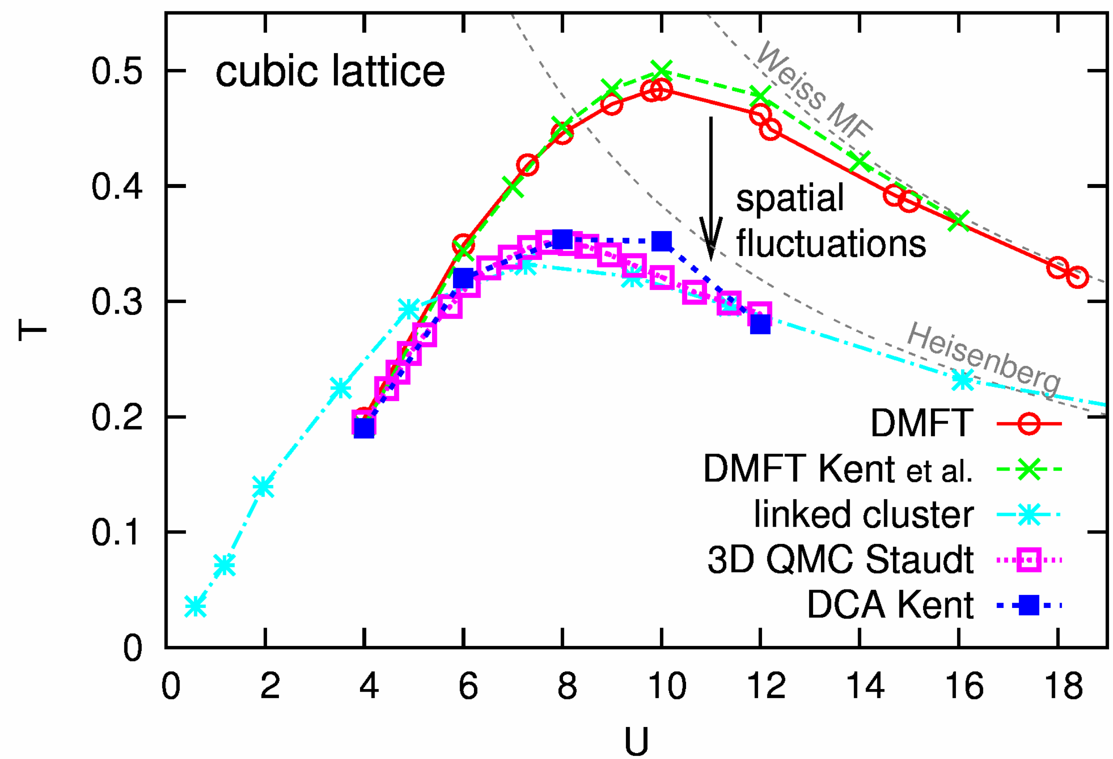

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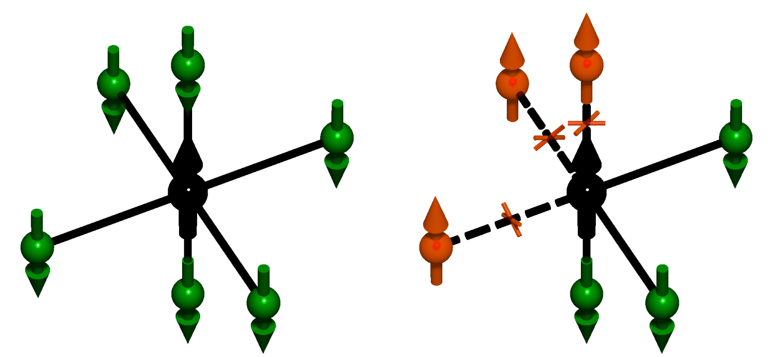

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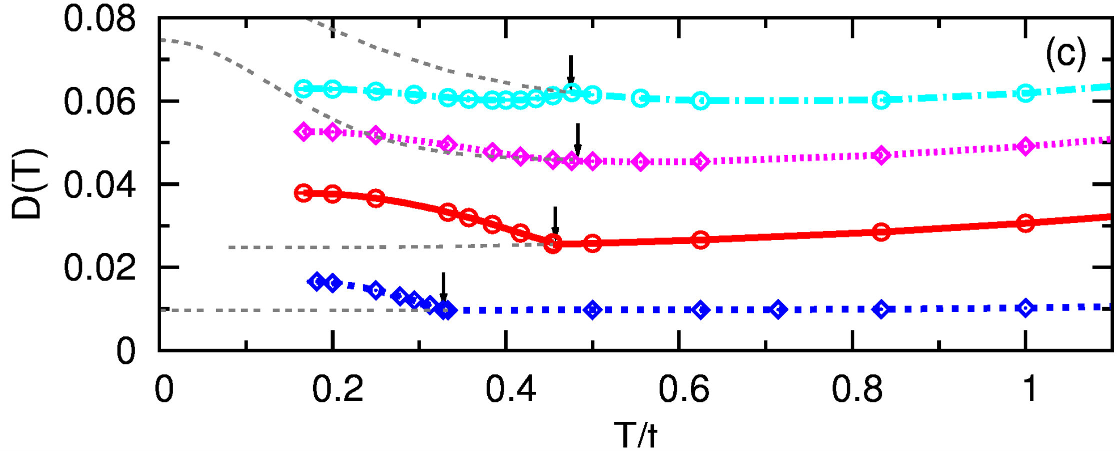

