Quantum Monte Carlo simulations of ultracold fermions on optical lattices within dynamical mean-field theory

Nils Blümer and Elena Gorelik

Gutenberg University Mainz, Germany

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]

Néel transition of lattice fermions in a harmonic trap

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

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Effect of nonlocal correlations? Comparisons with direct QMC

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

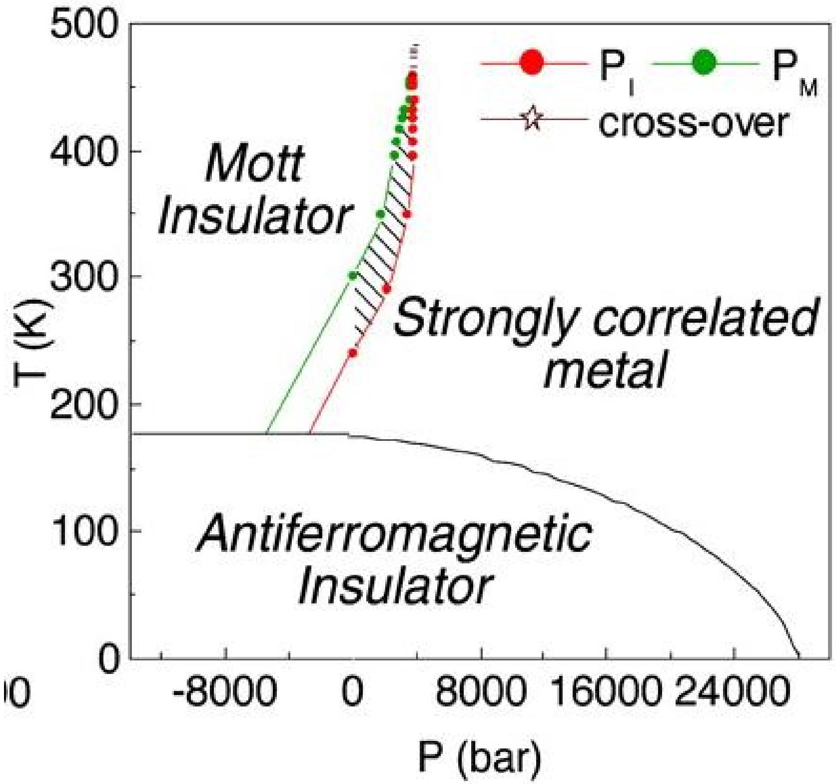
Impact of frustration, triangular lattice

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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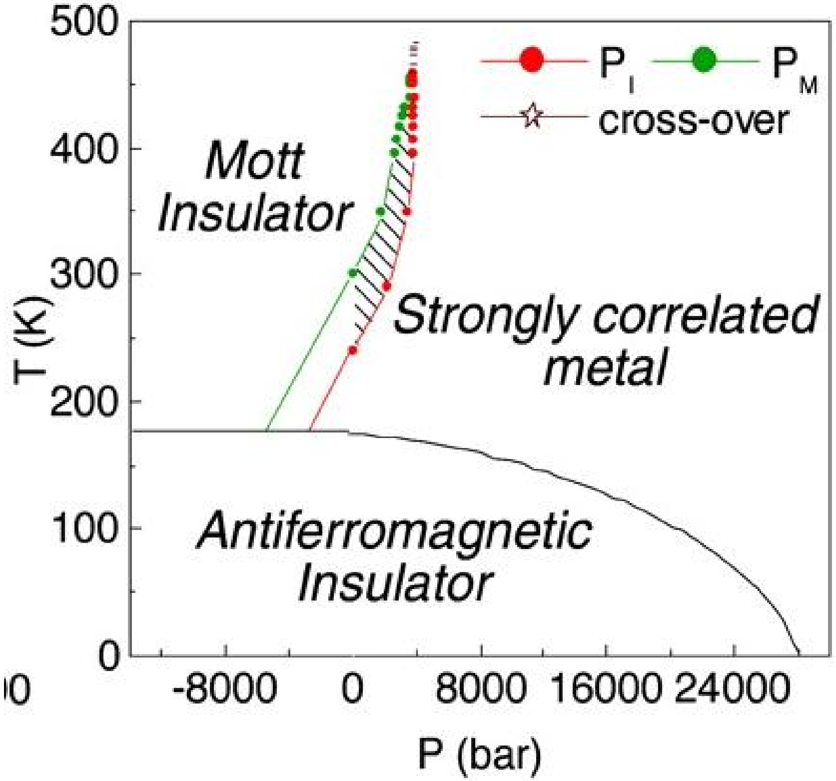

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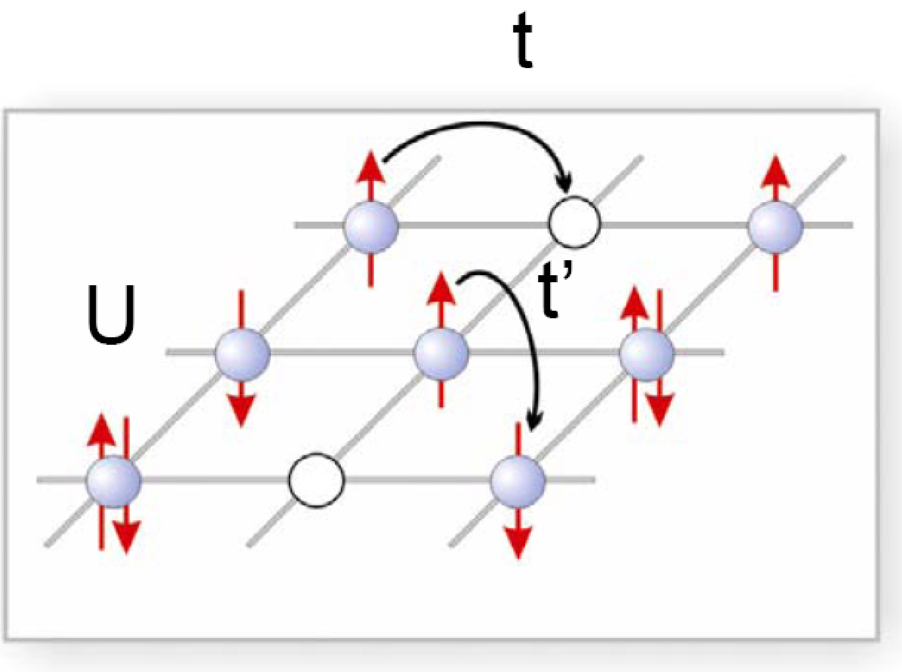
Mott metal-insulator transition and AF: generic physics of 1-band Hubbard model



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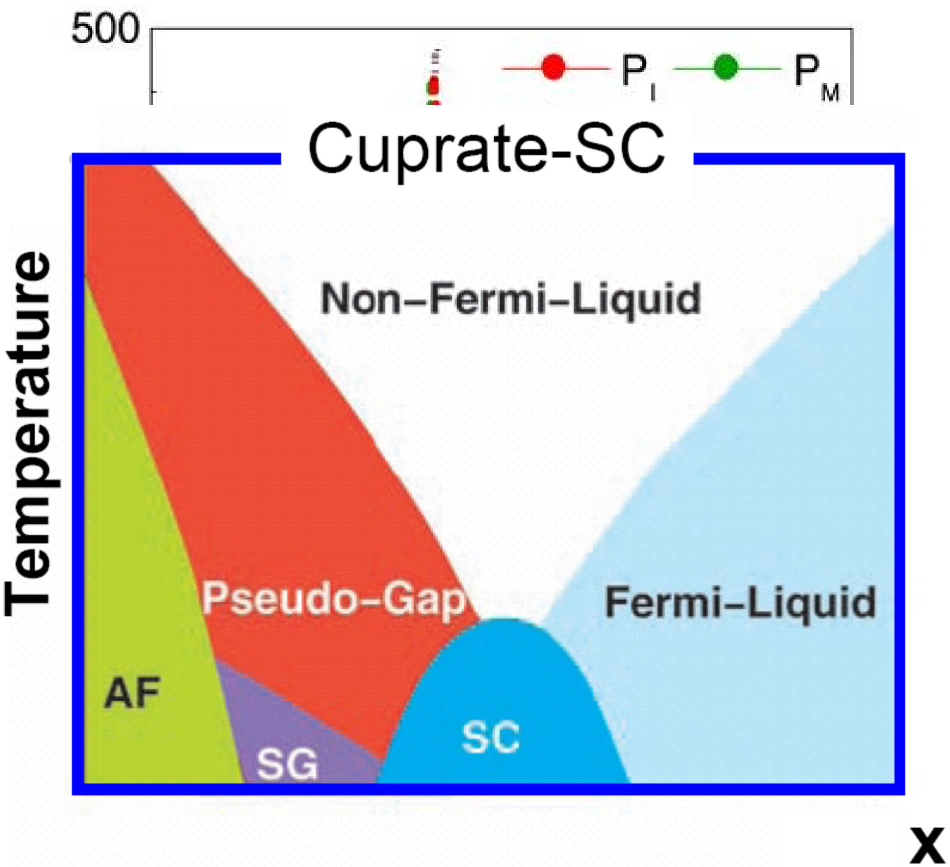

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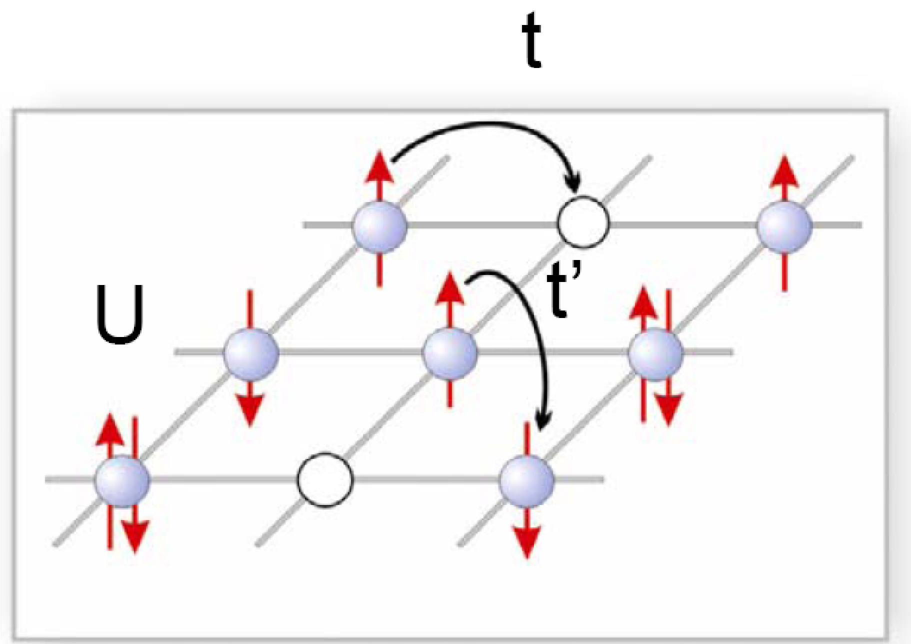

Are AF and Mott phases essential for superconductivity?

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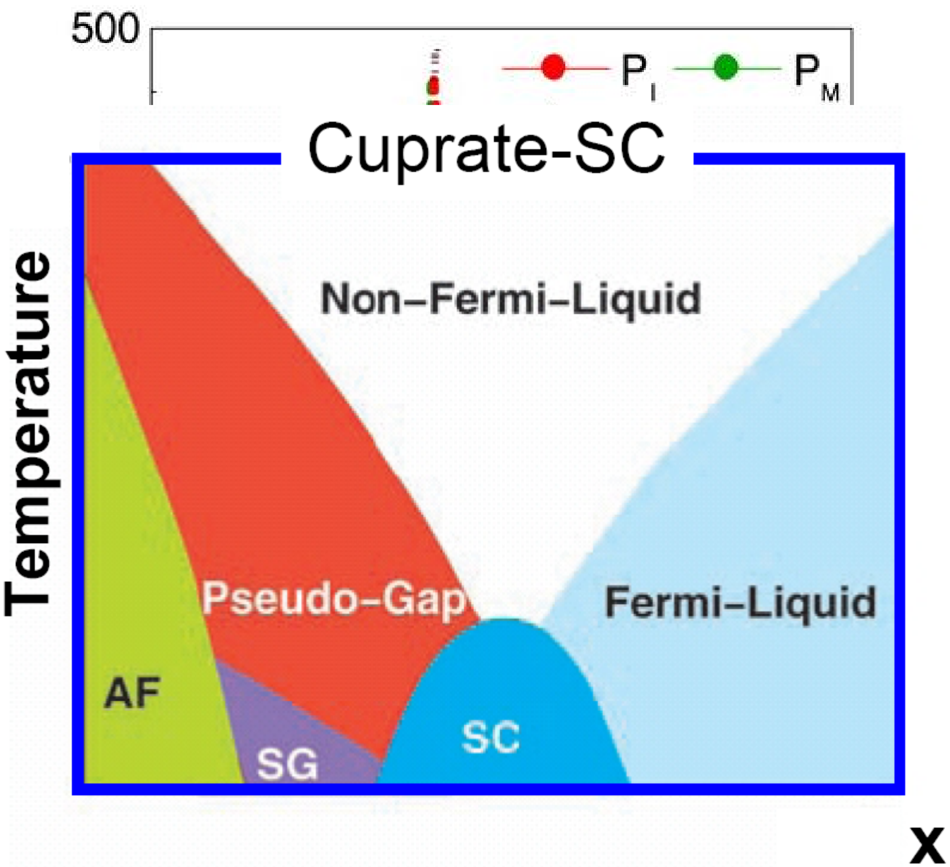

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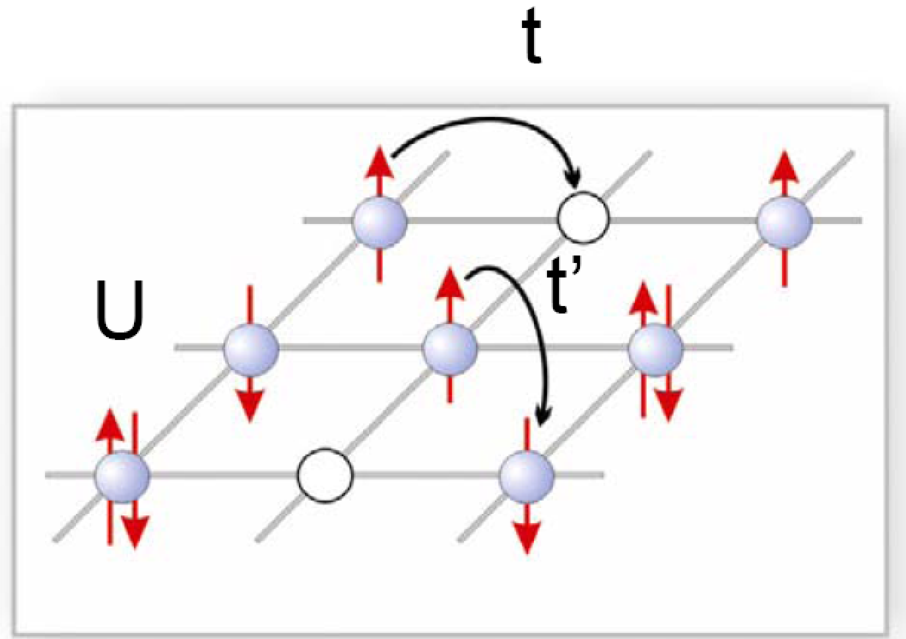


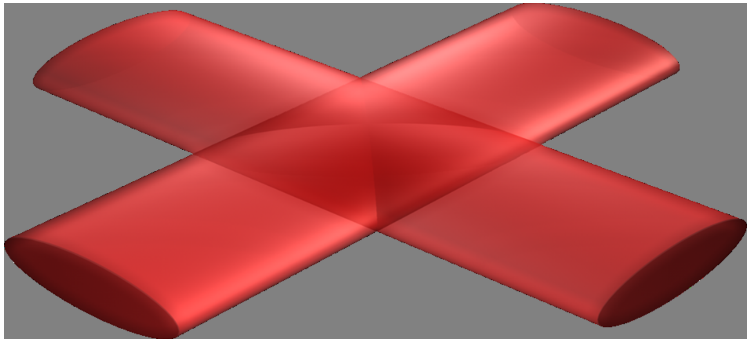
Are AF and Mott phases essential for superconductivity?