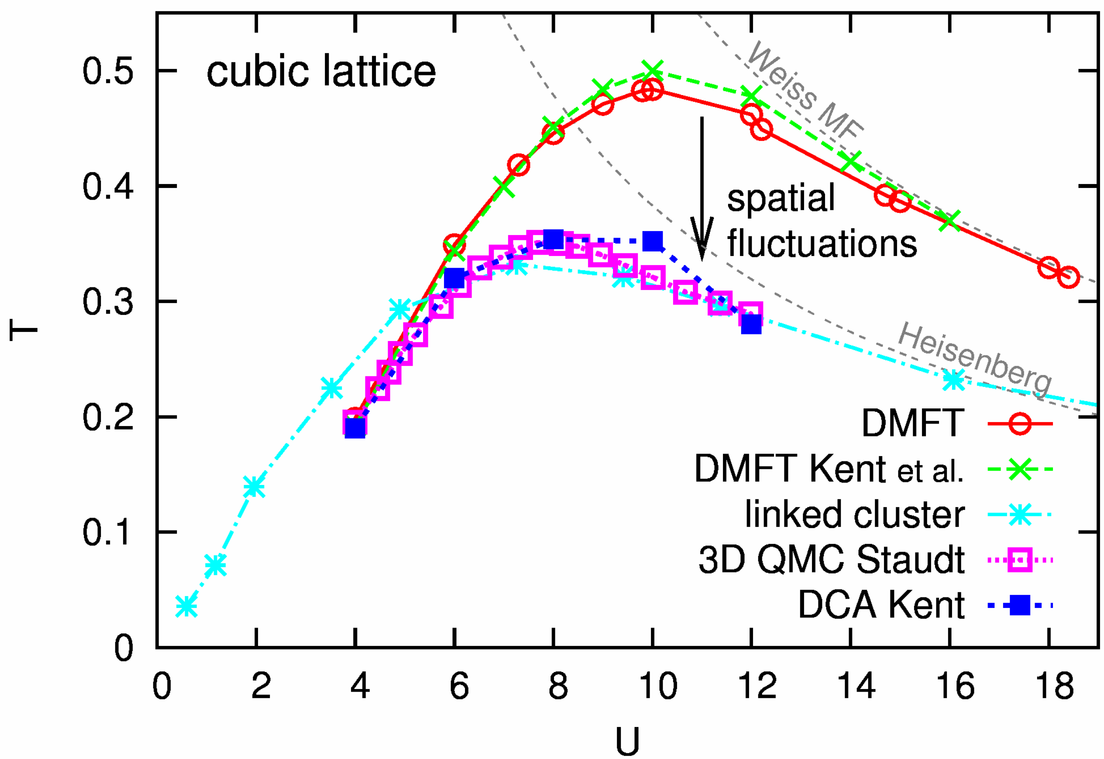

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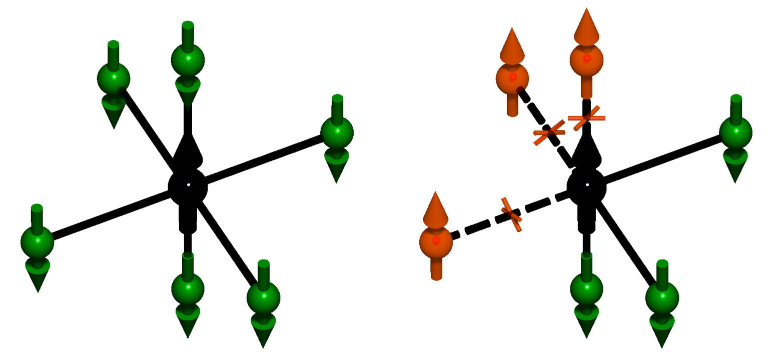
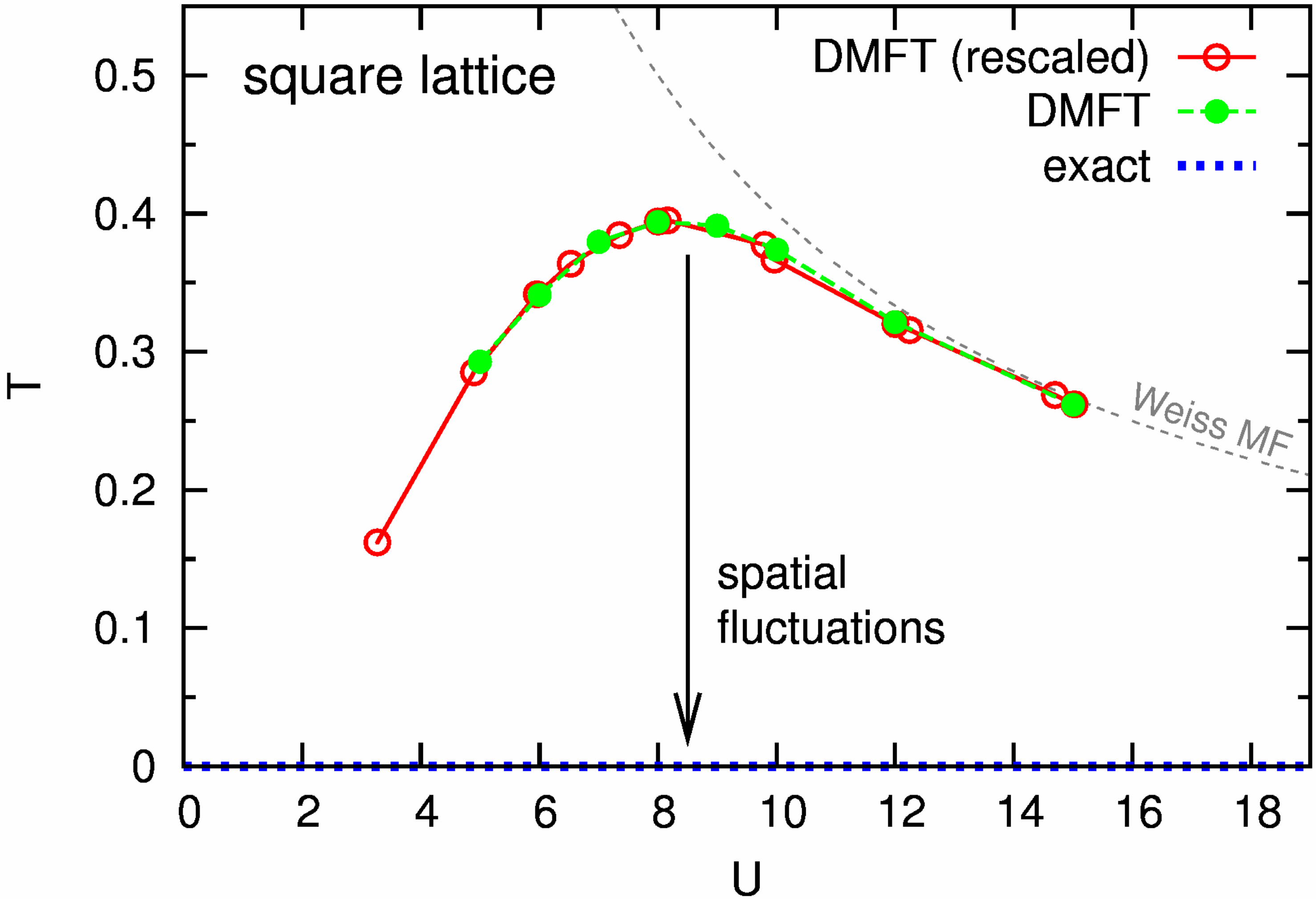


and independ. of long-range order

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



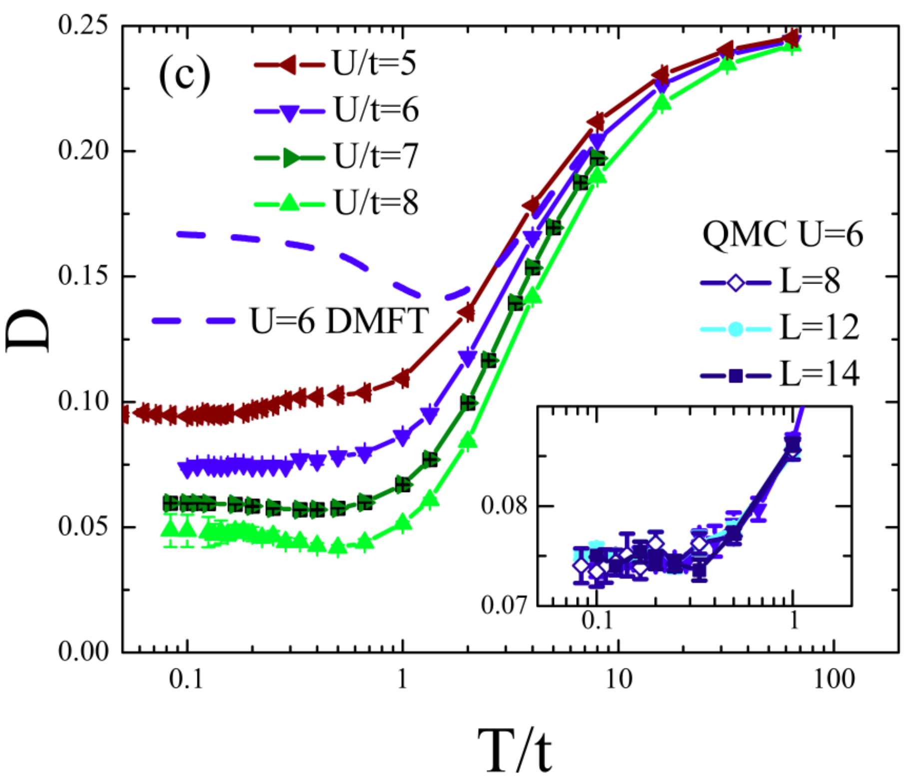
Will any enhancement of D at low T remain? At which temperature scale?

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

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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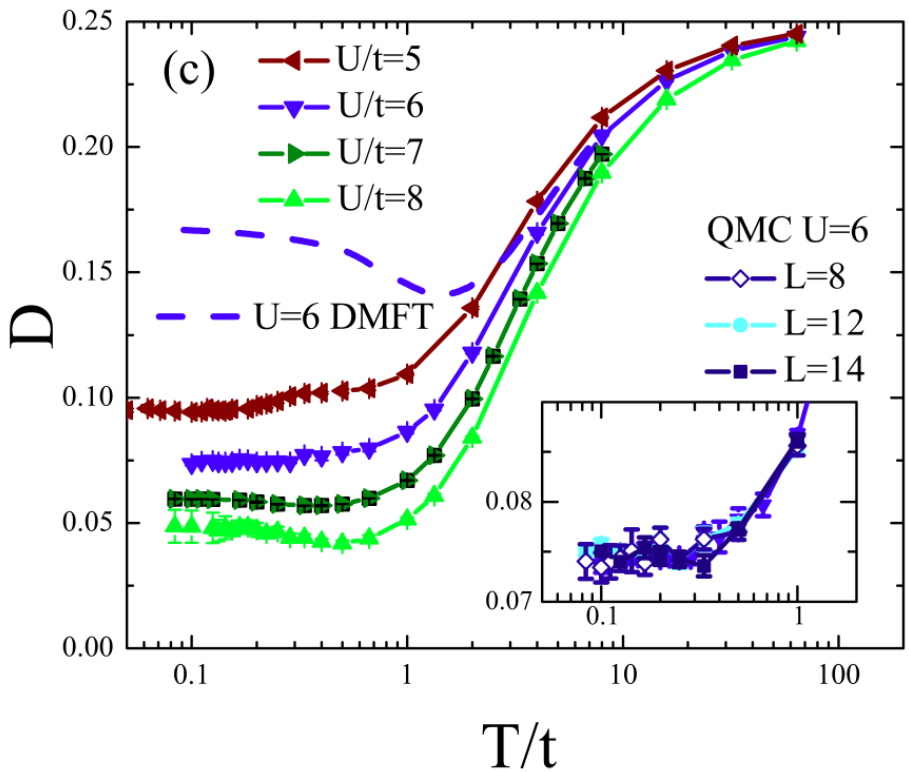
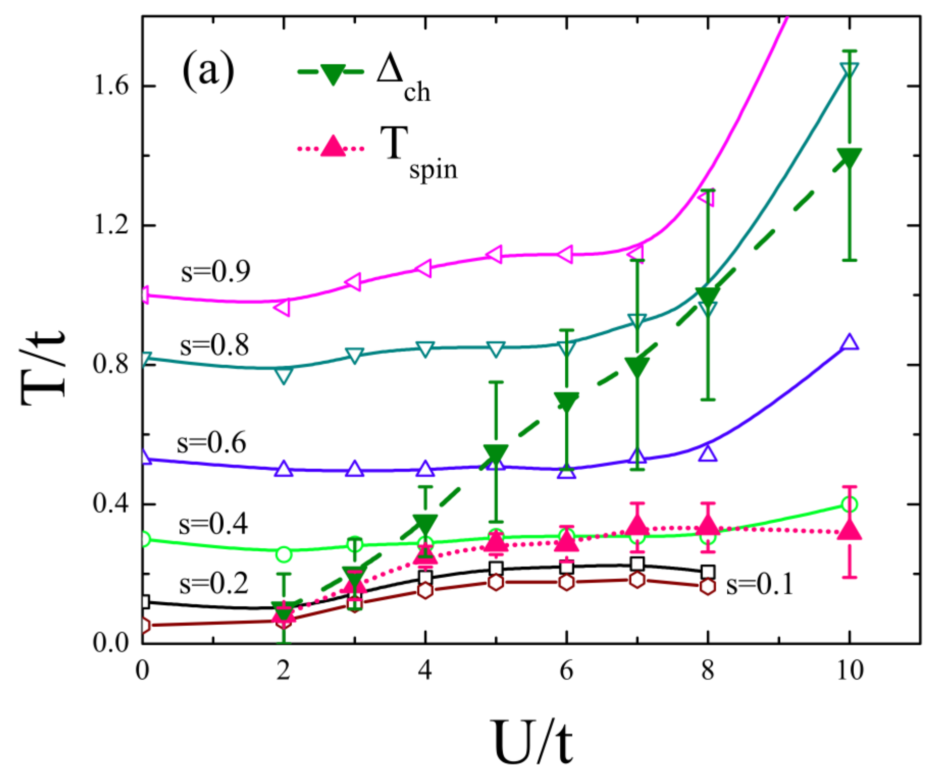
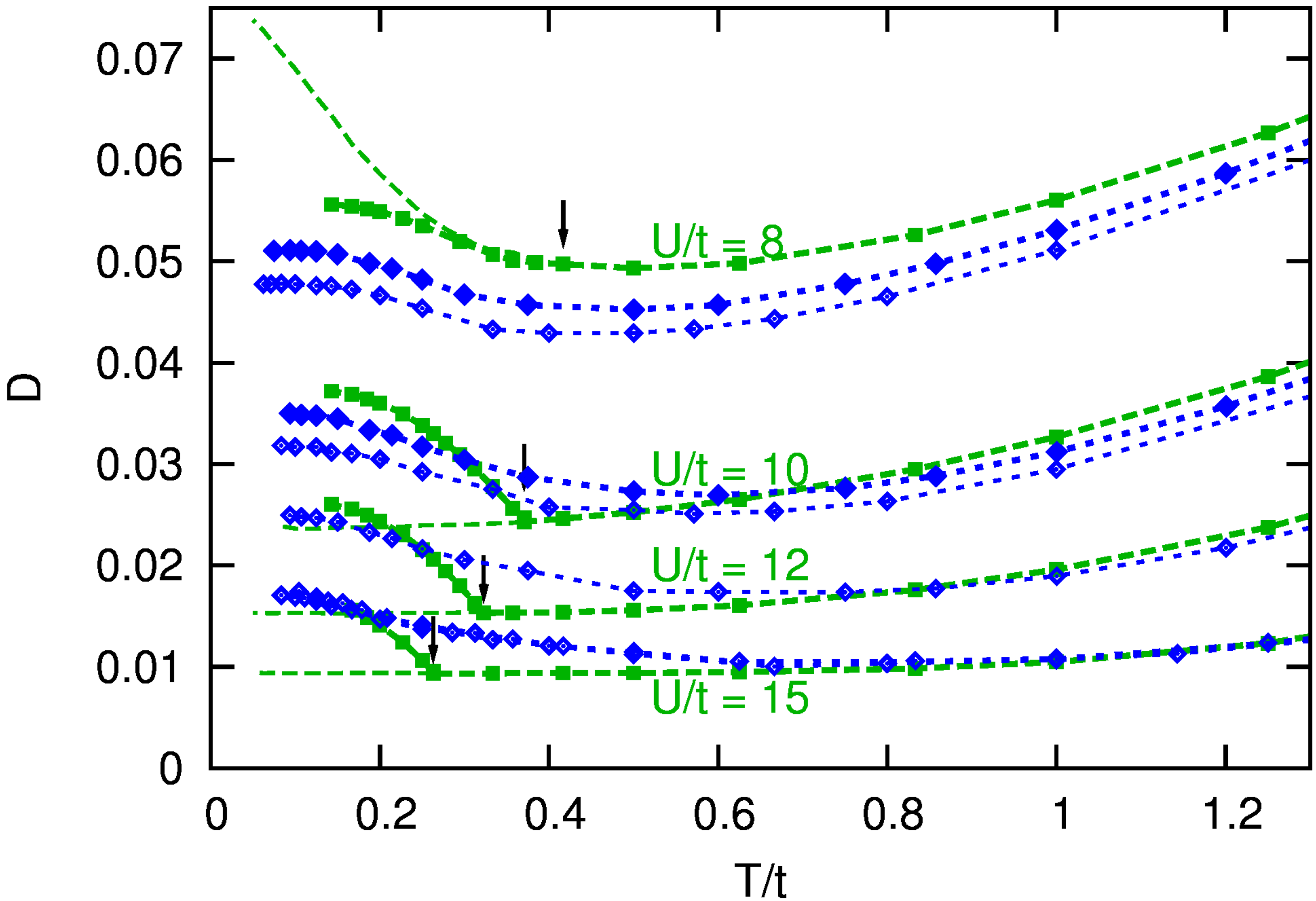