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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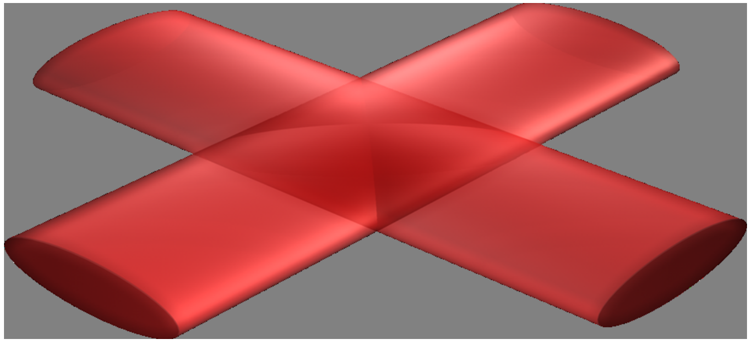

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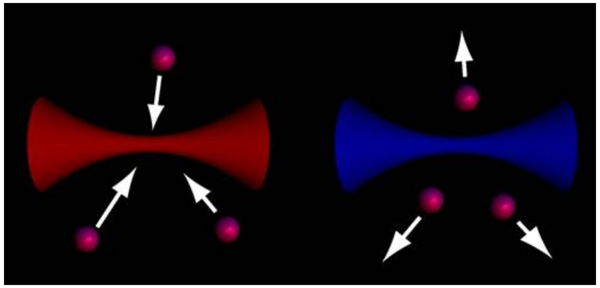

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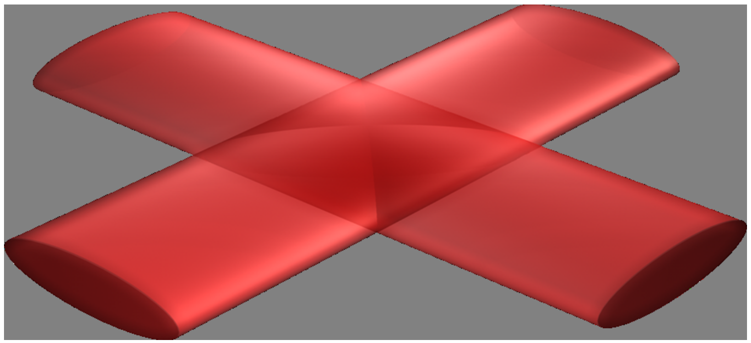

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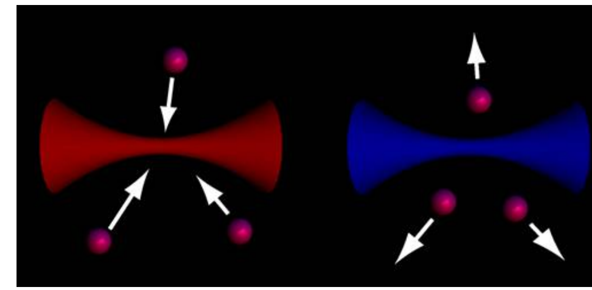
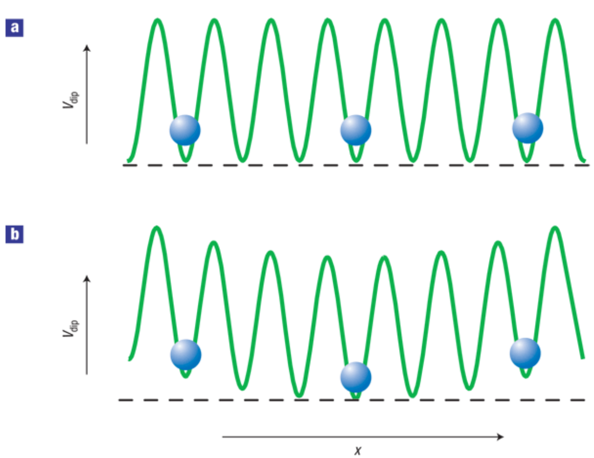


Standing wave (from coherent counterpropagating beams) $\rightsquigarrow$ modulated potential



Beam profile: (anti) trapping

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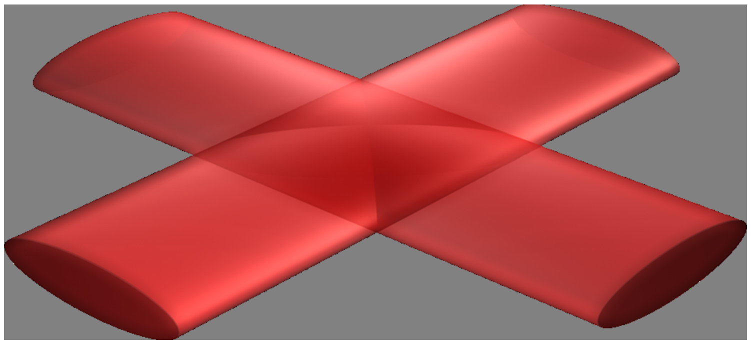

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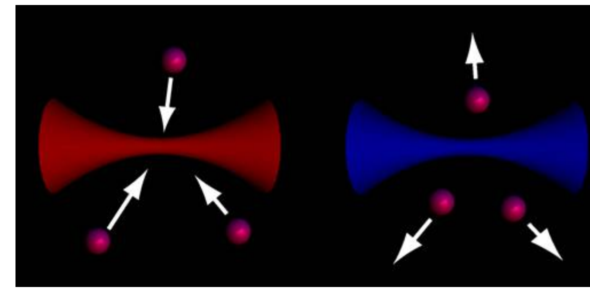

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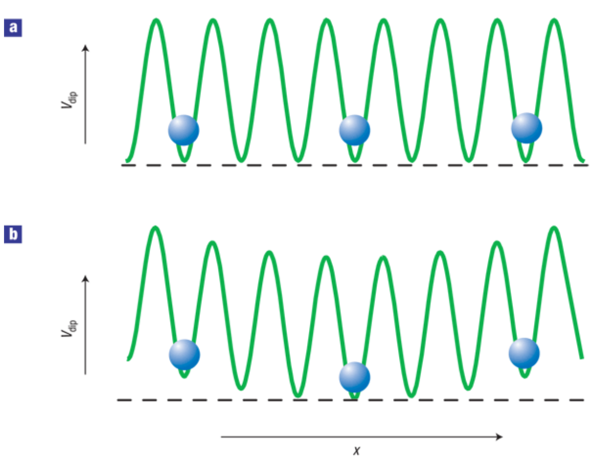


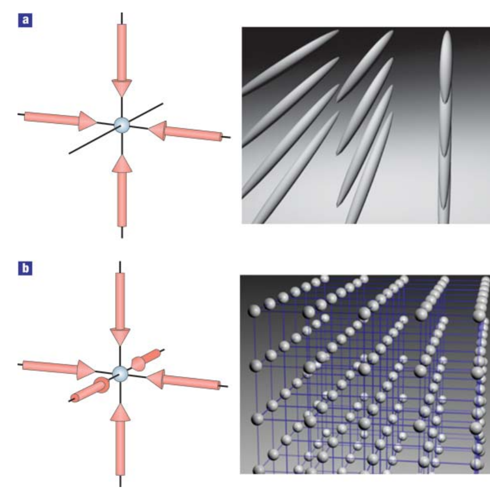
Beam profile: (anti) trapping

1 pair of lasers $\rightsquigarrow$ pancakes

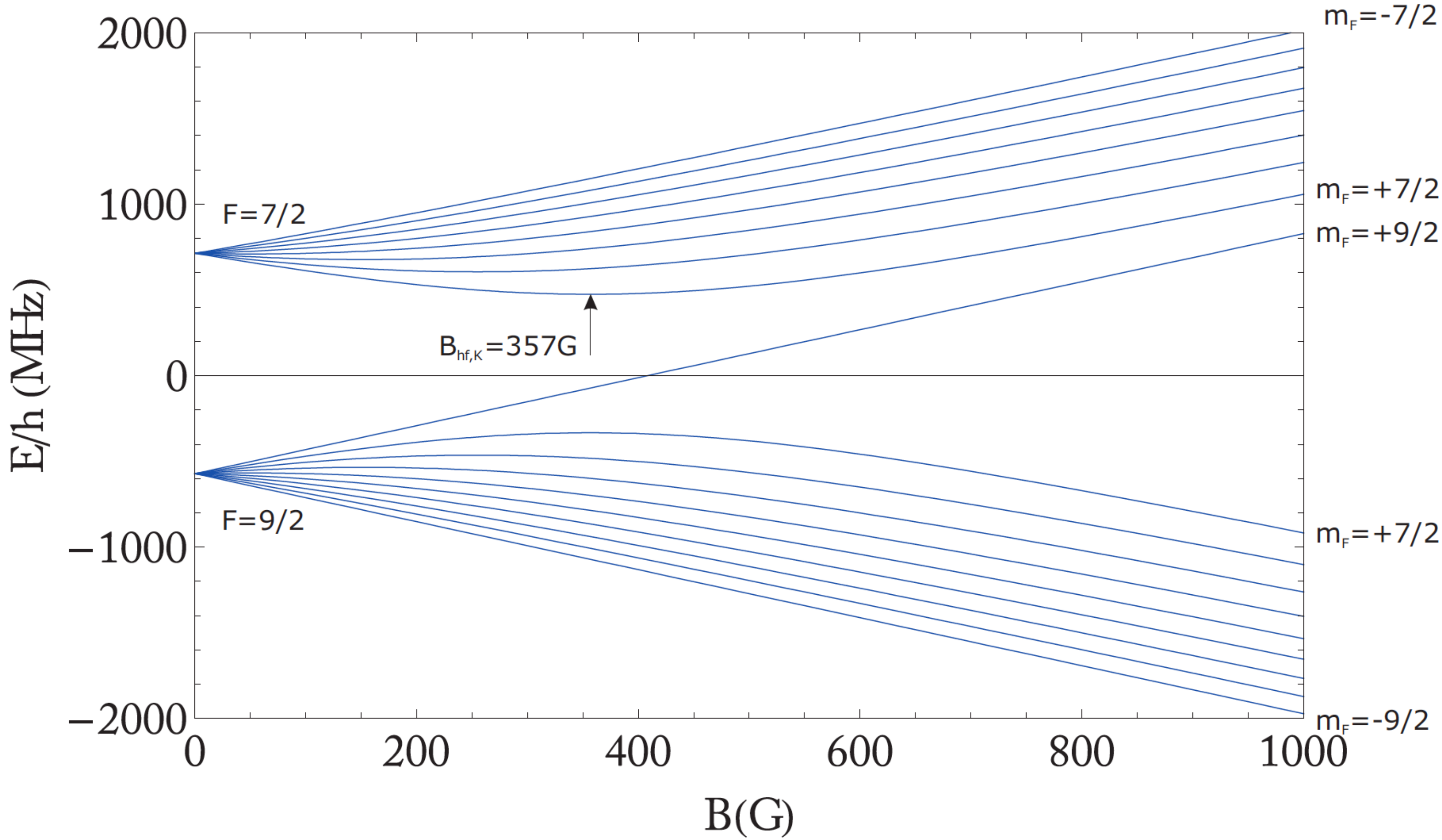
2 pairs of lasers $\rightsquigarrow$ tubes

3 pairs of lasers $\rightsquigarrow$ 3D lattice

hopping t tunable by laser



Large multiplets: reservoir of “flavors”

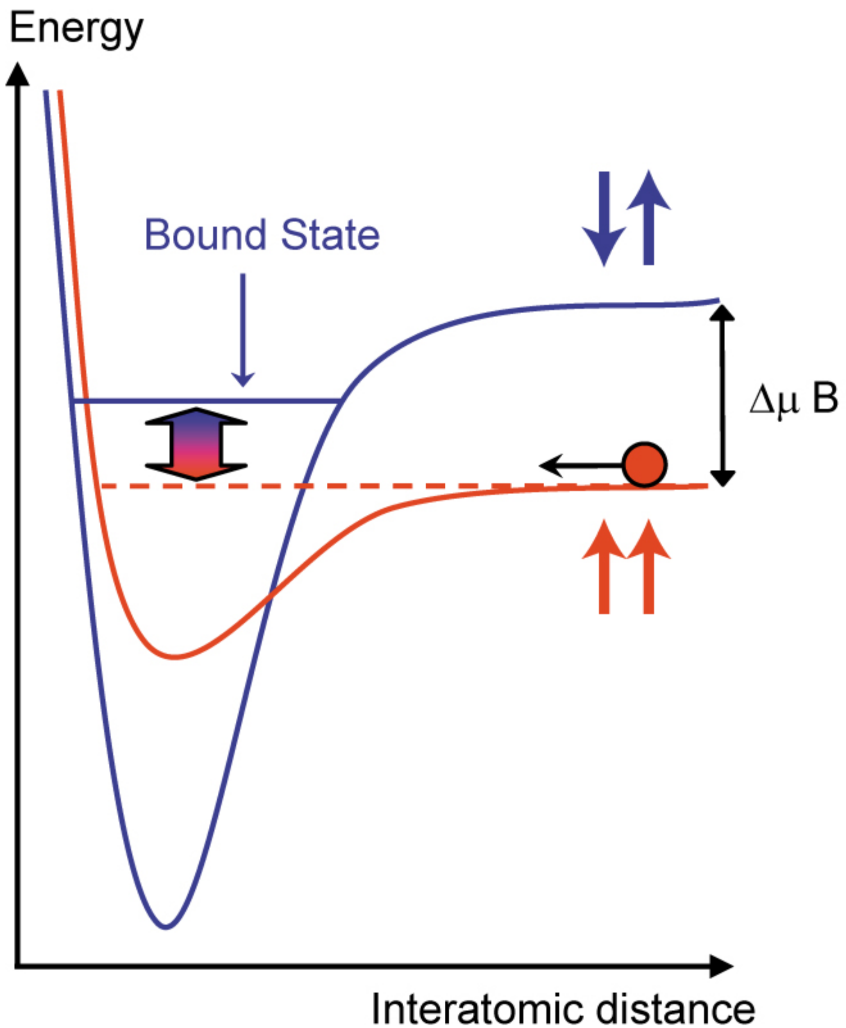


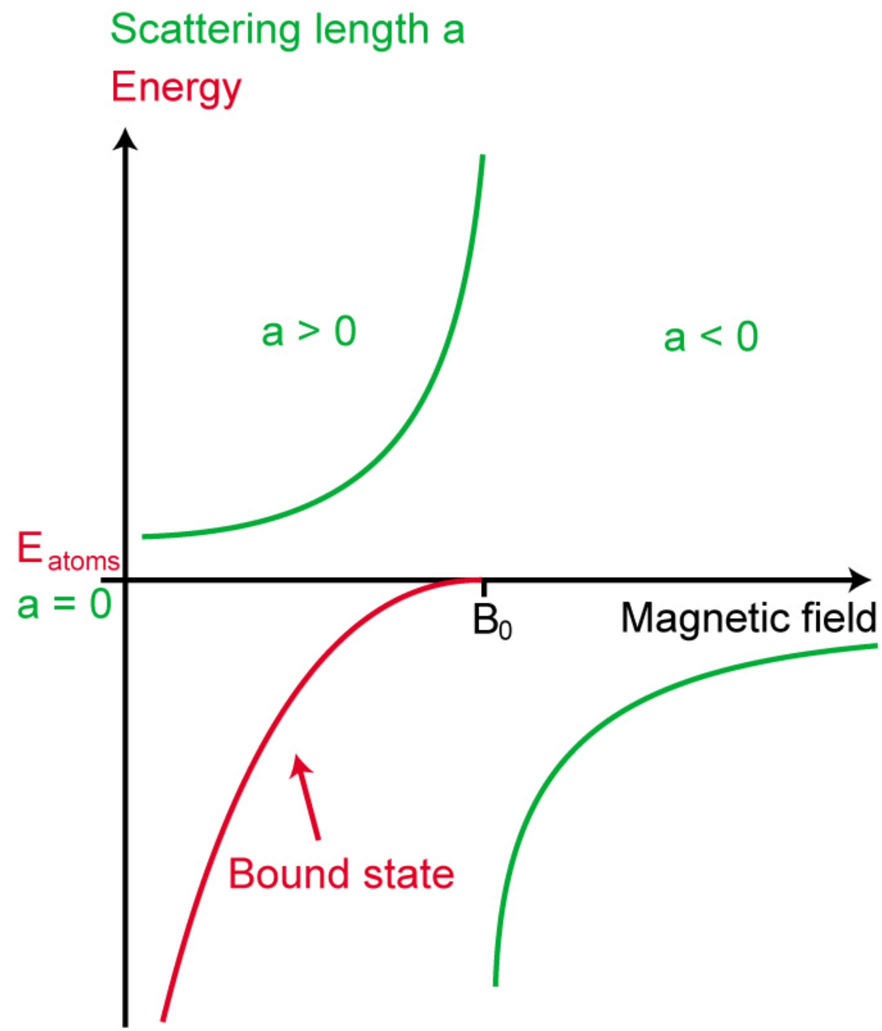
Hyperfine structure of the $^2S_{1/2}$ ground state of ^{40}K (Breit-Rabi formula)

[Tiecke, unpublished]

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

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





Main measurement technique: column density distribution, TOF

Send resonant parallel light through atomic cloud, detect by CCD

$\rightsquigarrow$ shadows $\propto$ column density (integrated over line of sight)

Use flavor sensitivity $\rightsquigarrow$ partial densities, "magnetization" profiles

In situ atomic (site) resolution only for 2-dimensional lattice systems:

large-aperture lens [Kuhr, Greiner], electron microscopy [Ott]

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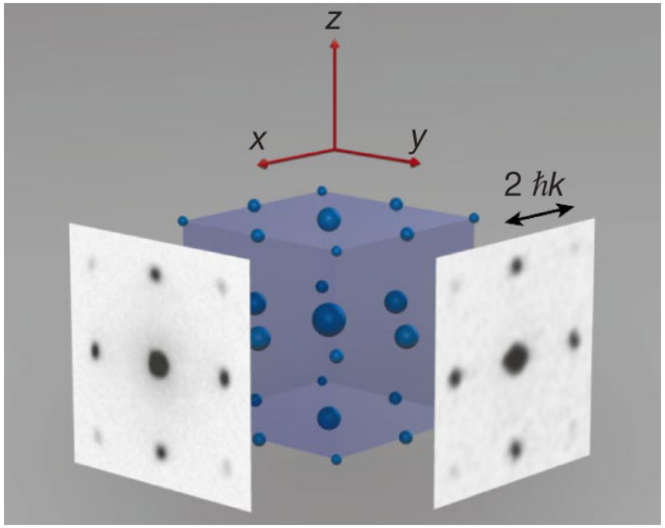

$$\boldsymbol{r}_i(t) = \boldsymbol{r}_i(0) + \boldsymbol{v}_i(0)t - \frac{1}{2} g\, \hat{\boldsymbol{e}}_z t^2$$

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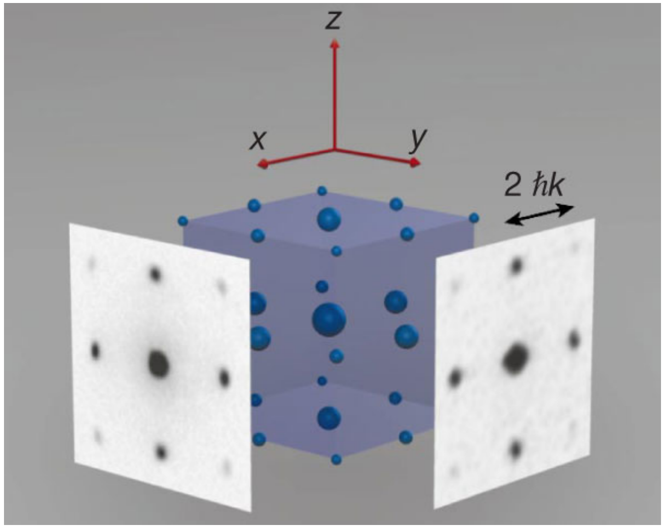