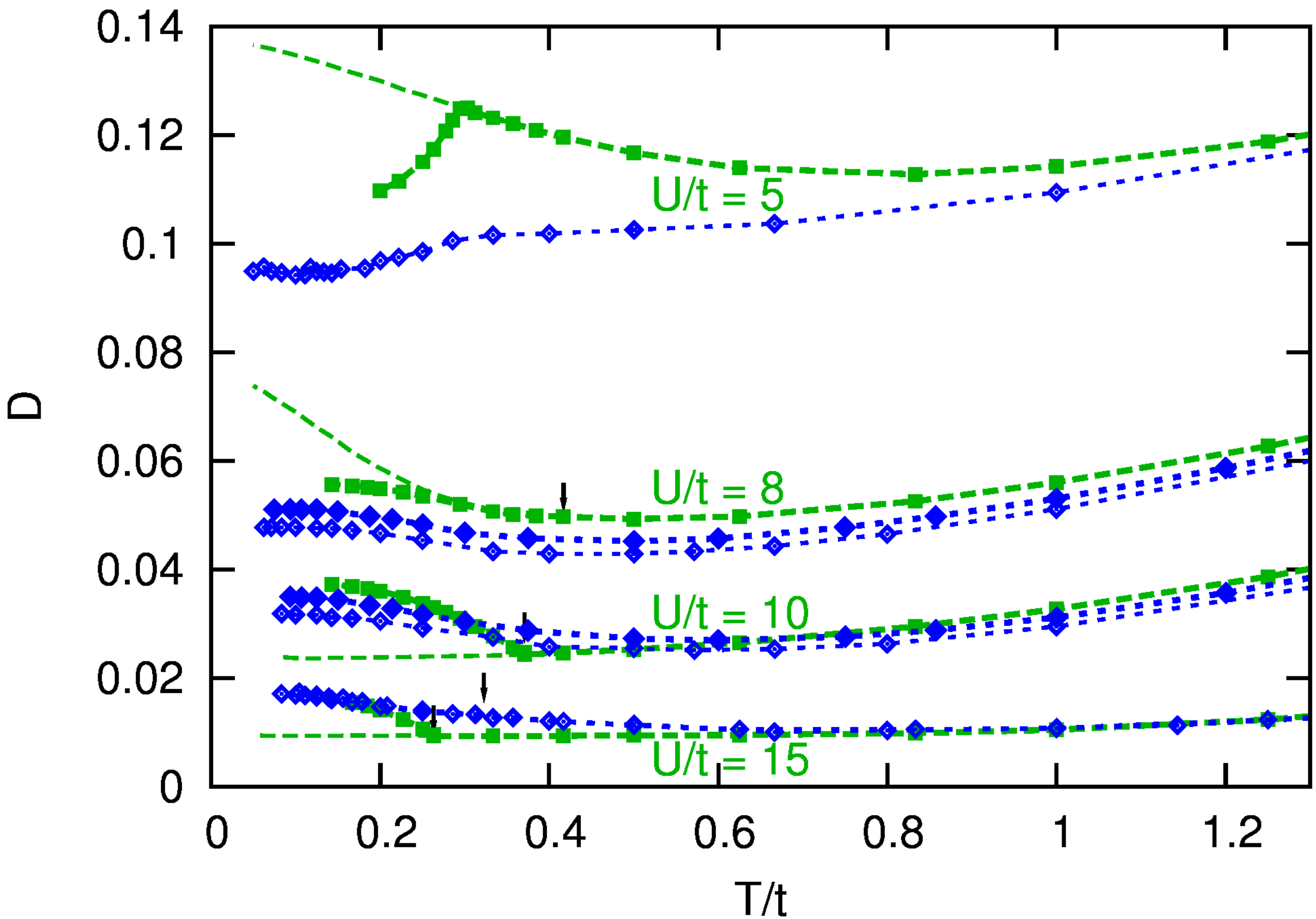
Comparison DMFT – direct QMC for the 2d square lattice ($n = 1$)



green: DMFT, blue: BSS-QMC (thicker lines: smaller $\Delta\tau$)

excellent agreement at $U = 8$; rounding off at $T \gtrsim T_N^{\text{DMFT}}$ for larger U

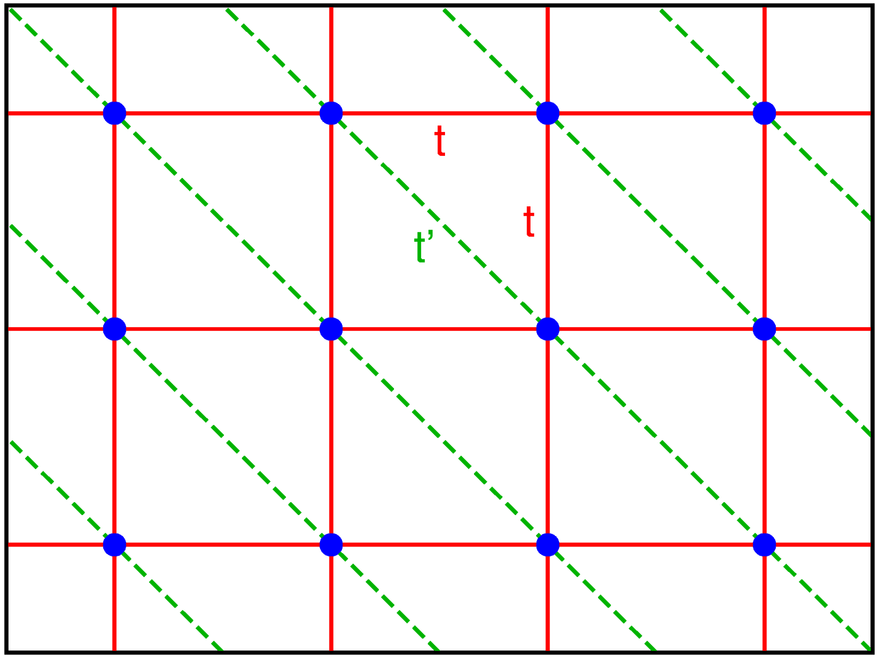
Even the low-T suppression of D at small U corresponds with direct QMC:



Not shown: agreement even better in 3 dimensions!

Impact of frustration: towards the triangular lattice

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



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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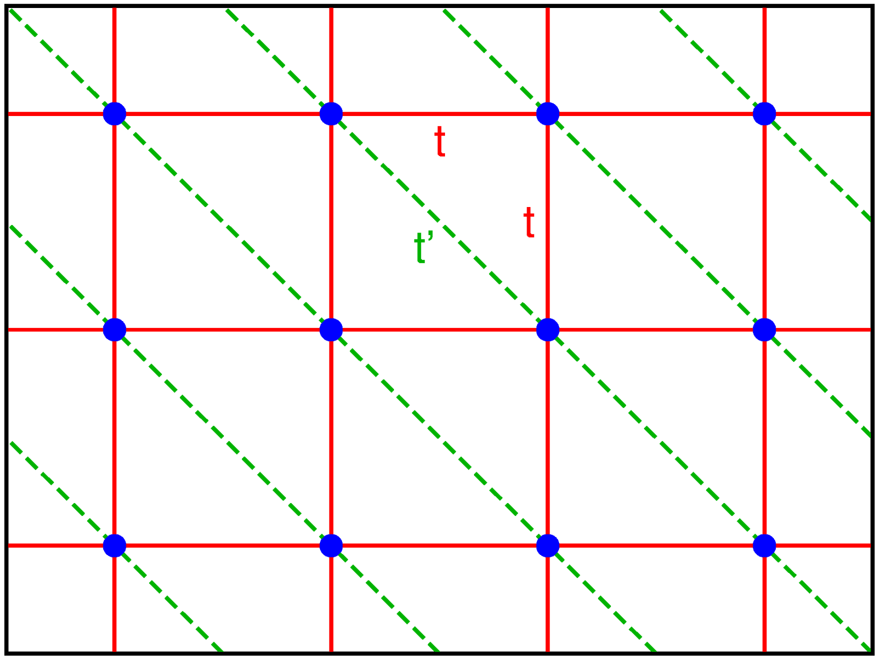

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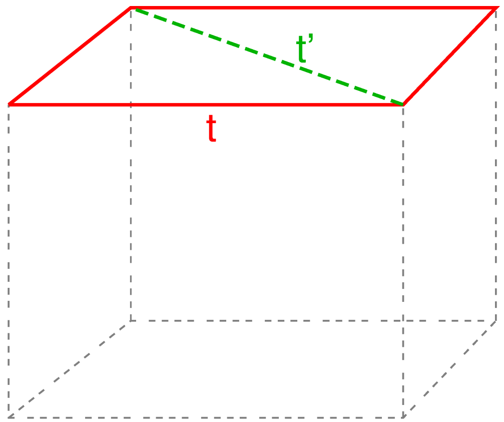
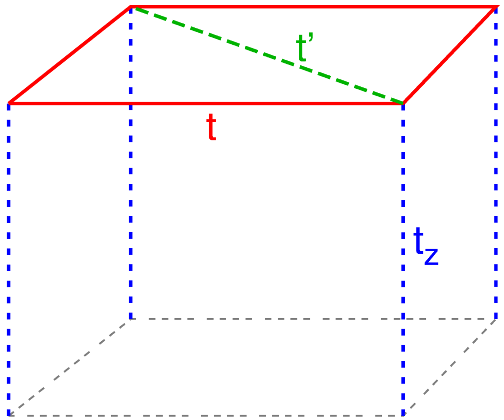
Solution: add third dimension