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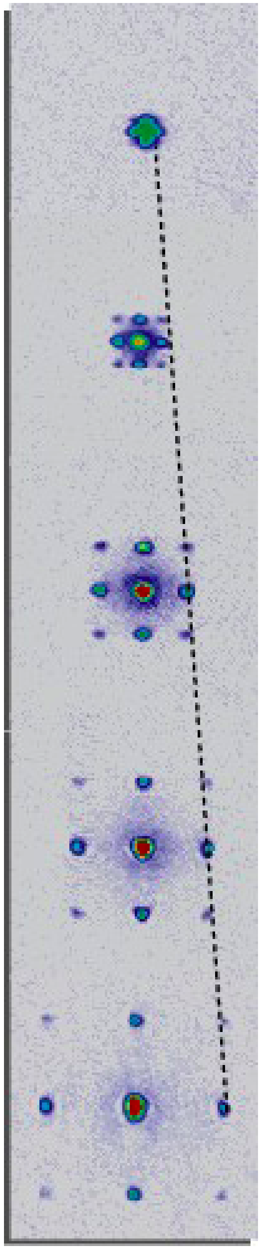
assume $\hbar\,\boldsymbol{k}_i = m\,\boldsymbol{v}_i(0)$

$$\rightsquigarrow \left(\boldsymbol{r}_i(t) + \tfrac{1}{2}g\,\hat{\boldsymbol{e}}_z t^2\right)\frac{m}{\hbar t} \approx \boldsymbol{k}_i$$

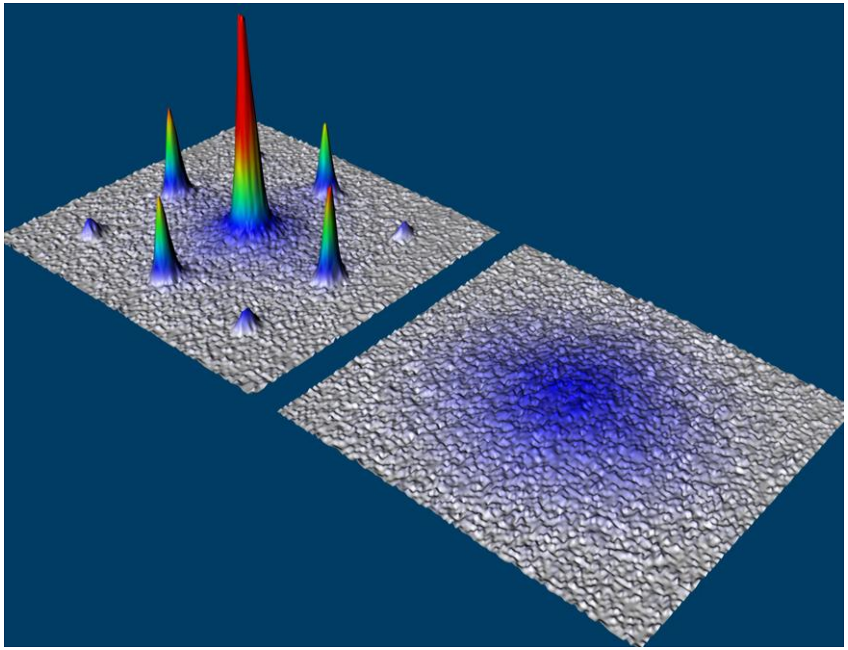
for $t \gg \sqrt{\langle r^2\rangle} \,/\, \sqrt{\langle \boldsymbol{v}^2\rangle}$



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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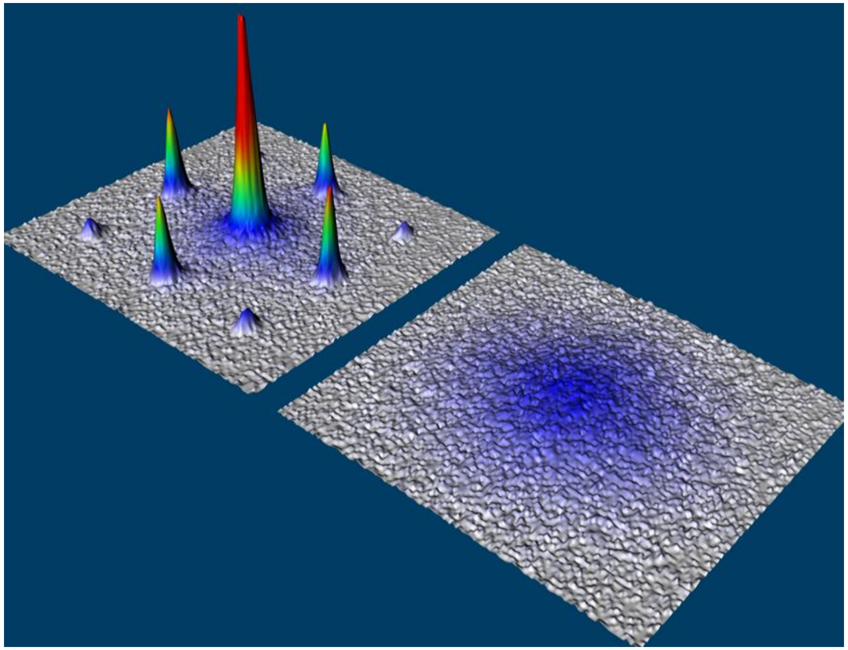

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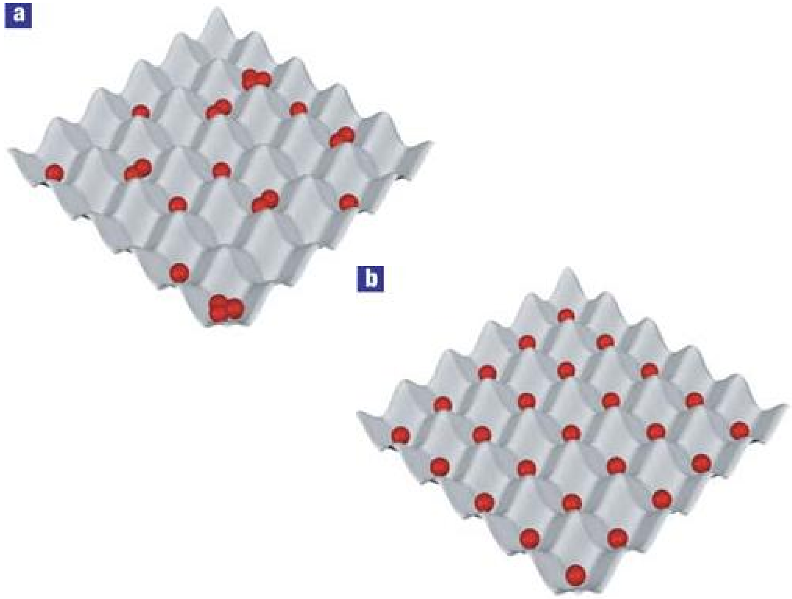
corresponding real-space picture



Superfluidity destroyed by density constraint at large U

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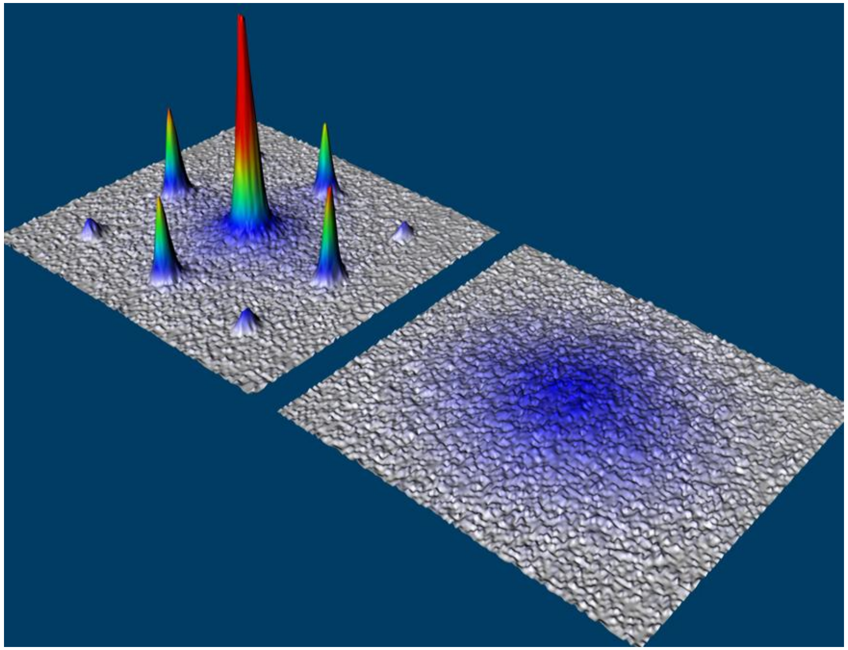

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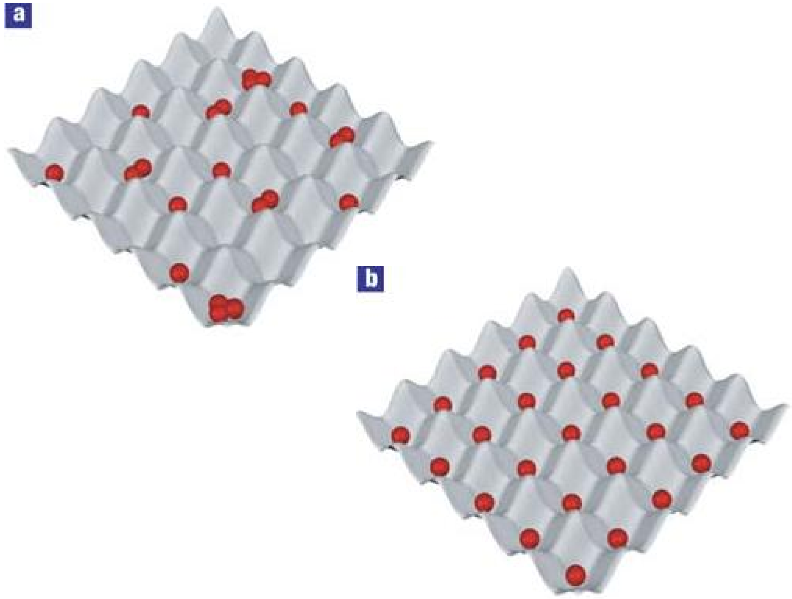
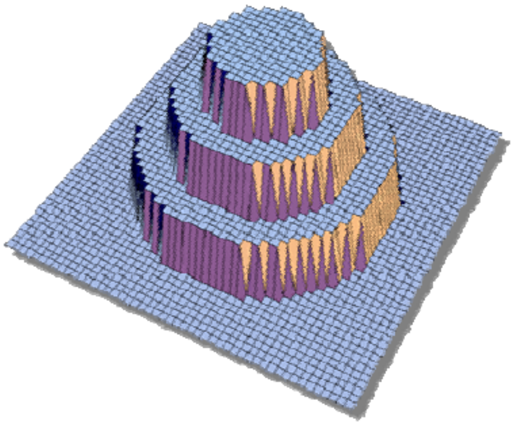


Superfluidity destroyed by density constraint at large U

Trapping potential $\rightsquigarrow$ wedding cake structure



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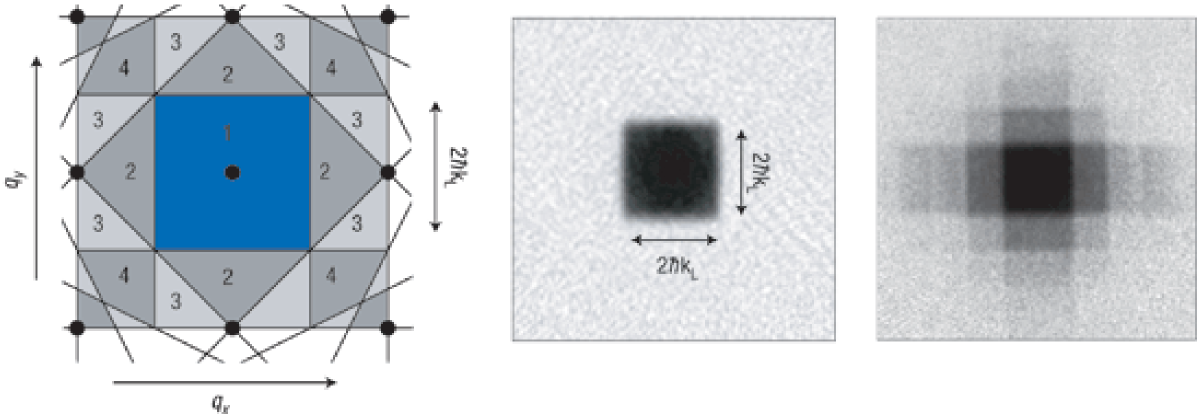

1 species: band insulator for filled 1st Brillouin zone:

[Köhl et al, PRL (2005)]

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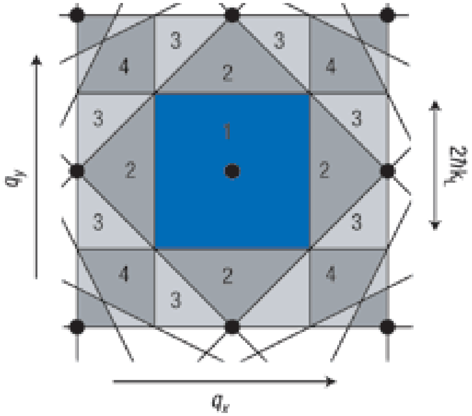

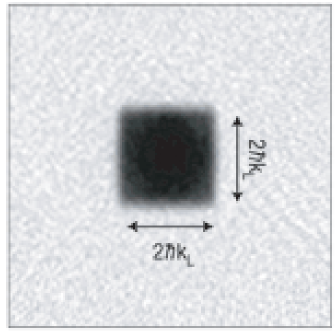

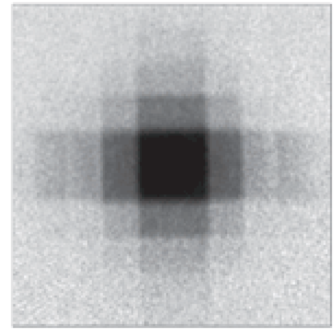

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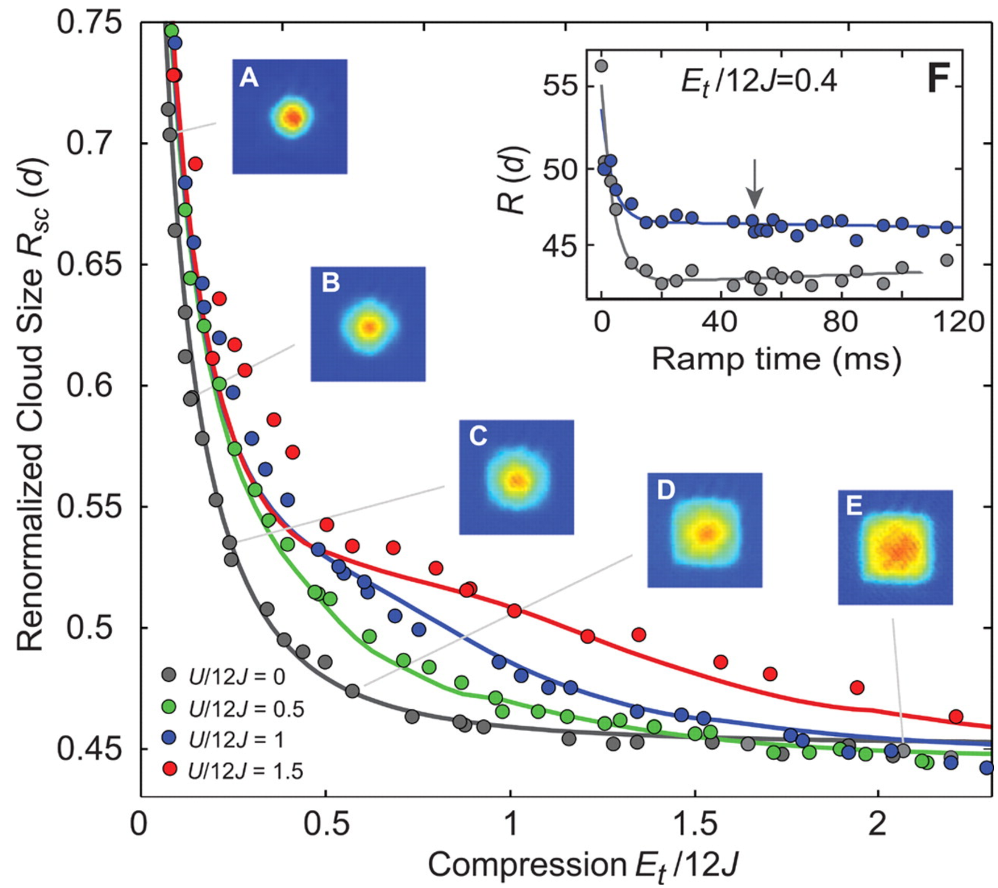
Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

Detection method: measure cloud diameter vs. trap strength

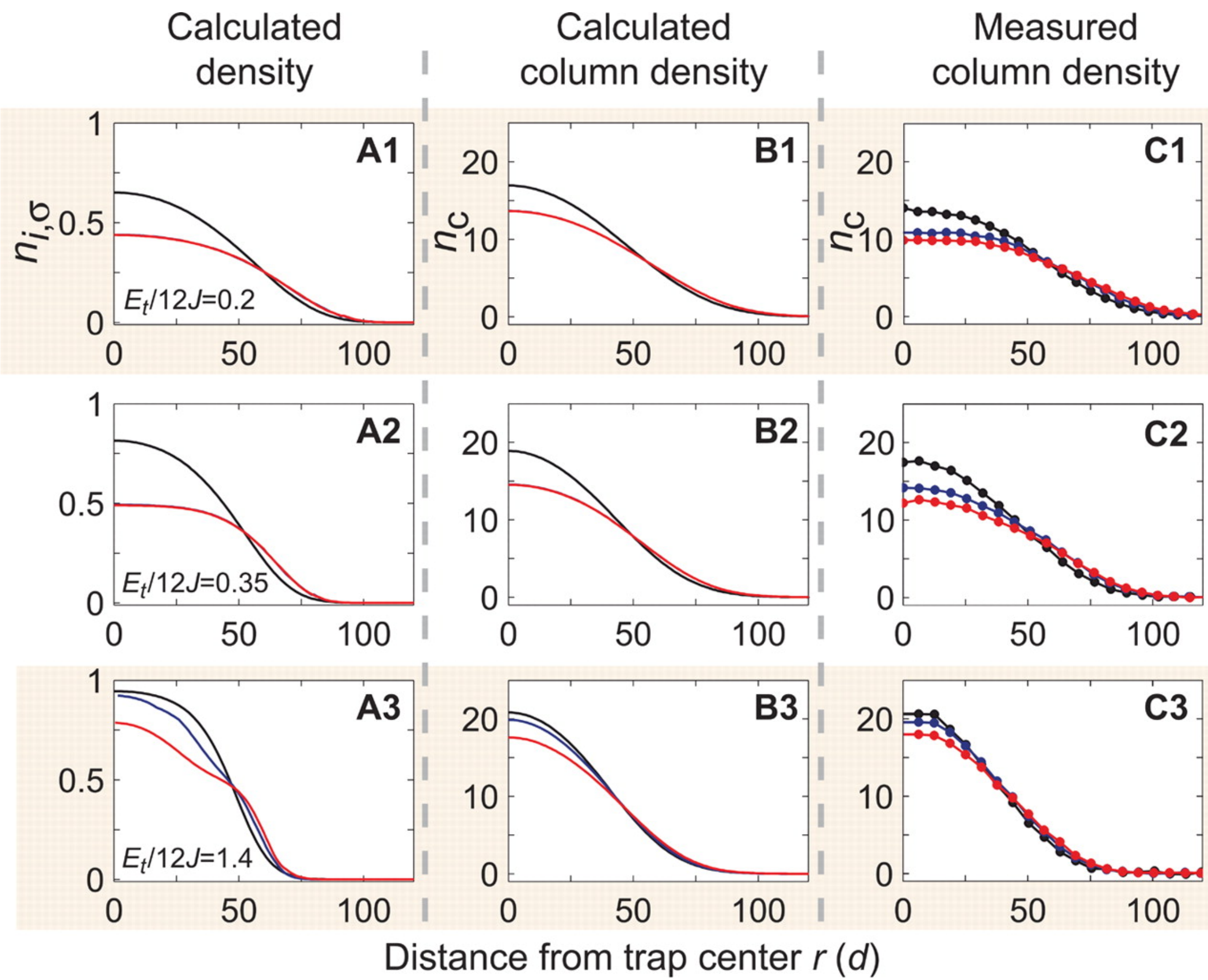
MIT signature: plateau in $R_{SC}(E_t)$

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

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



Further MIT observables: column density . . .



MIT signature: density plateau at $n_{i,\sigma} = 0.5$

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

. . . and 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 (∼ Stern-Gerlach)

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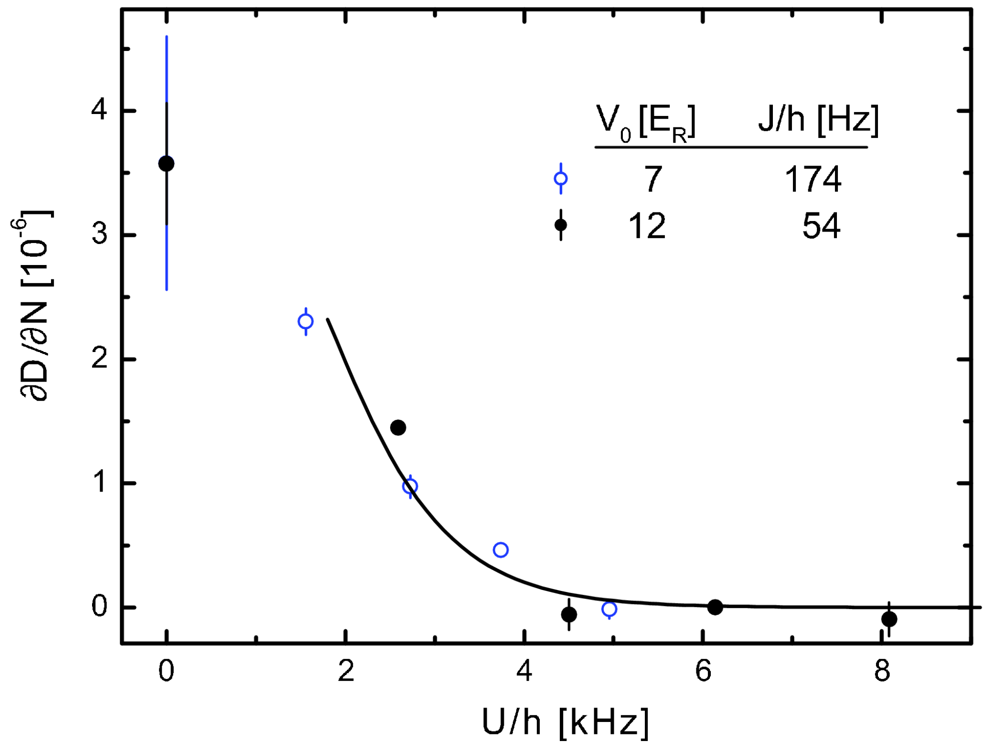

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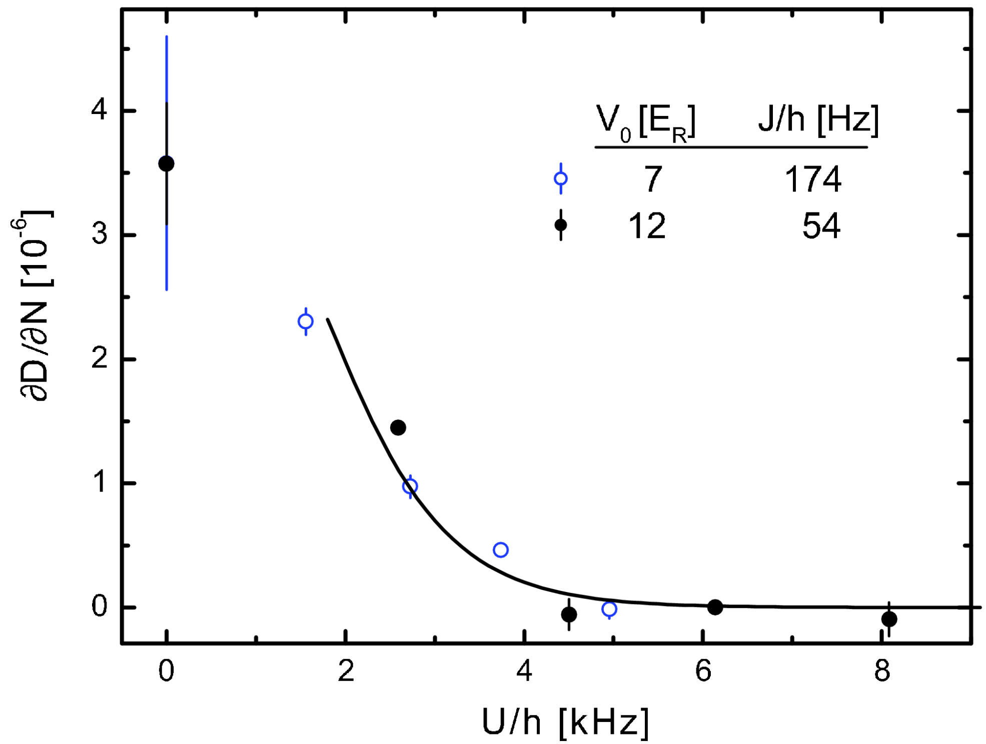

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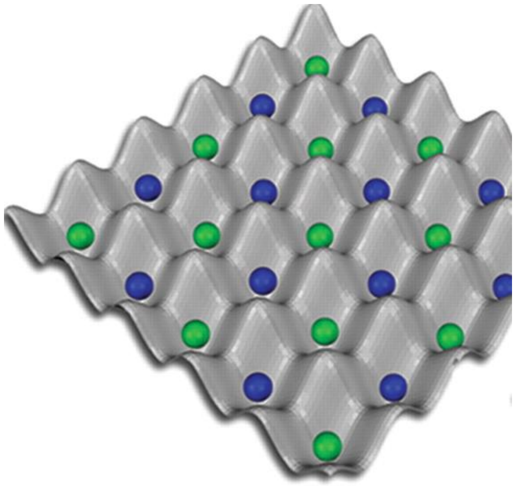
Many other phenomena seen: superconductivity, vortices, BEC-BCS crossover, . . .

Next grand challenges:

Antiferromagnetism (staggered order) in ultracold fermions



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(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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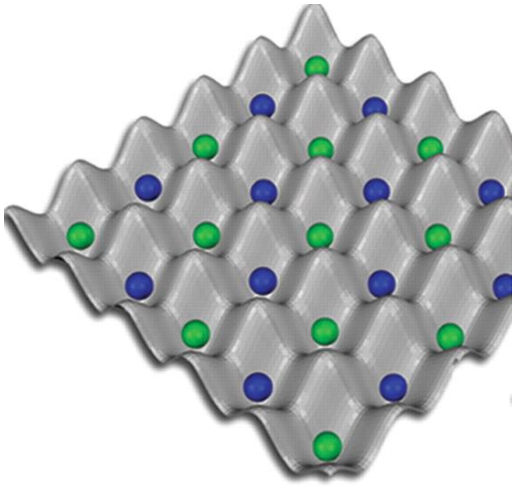

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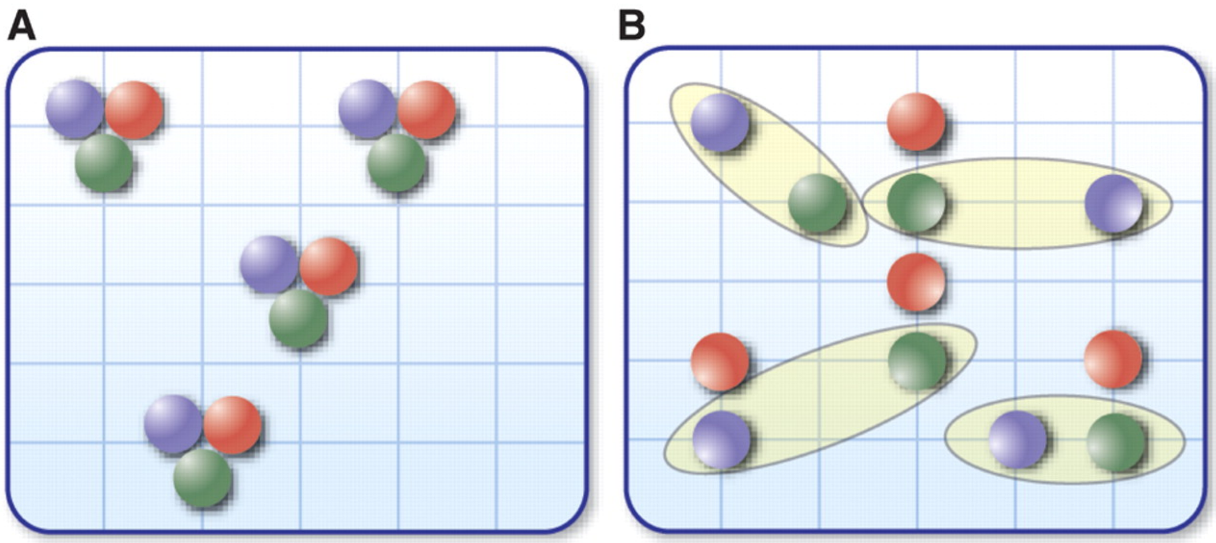
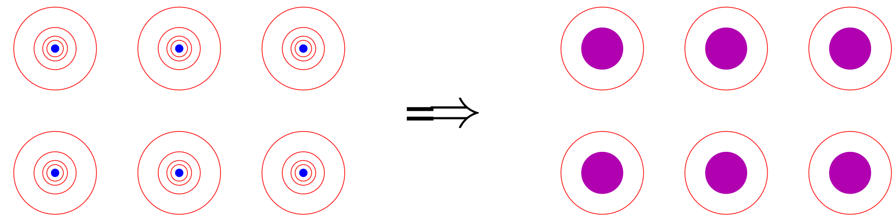
Multiflavor phenomena, e.g. trions versus color superconductivity



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 $\downarrow$



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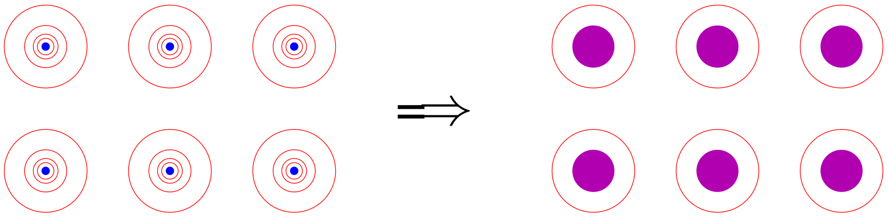

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occupation number formalism $\downarrow$ Wannier orbitals

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

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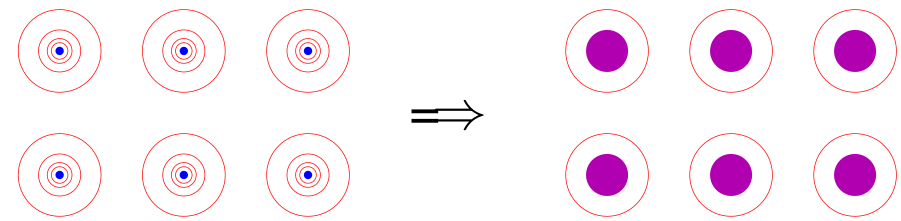

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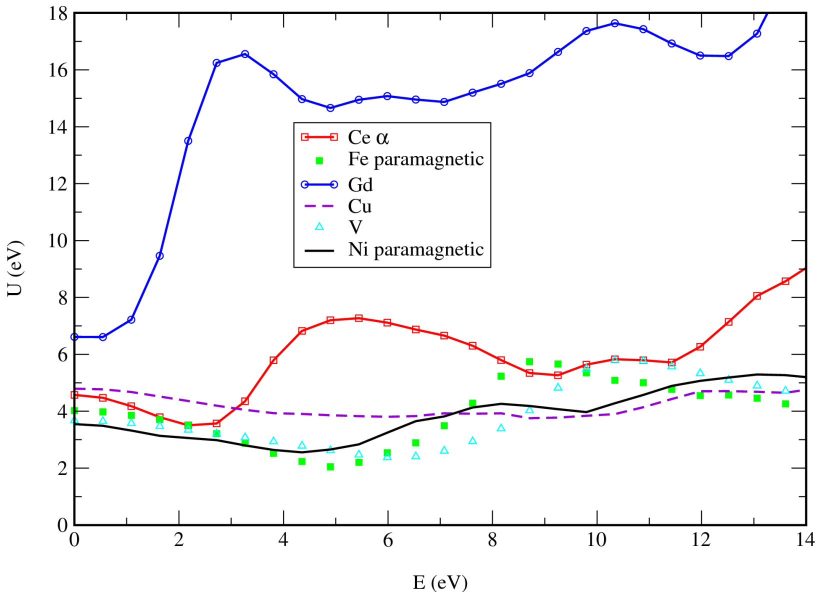
$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu}\, \hat{c}^{\dagger}_{i\nu\sigma}\, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'}\, \hat{c}^{\dagger}_{i\nu\sigma}\, \hat{c}^{\dagger}_{j\nu'\sigma'}\, \hat{c}_{n\mu'\sigma'}\,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

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

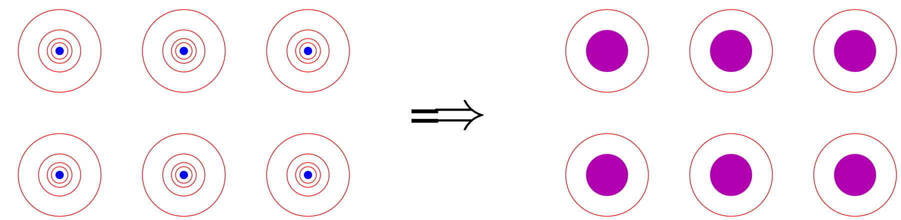
elated lattice Fermi systems



[Aryasetiawan et al., PRB 2006]

$$+ \sum_i V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

trons



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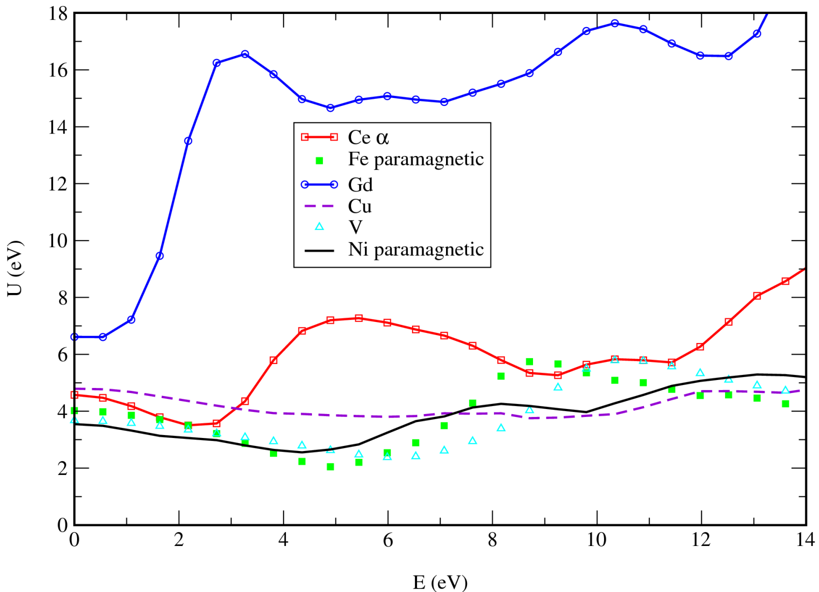

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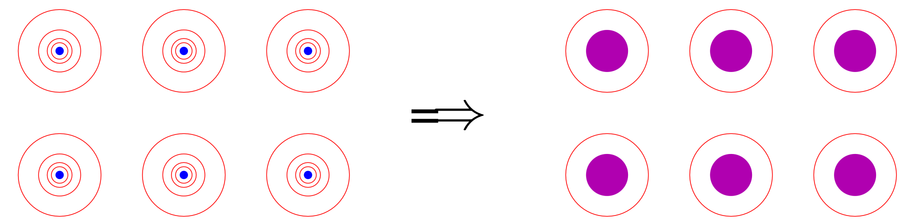

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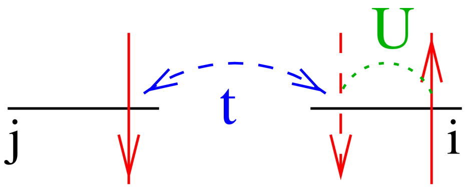
Note: no core states in quantum gas case!