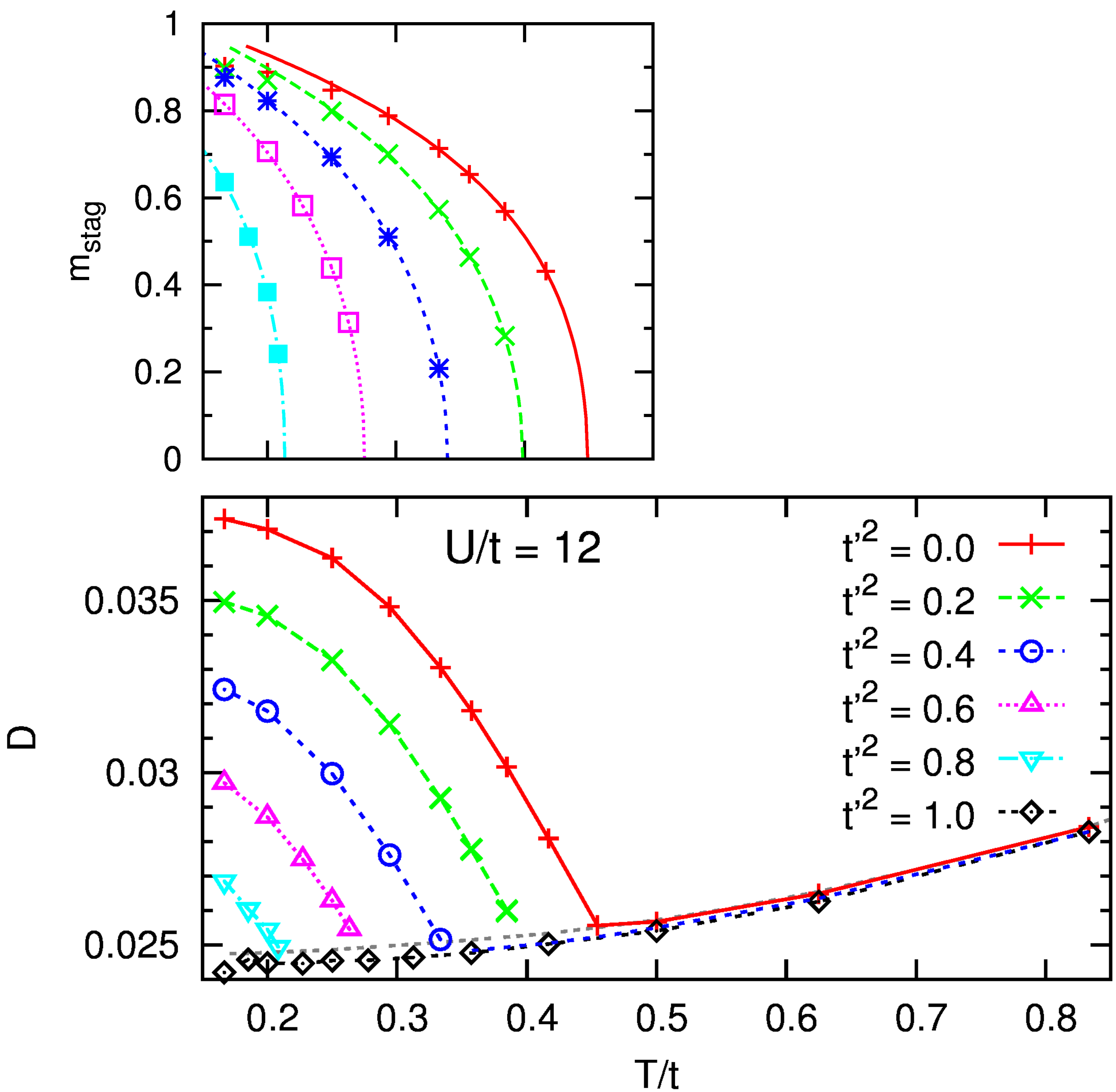


and hopping t_z between planes



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

Tuning the frustration from the cubic to the triangular lattice



with increasing t':

- param. phase unchanged!
- D suppressed in AF phase
- T_N decreases

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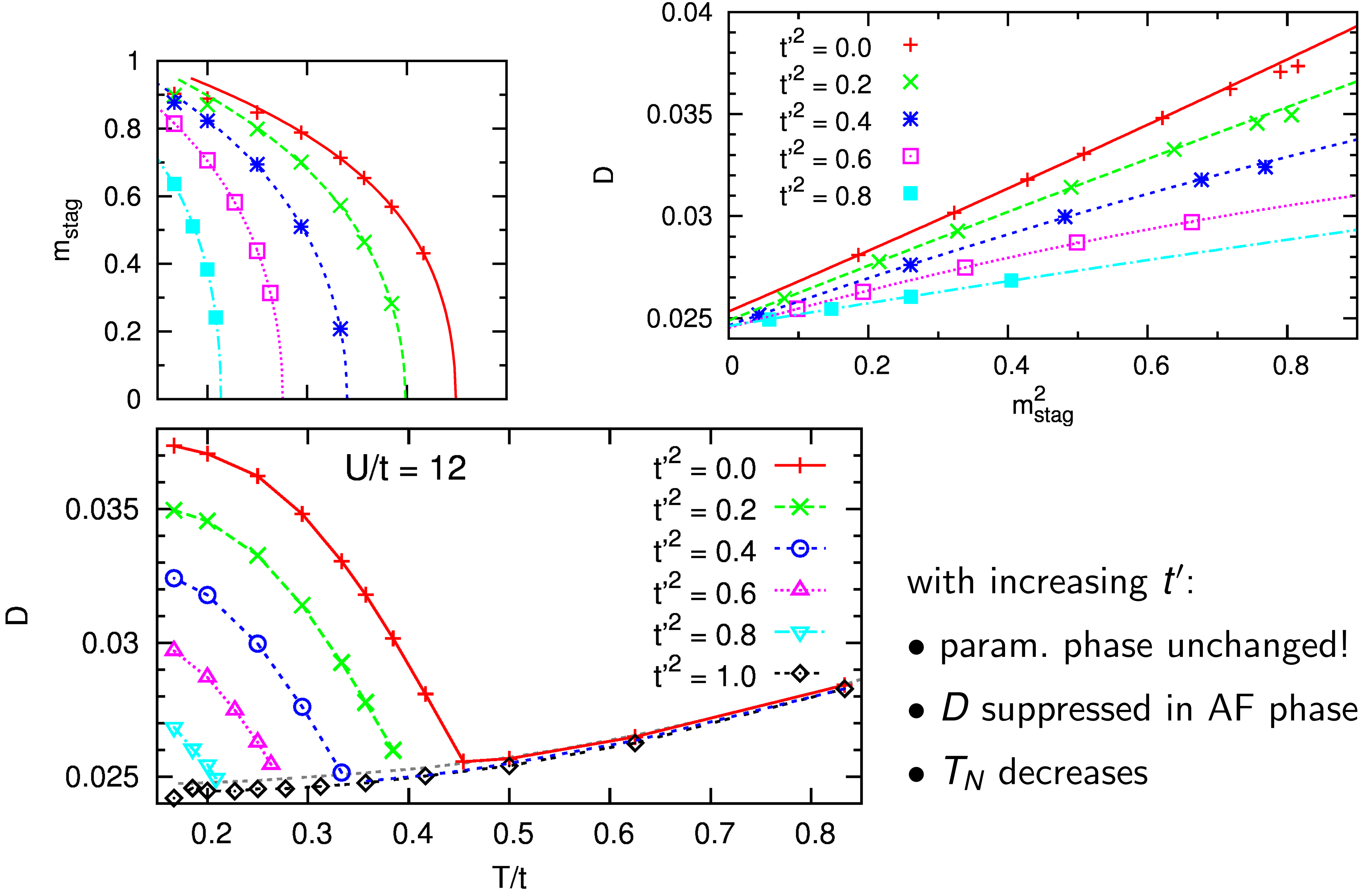