Approaches for Hubbard-type models

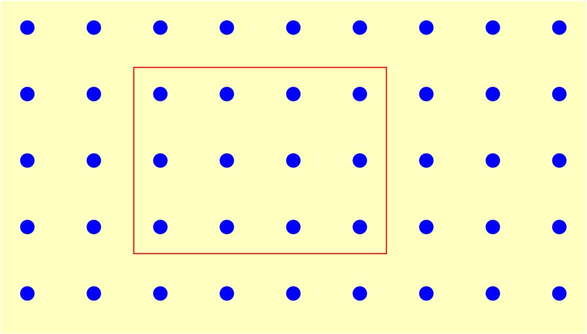
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij}\,(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



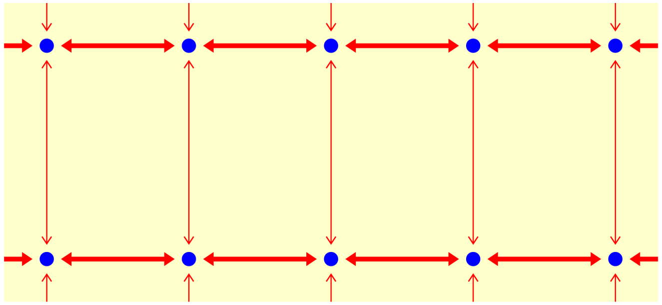
Perturbation theory

- $U \to 0$: 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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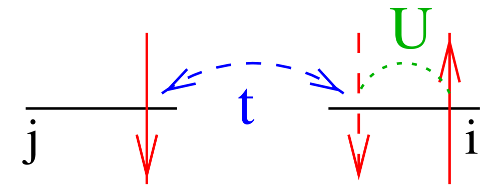

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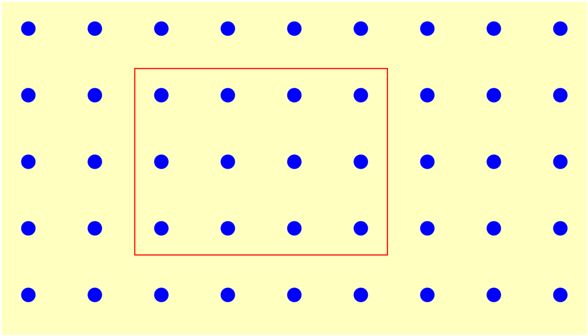

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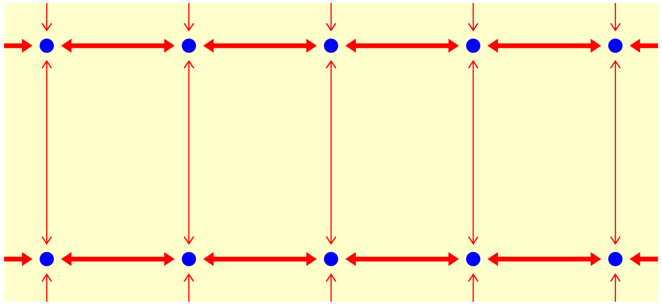
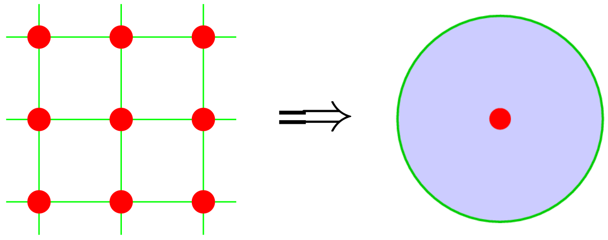


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

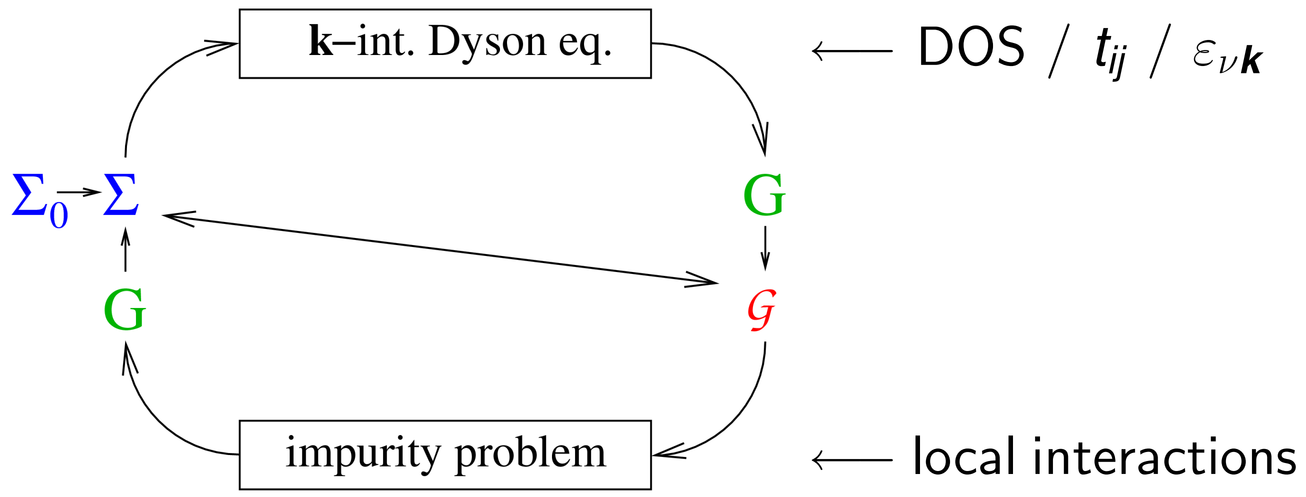
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

+	non-perturbative $\rightsquigarrow$ valid at MIT
+	dynamical on-site correlations preserved
+	in thermodynamic limit
+/−	exact for coordination $Z \to \infty$



Iterative solution of DMFT equations

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



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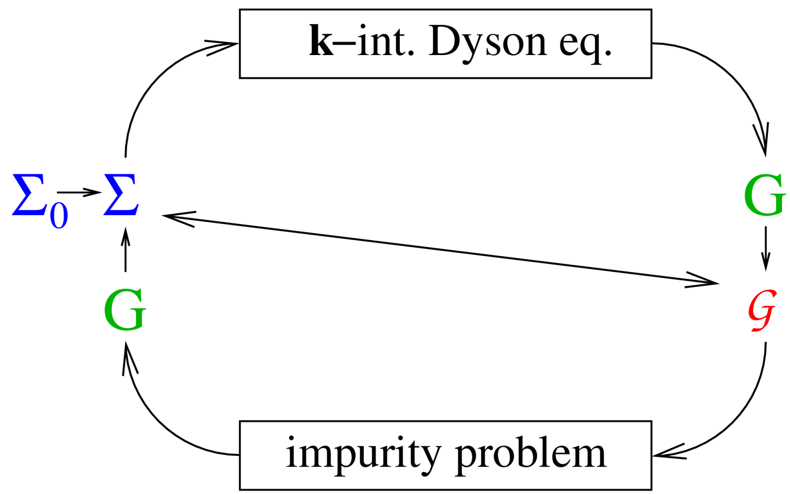
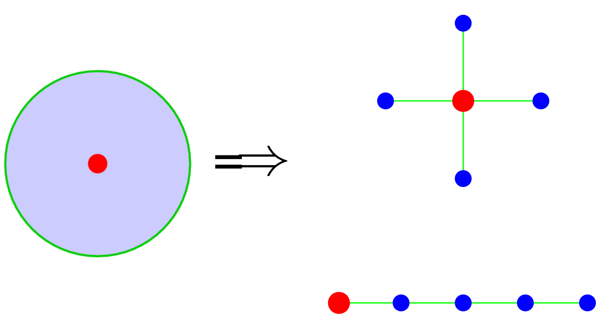


$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu \boldsymbol{k}}$

$\longleftarrow$ local interactions

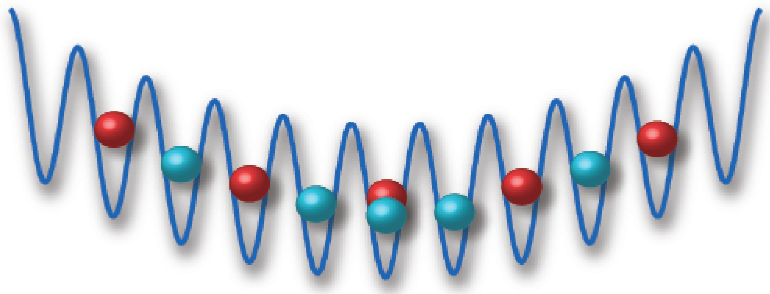
Impurity solver:

- 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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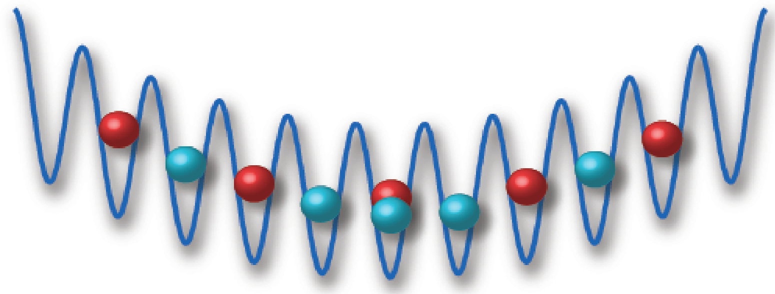

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Real-space DMFT: use local, but site-dependent, self-energy

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

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

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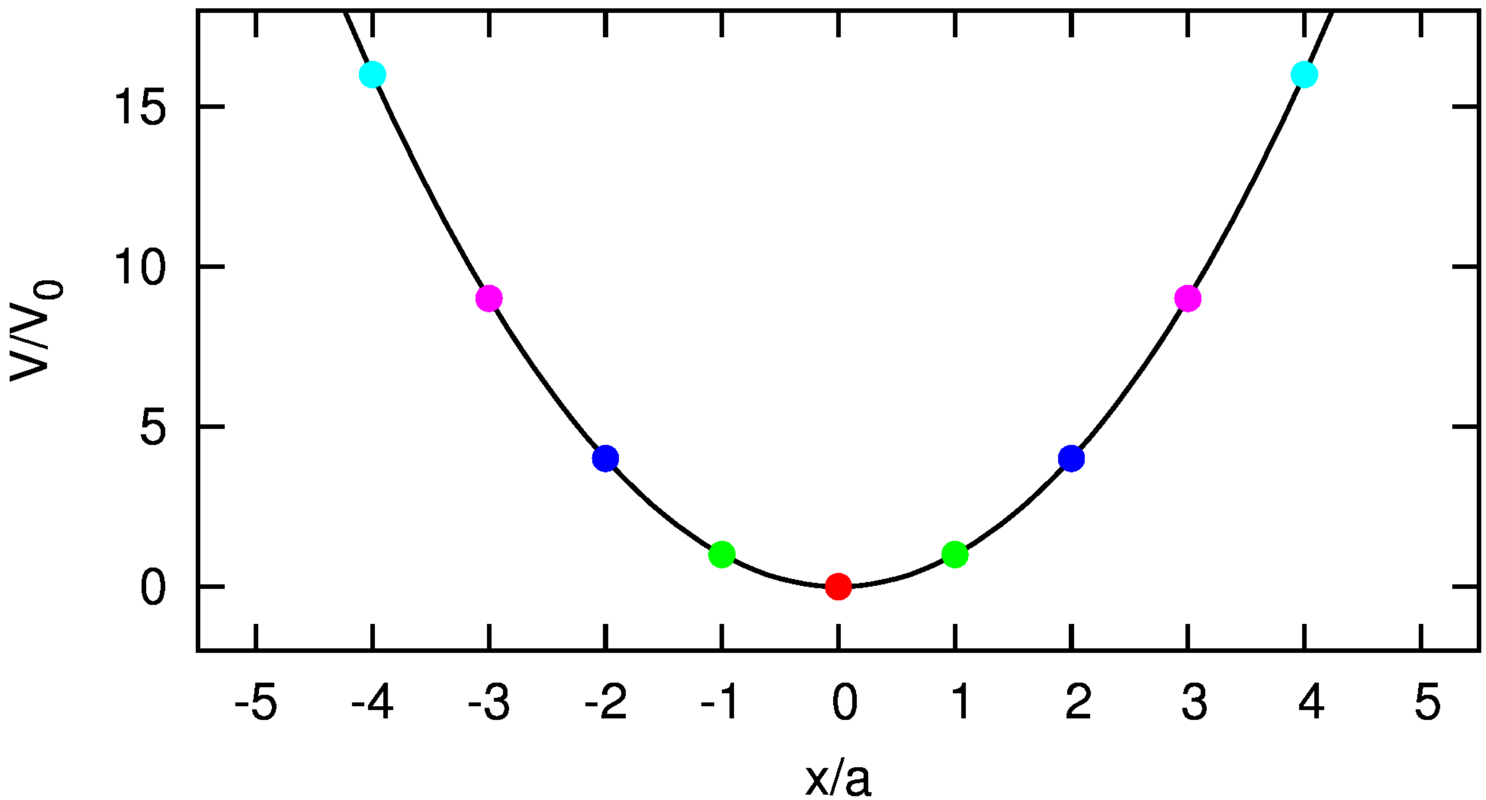
Note: impurity problem is site-parallel, lattice Dyson equation is frequency-parallel

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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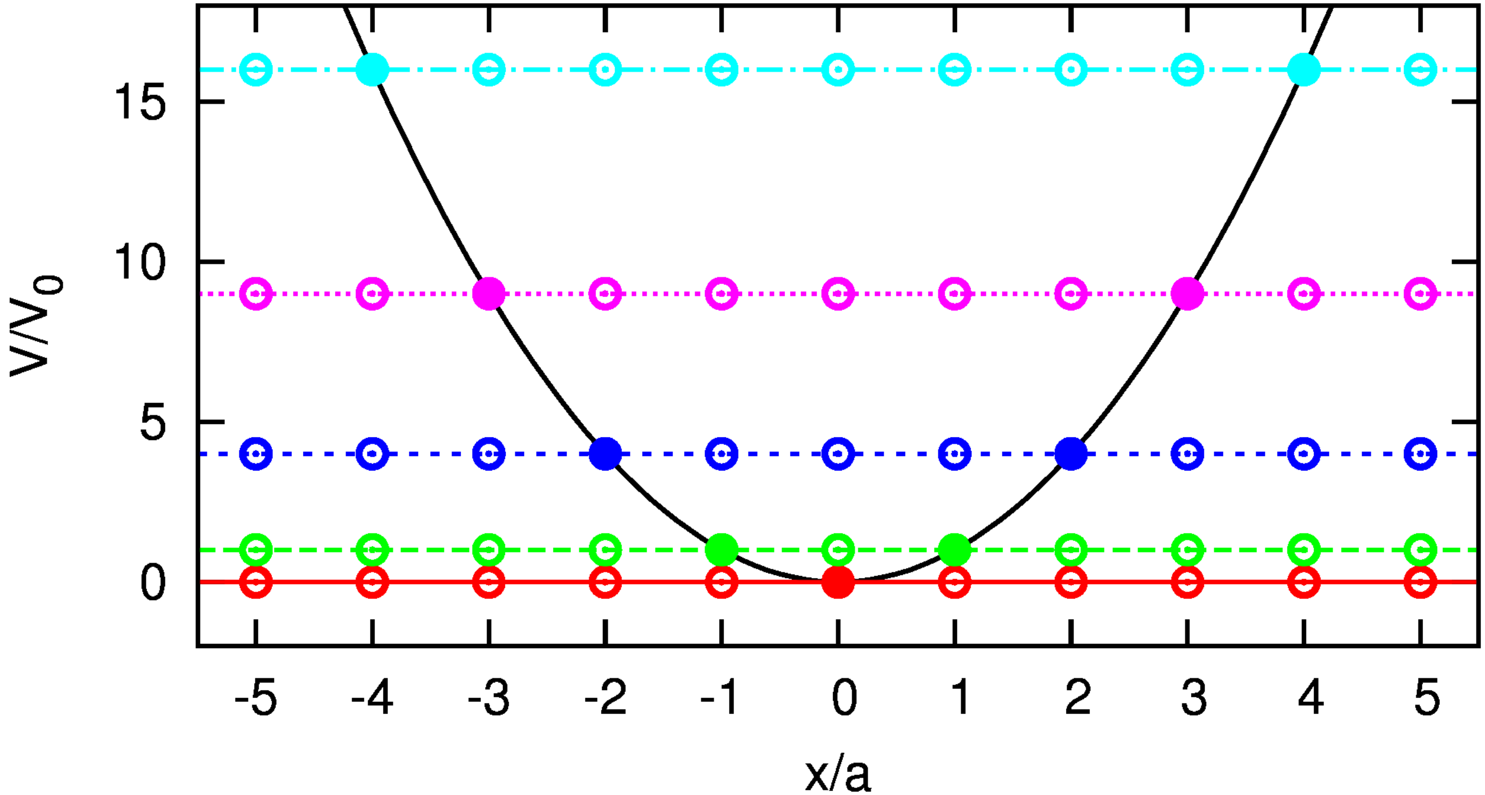

. . . will be used for comparison to RDMFT

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

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

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

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

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(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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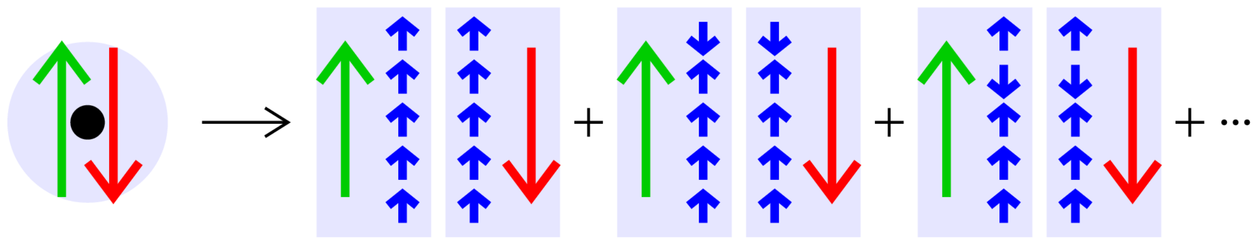