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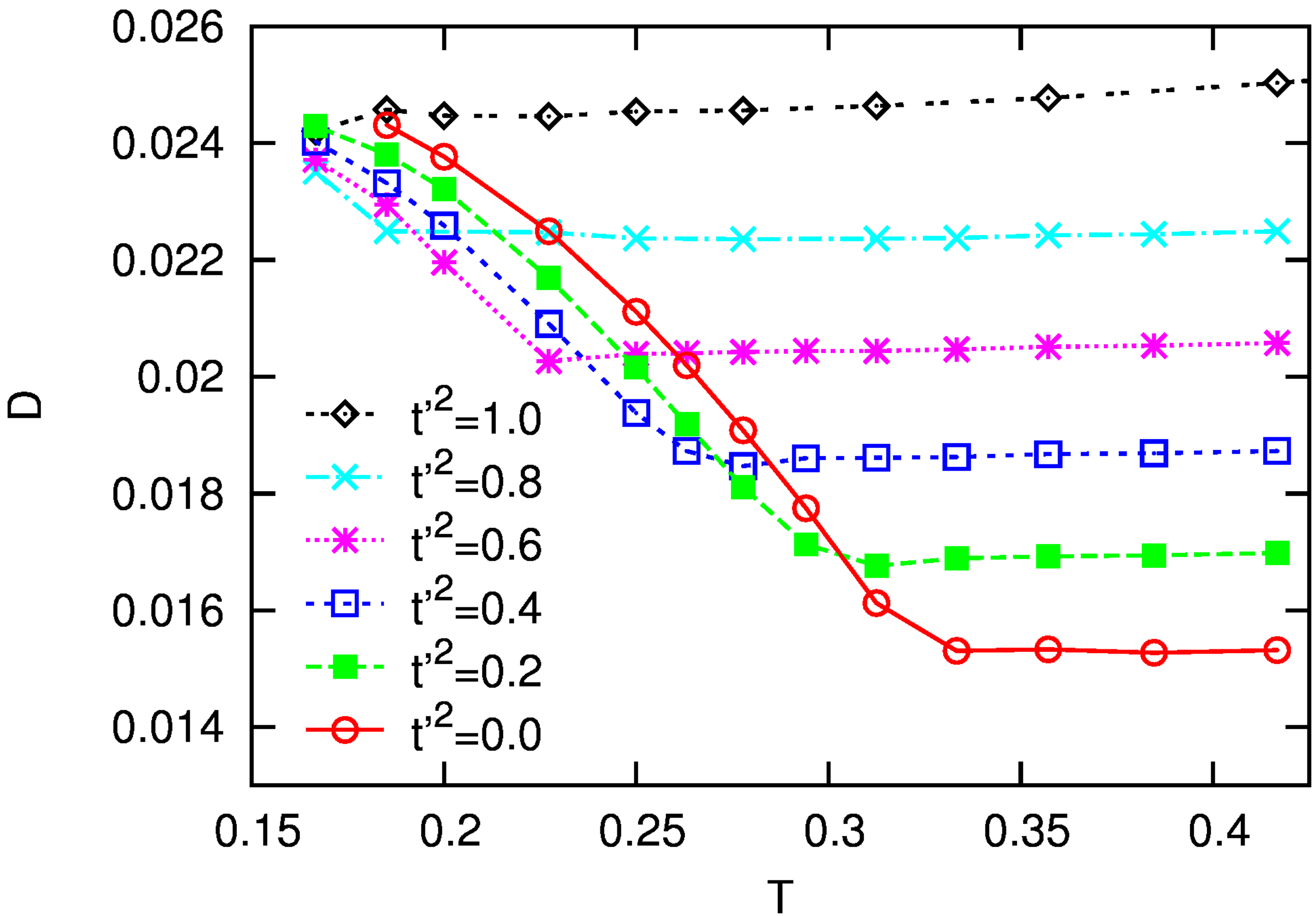

Now situation reversed: strong t'^2 dependence only in paramagnetic phase

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 order/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

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

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

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

Outlook

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, . . .)

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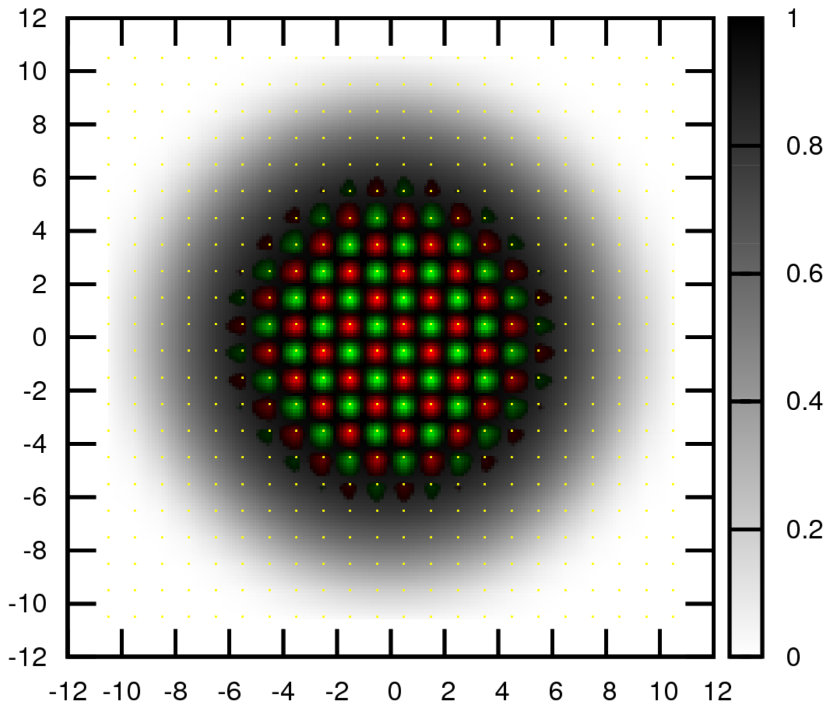

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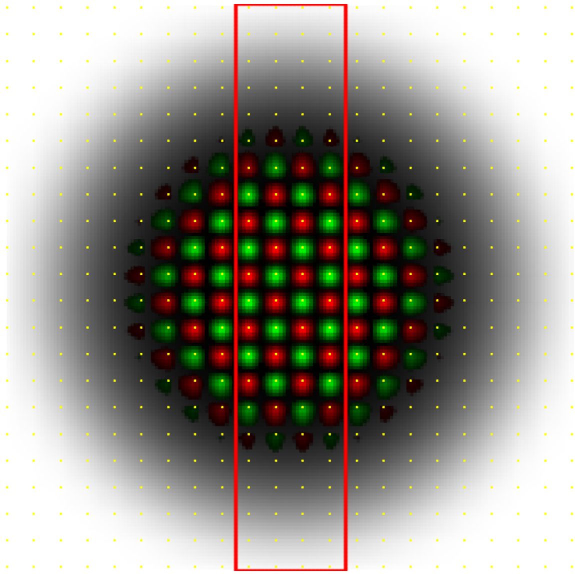