Wick theorem:

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

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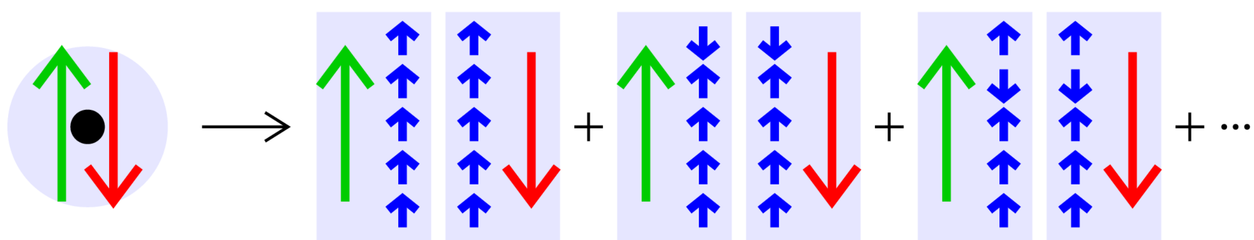


Wick theorem:

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

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

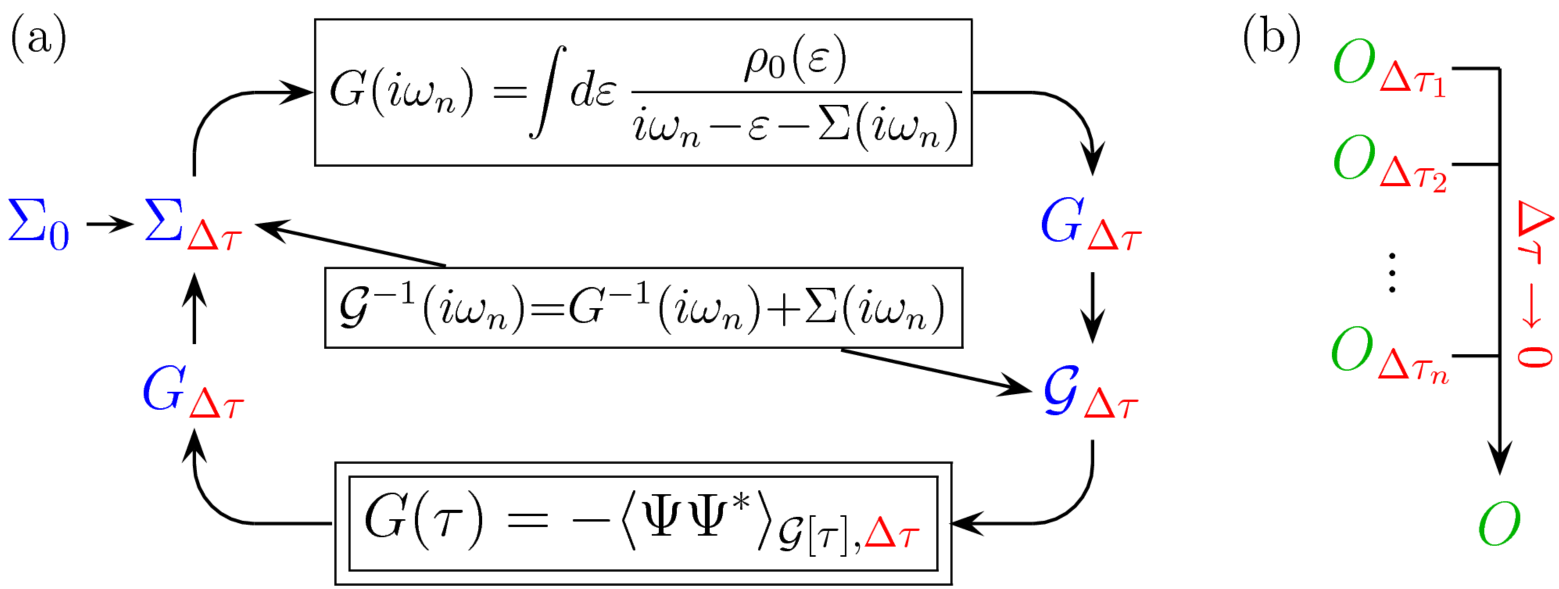
+ numerically exact, + no sign problem, $-$ effort scales as T^{-3}

(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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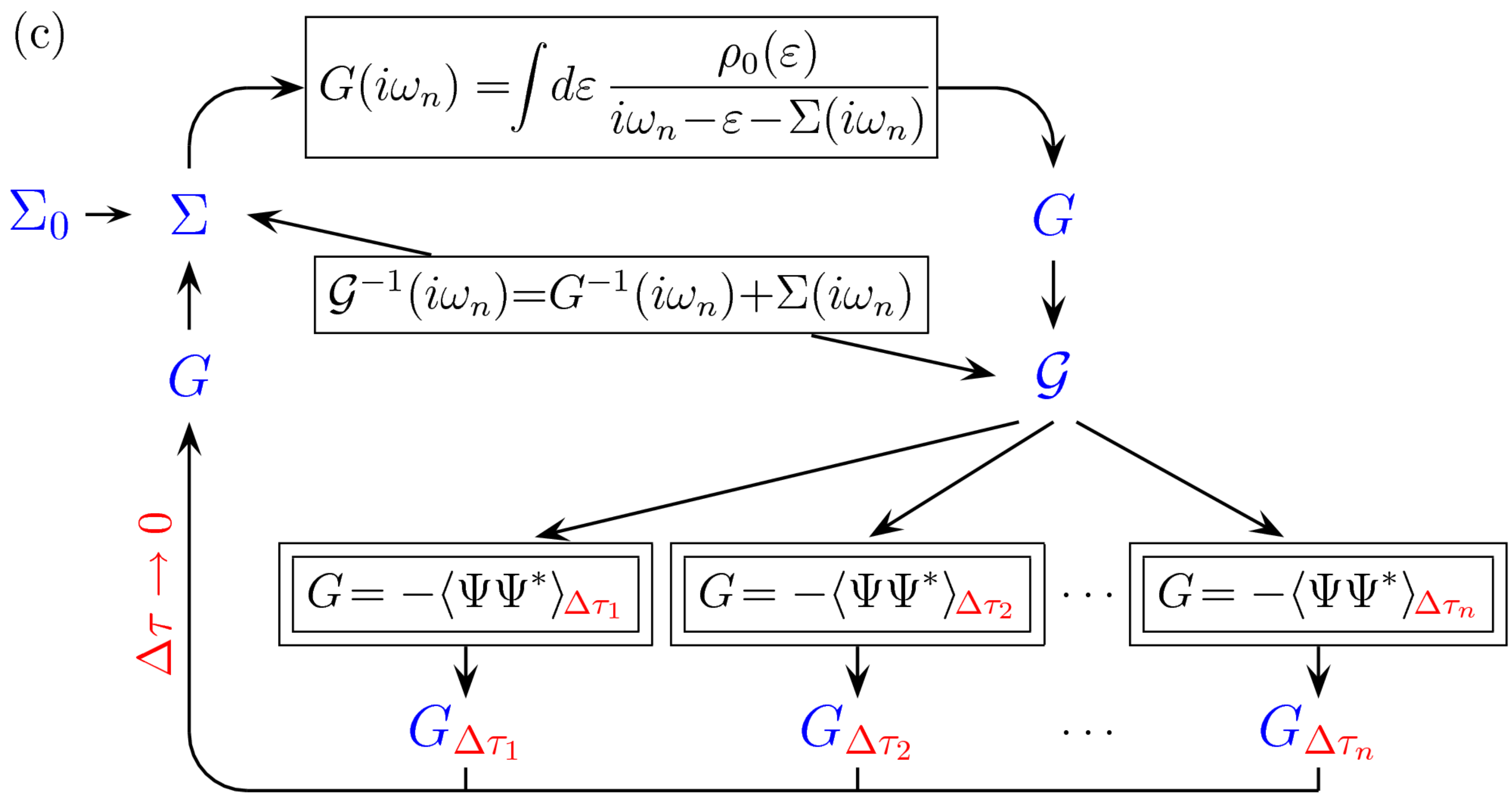


(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ 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 ($T = 0$)

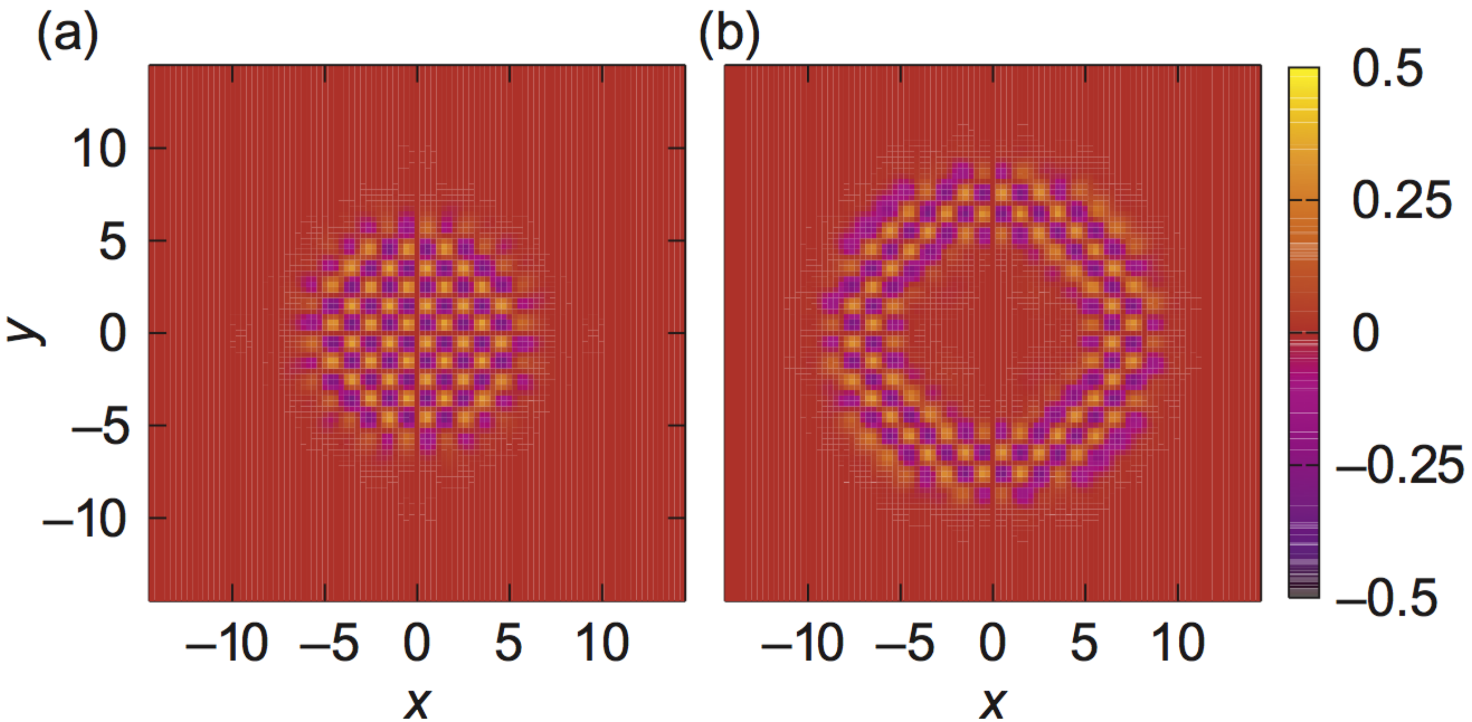
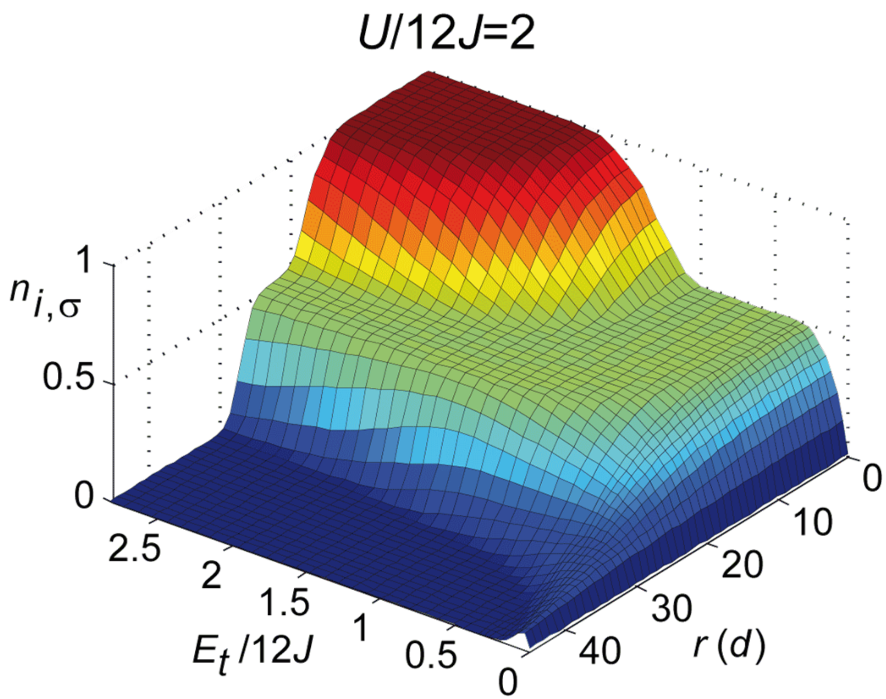


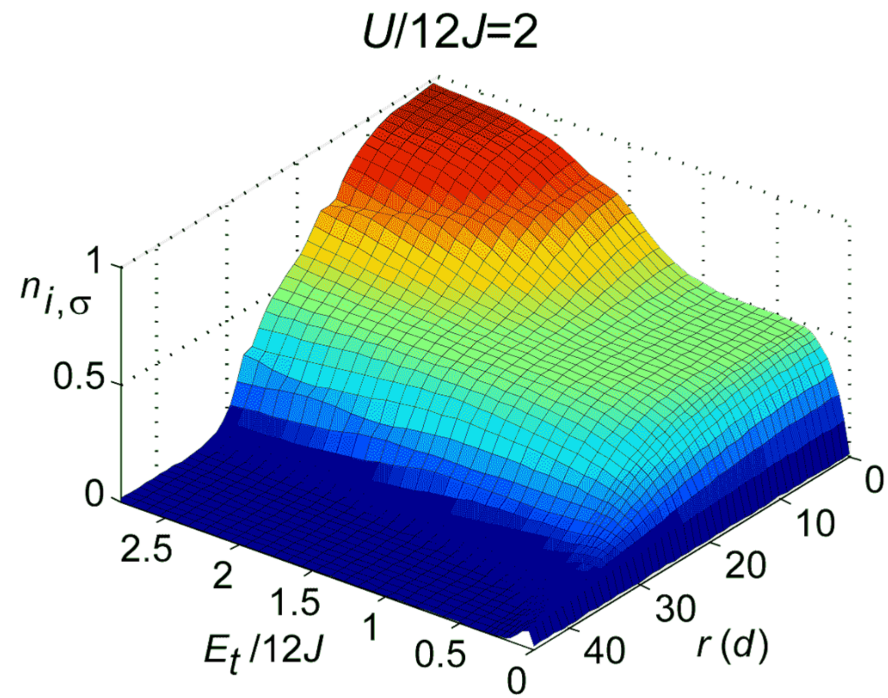
Figure 1. Real-space magnetization profiles for $U = 10$ on a square (30×30) lattice; (a) $V = 0.1$ and $\mu_\uparrow = \mu_\downarrow = 5$; (b) $V = 0.2$ and $\mu_\uparrow = \mu_\downarrow = 15$. Energies are expressed in units of the hopping parameter J.