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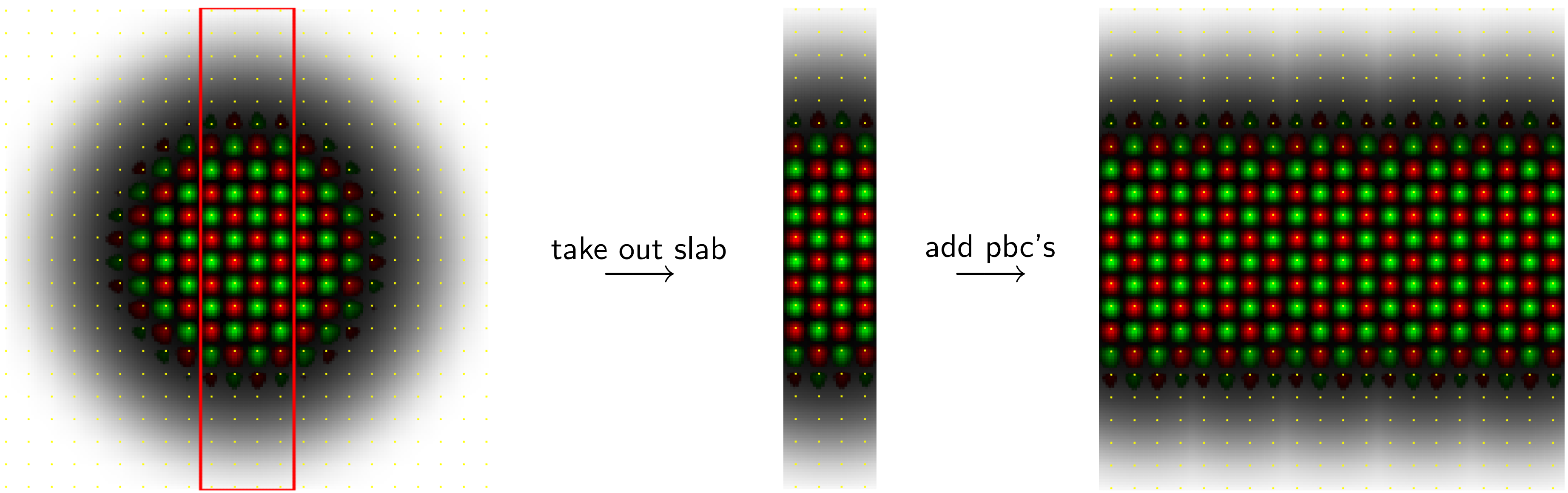
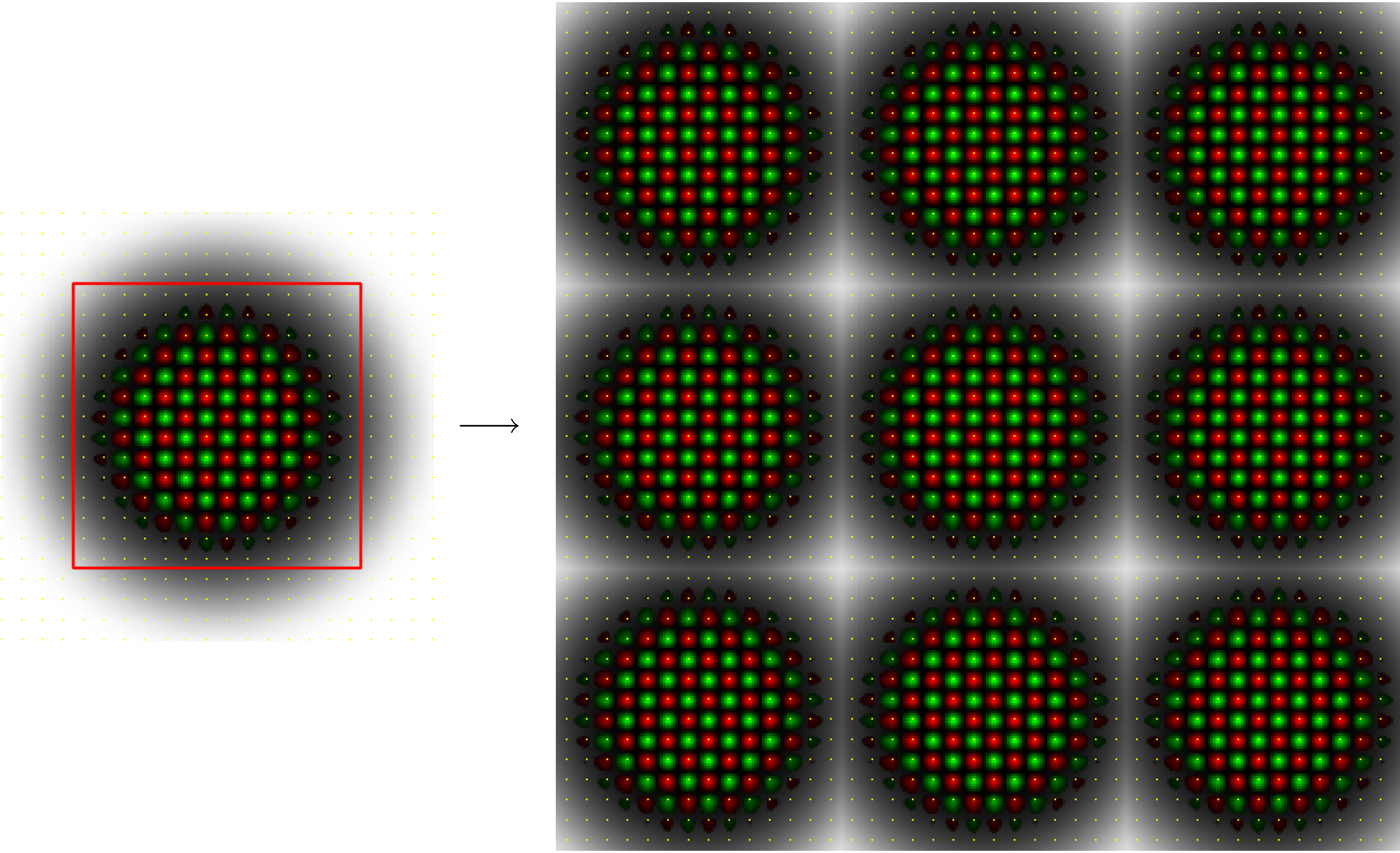


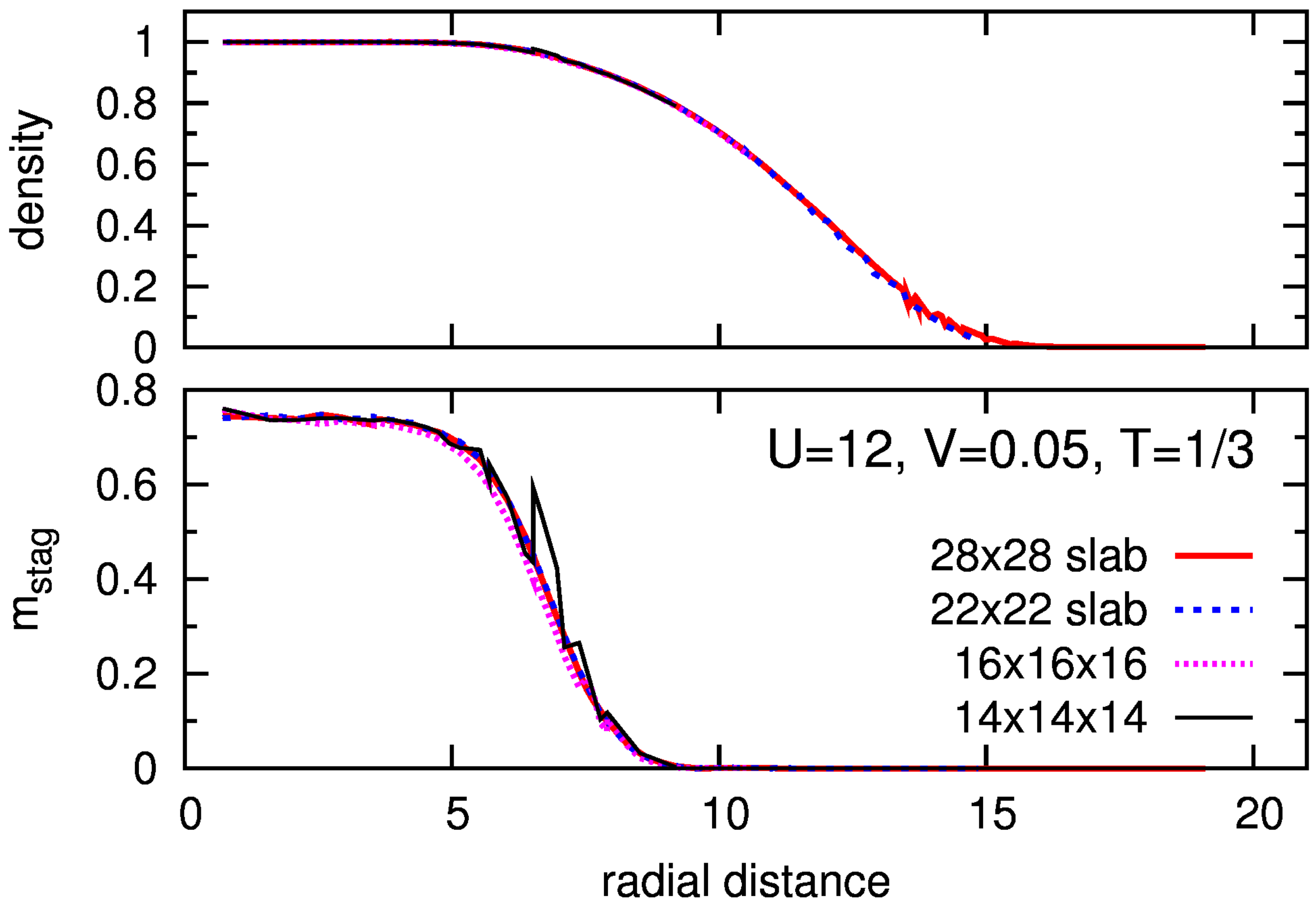
In practice: cylindrical potential (equivalent layers)