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

But: NRG problematic at elevated temperatures



$T = 0.07t$

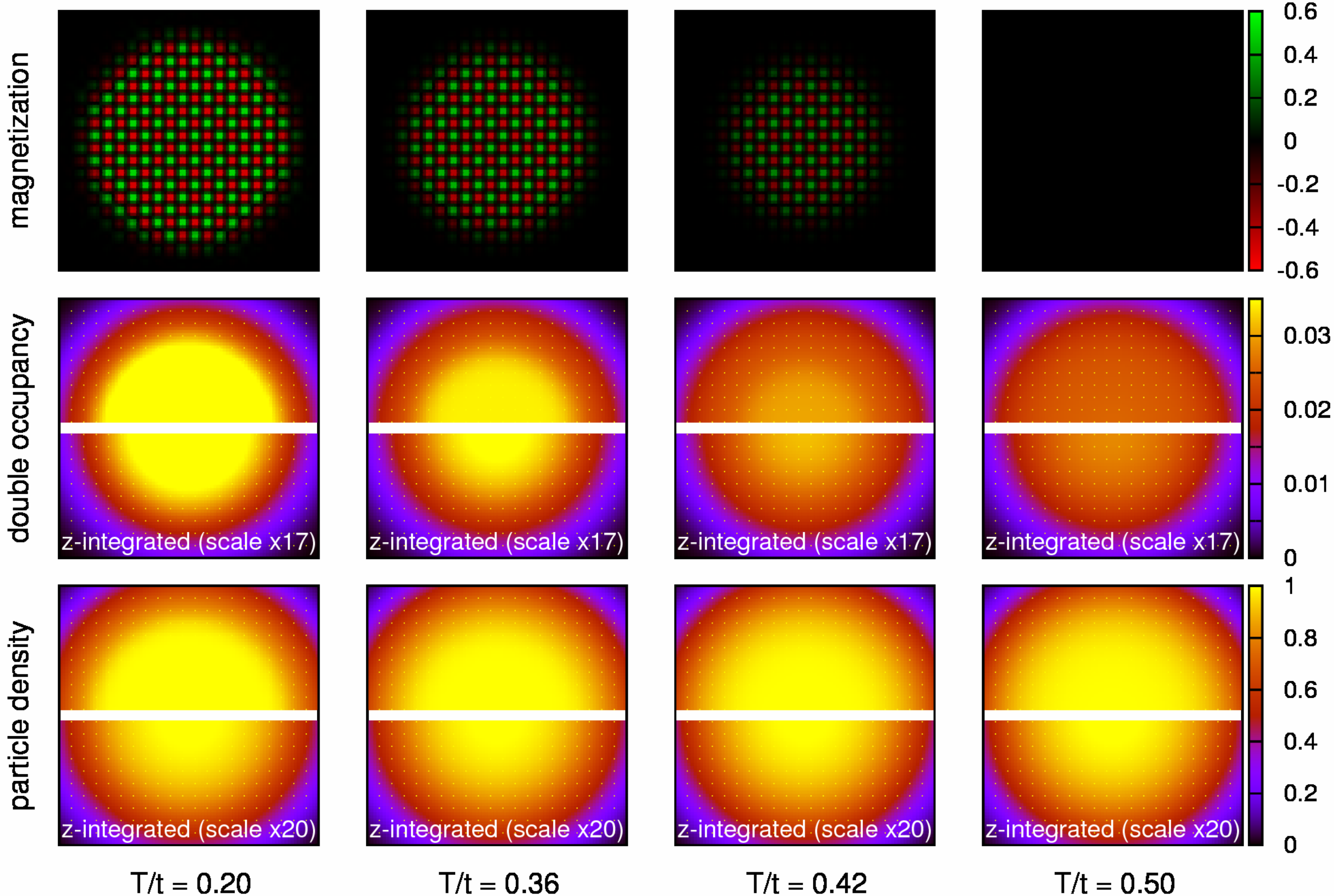


$T = 0.15t$

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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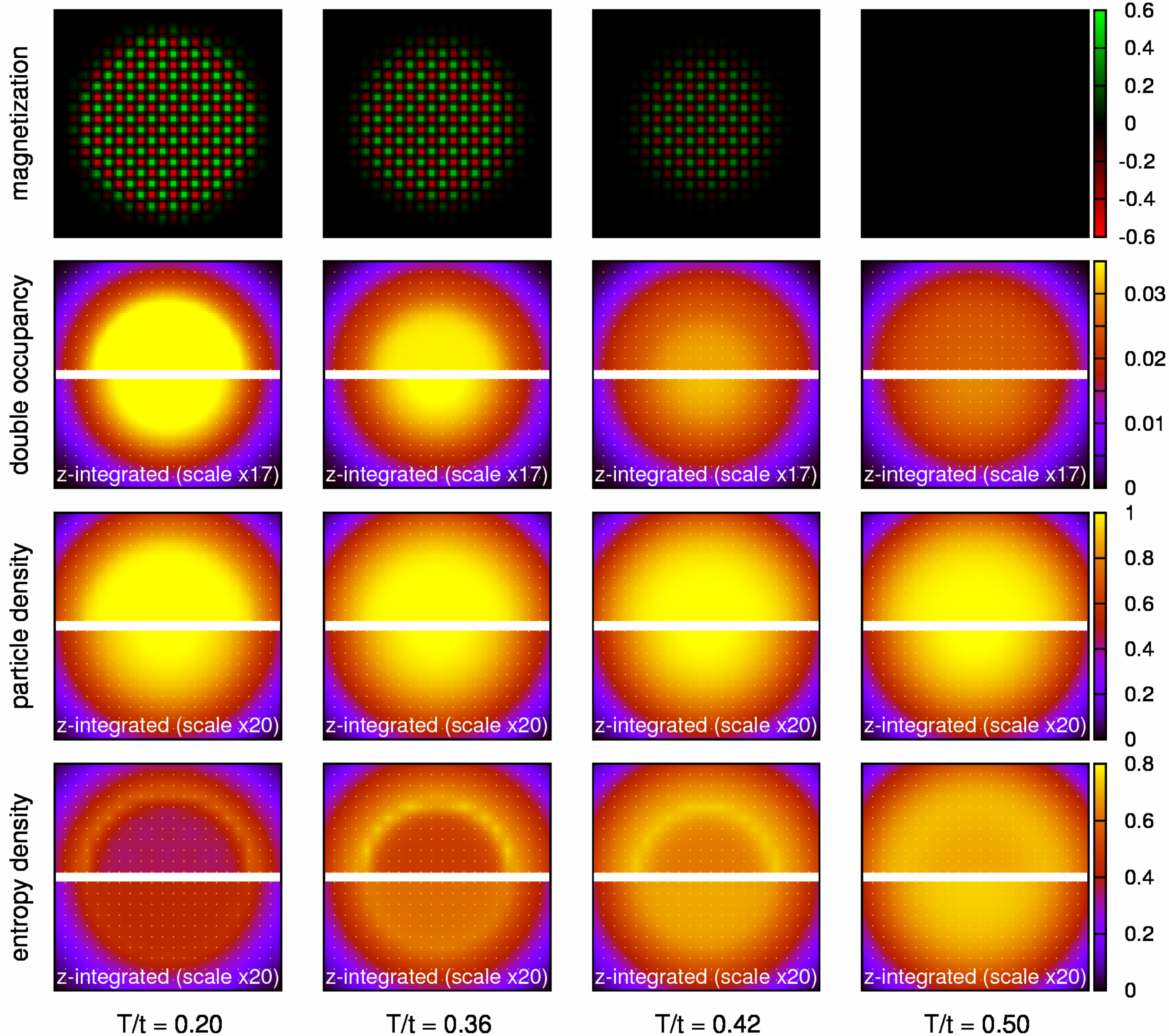


AF core:

nearly fully polarized at $T = 0.20t$

vanishes at $T_N \approx 0.46t$

AF $\leftrightarrow$ enhanced D!

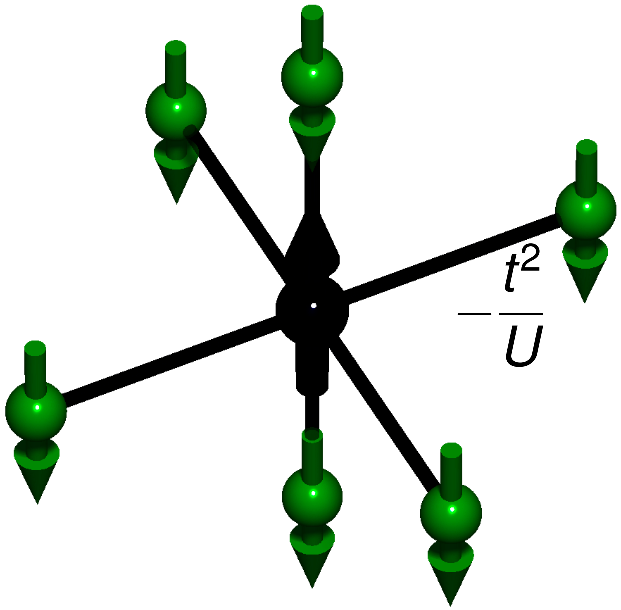
$\sim$ 6000 atoms (naively $\sim 30^3 = 27000$ sites needed)

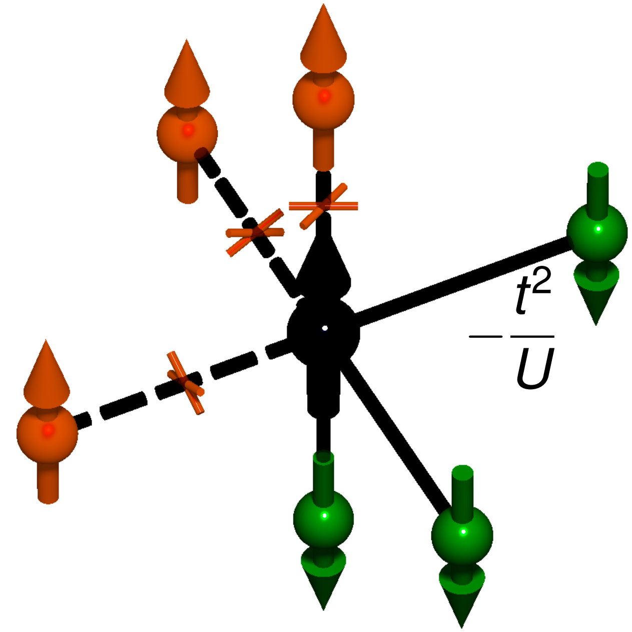
Entropy

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

Enhanced double occupancy: a signature of AF order

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





AF state:

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

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

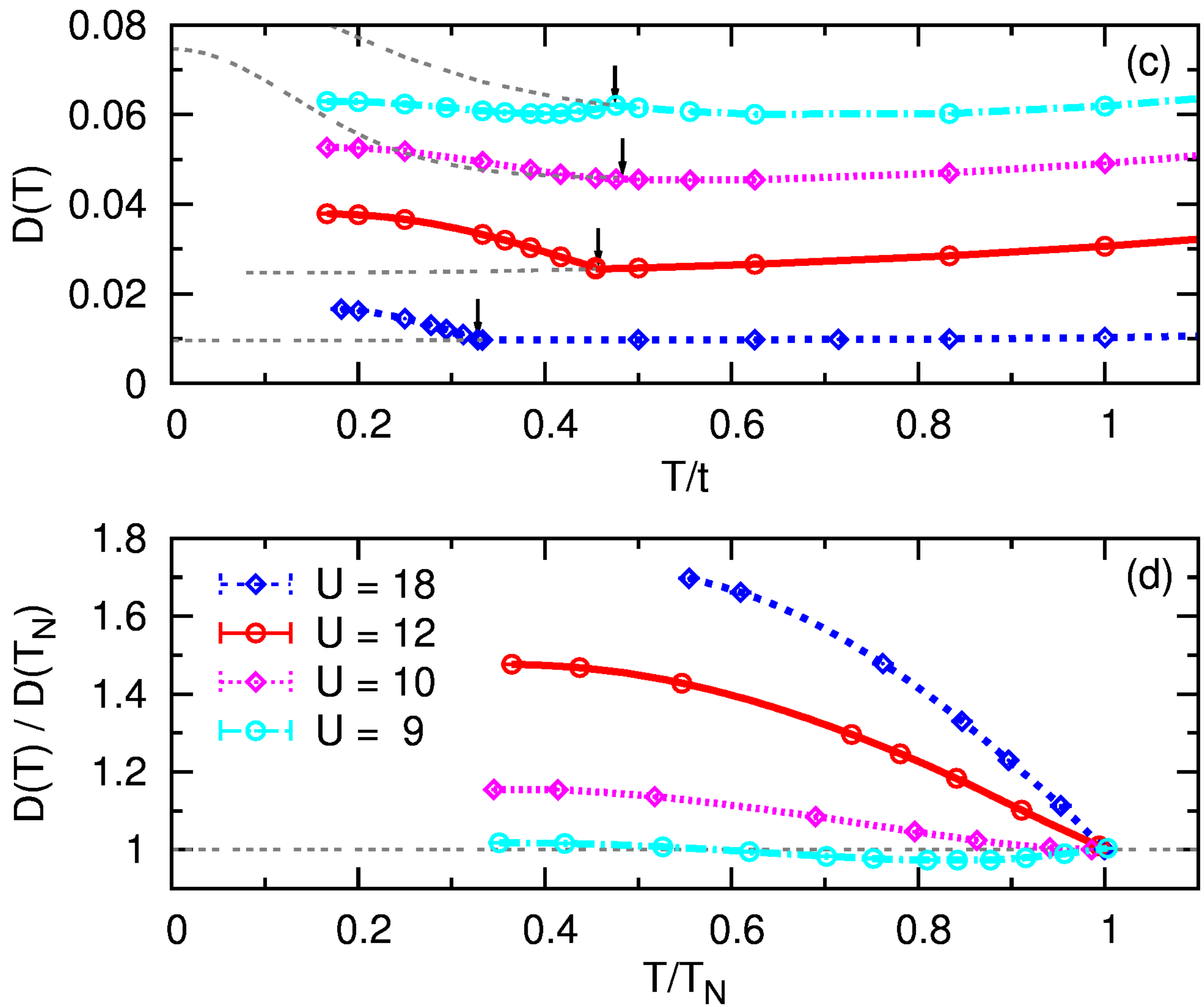
Paramagnetic state:

1/2 of the neighboring sites
are forbidden for hopping

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

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

DMFT-QMC estimates of D at half filling



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

arrows: Néel temperatures

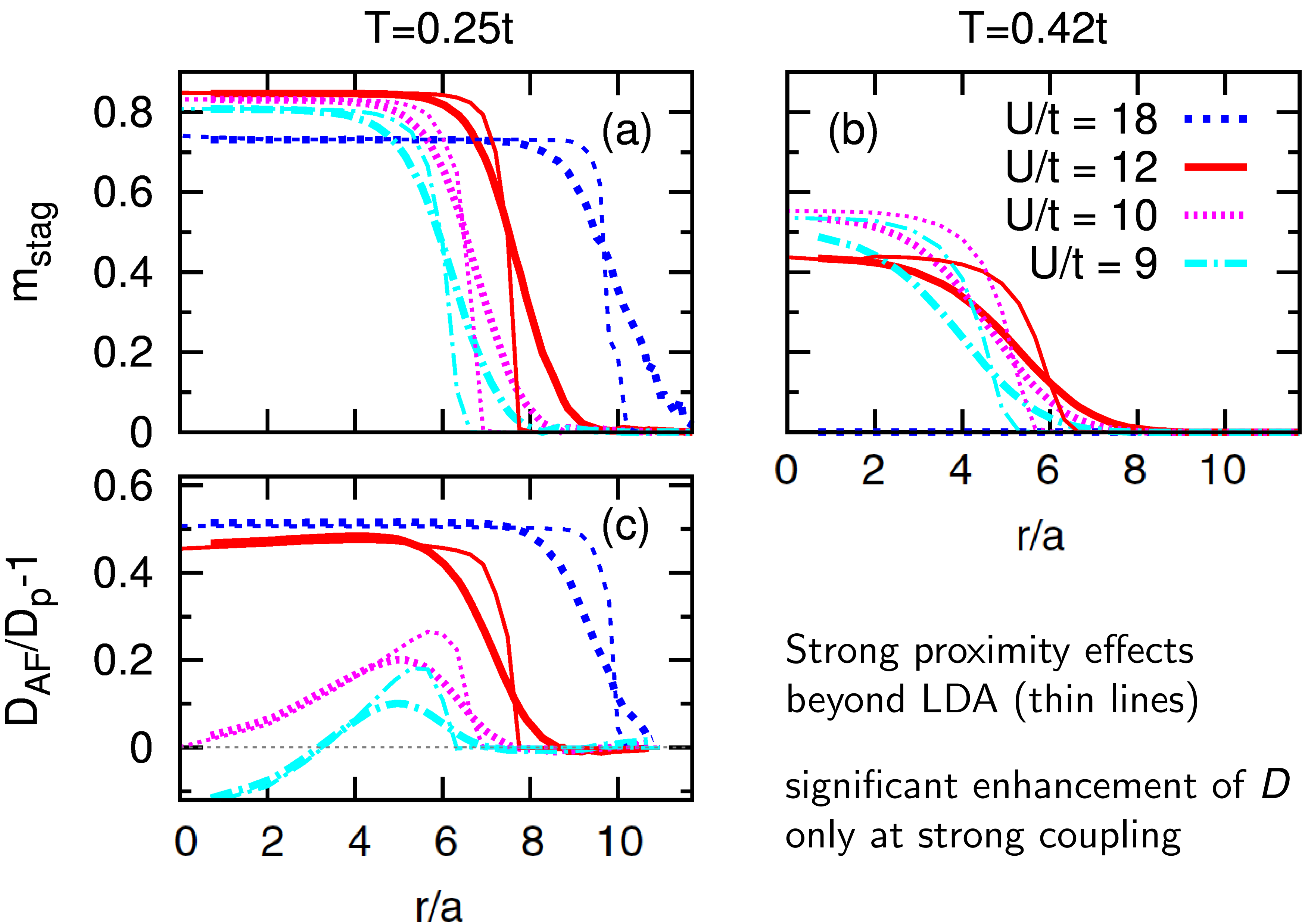
thin lines: metastable paramagnetic phase.