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



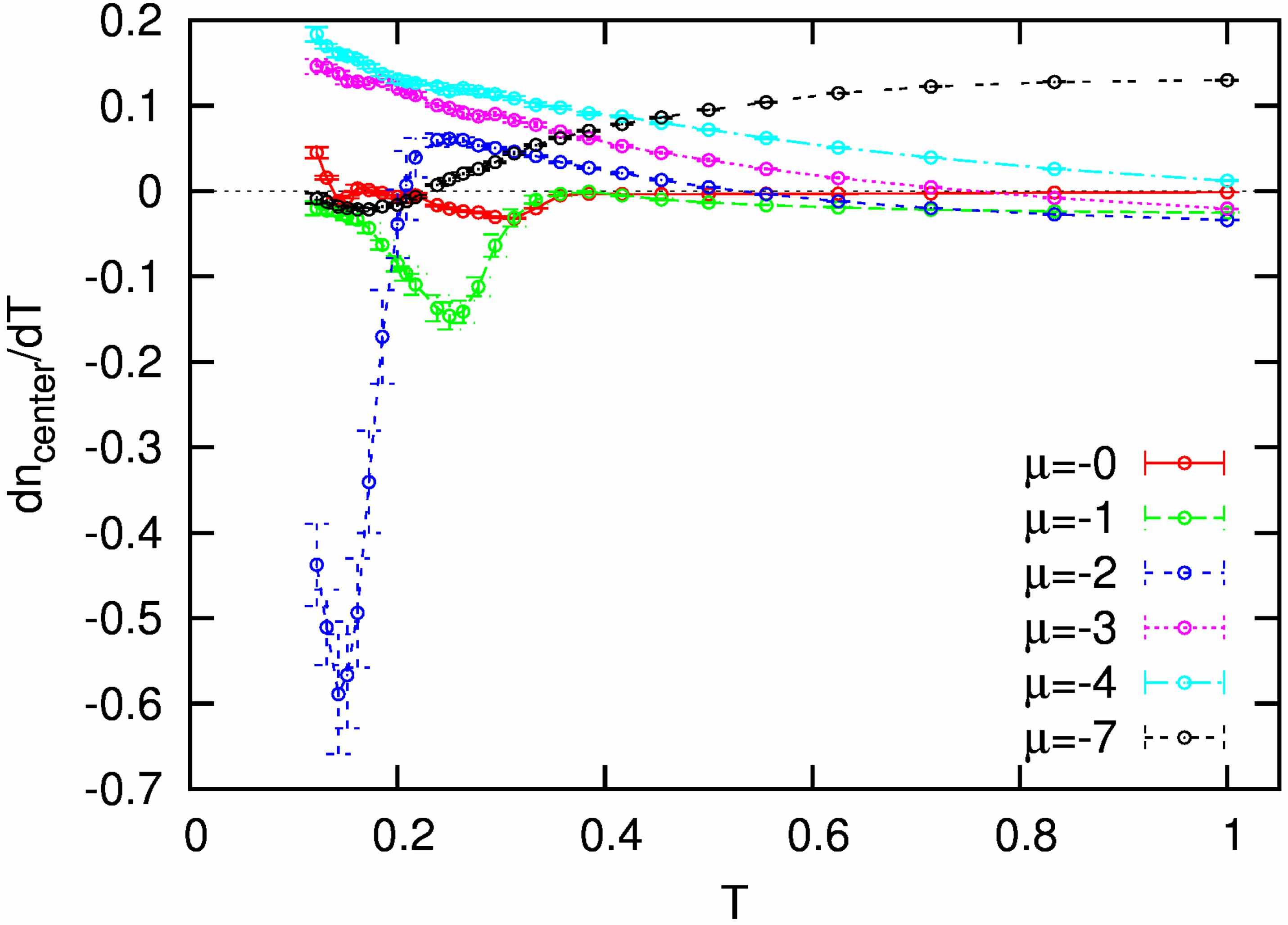
Most efficient: slab calculation focussing on AF core (with pbc)

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



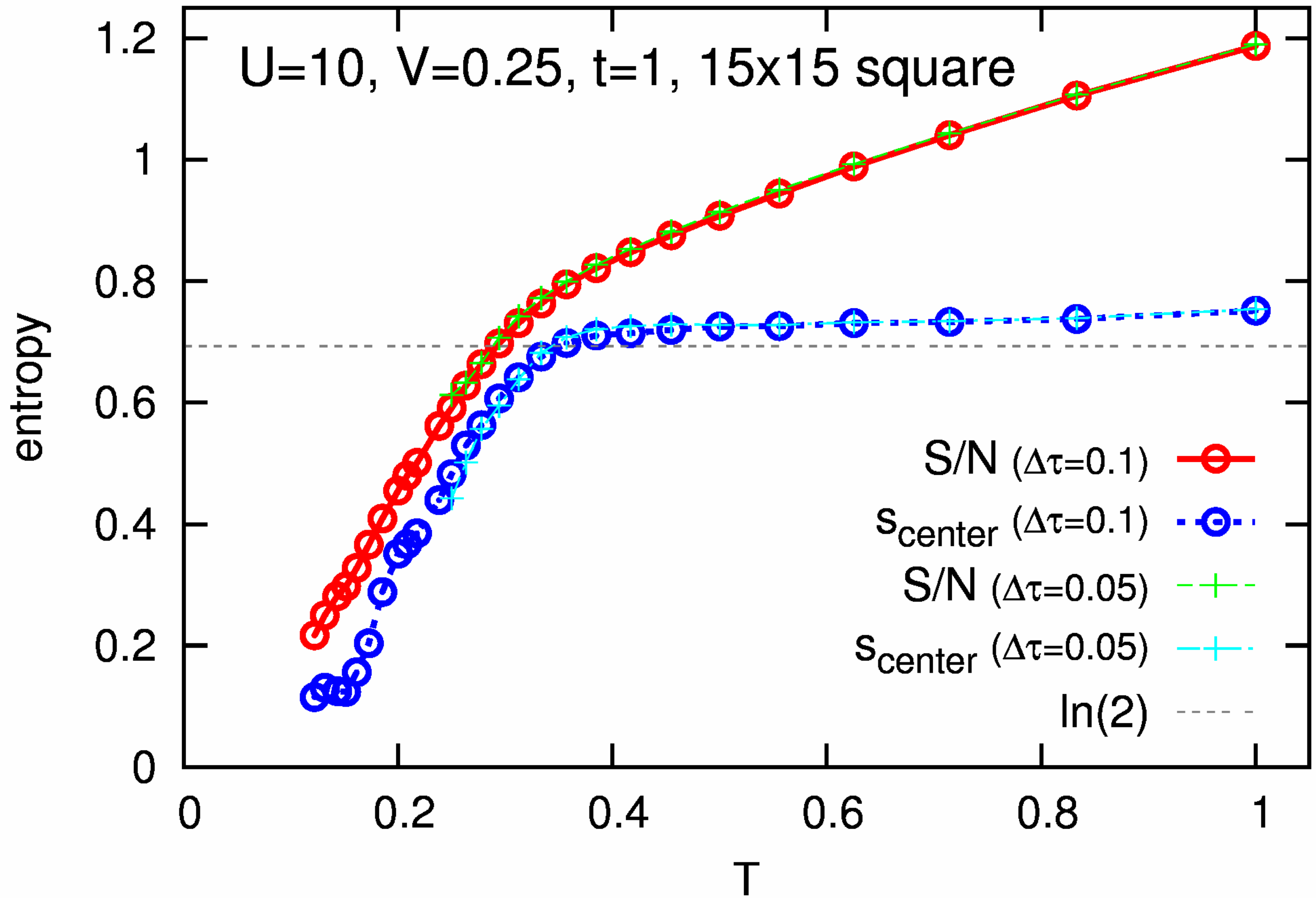
Significant deviations only if core touches boundaries!

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!