Data scaled to values of critical point:

relative enhancement
$D/D(T_\mathrm{N}) \xrightarrow{U\to\infty} 2$

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

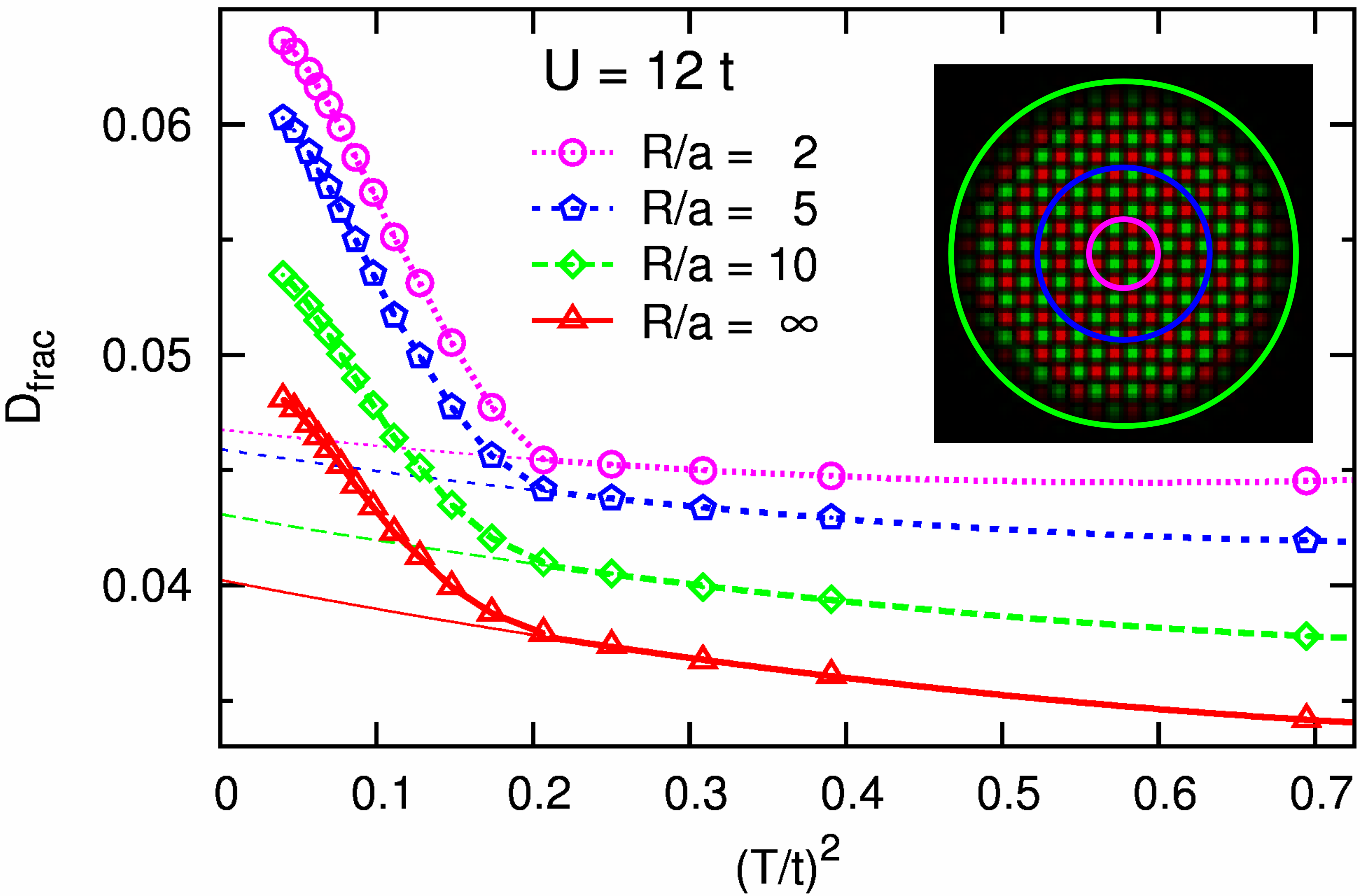
Radial dependence of m_{stag} and D: RDMFT calculations ($V = 0.05t$)



Strong proximity effects beyond LDA (thin lines)

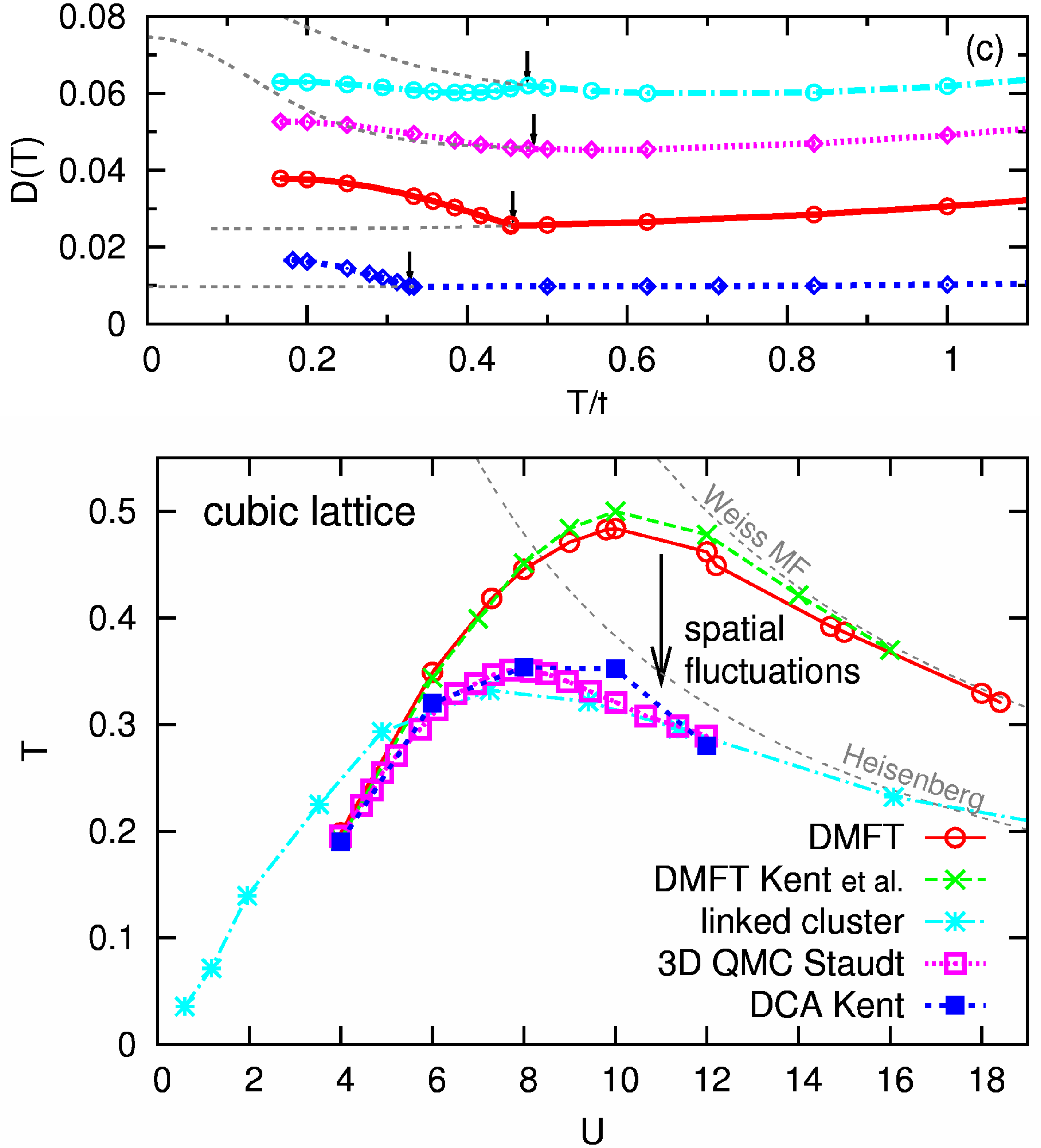
significant enhancement of D only at strong coupling

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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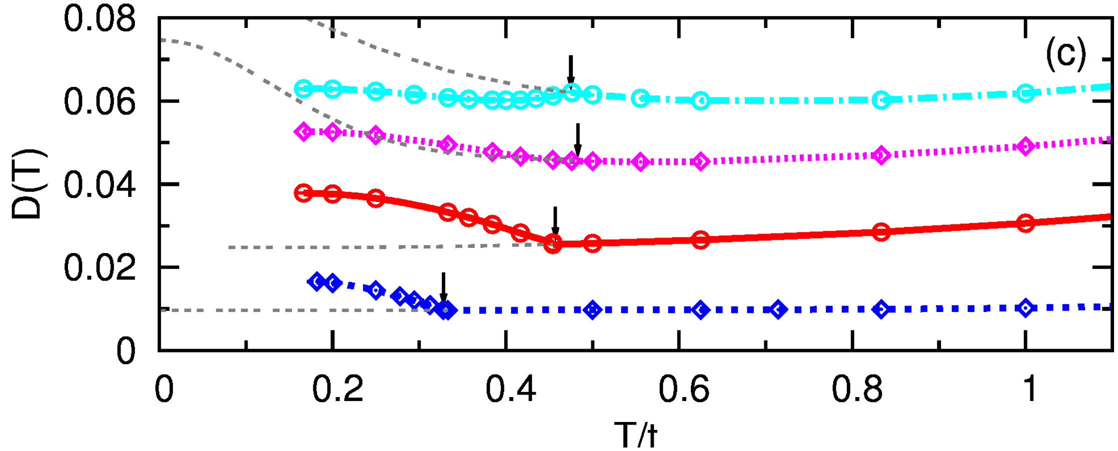

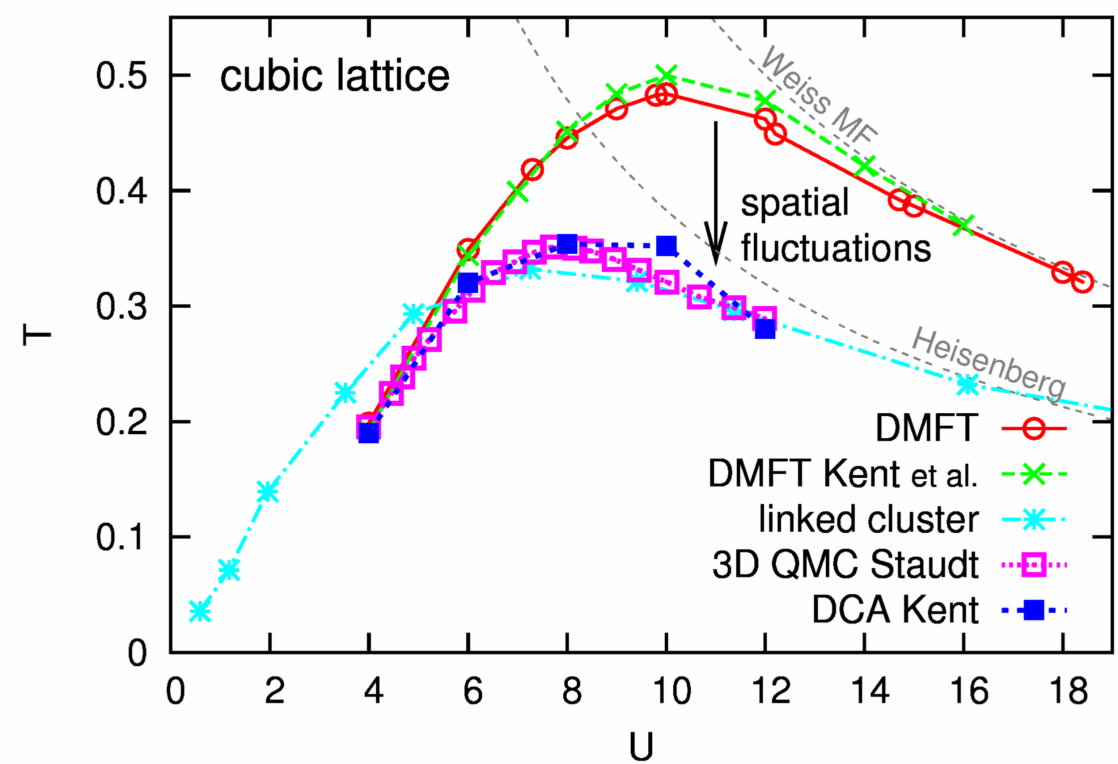

Unavoidable change: kinks cannot remain at $T = T_N^{DMFT} > T_N$!

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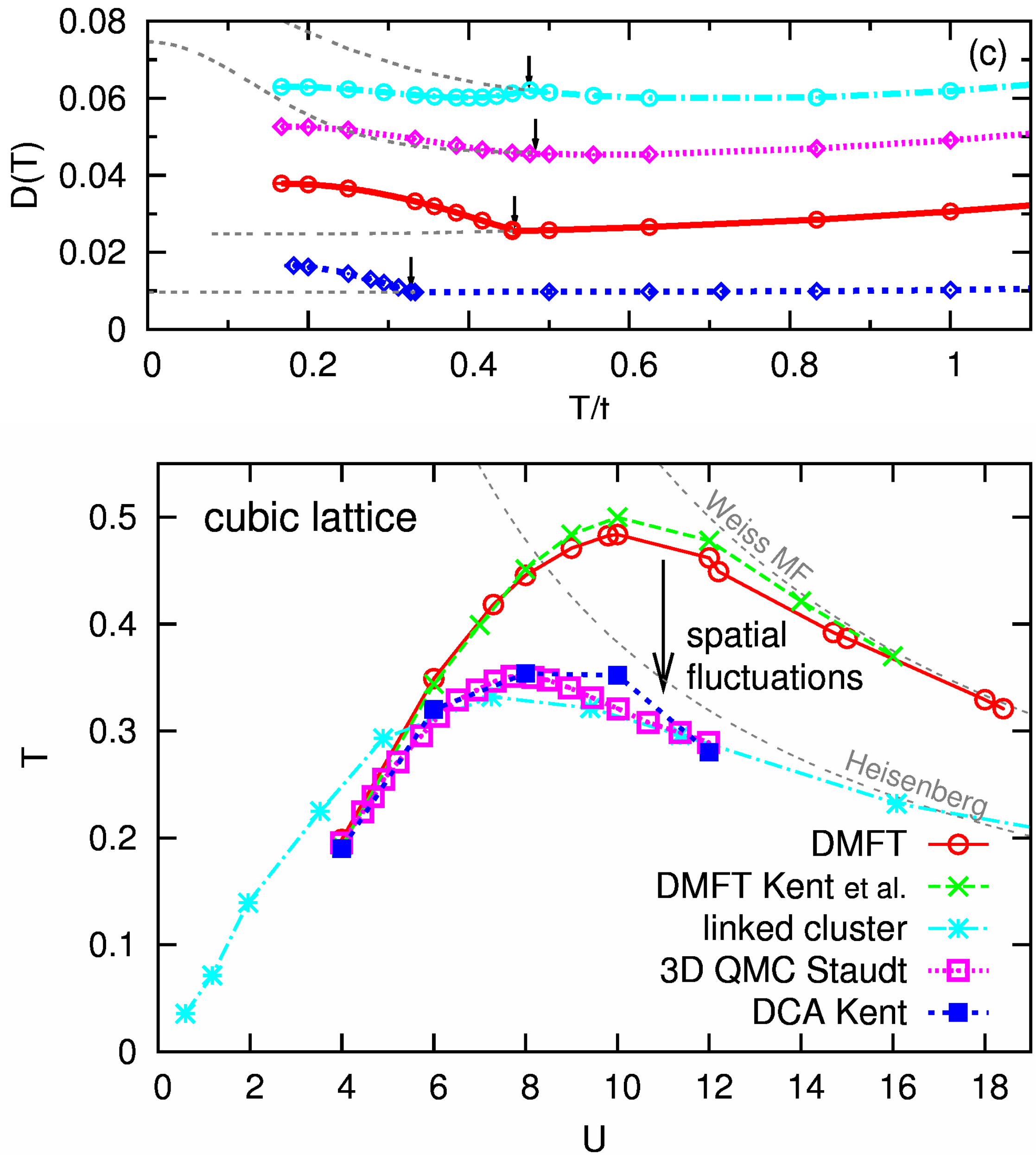

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Constraints:

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

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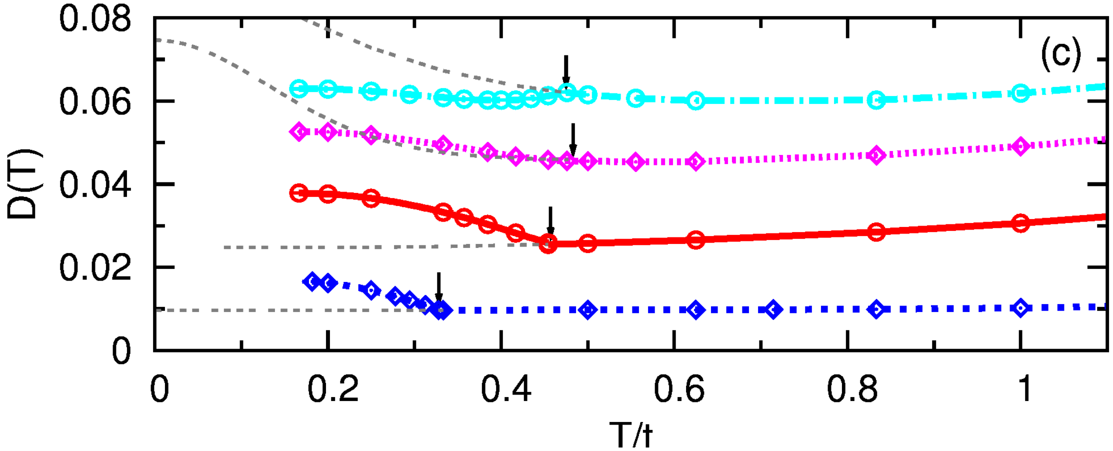

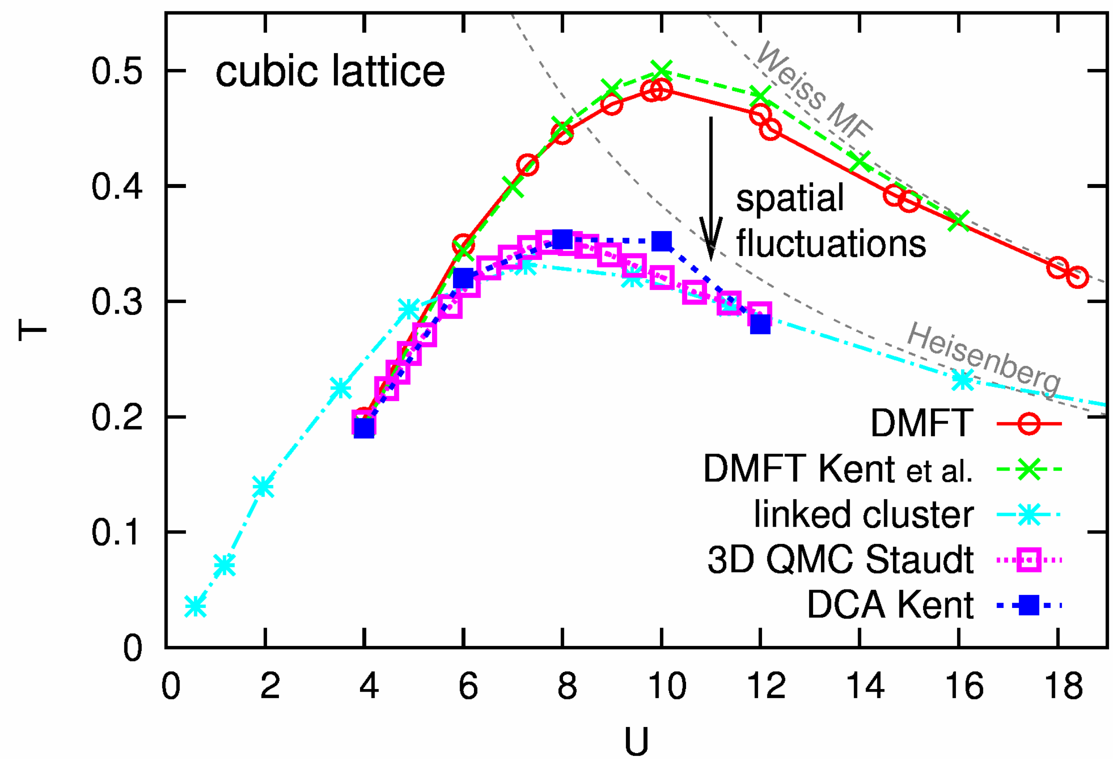

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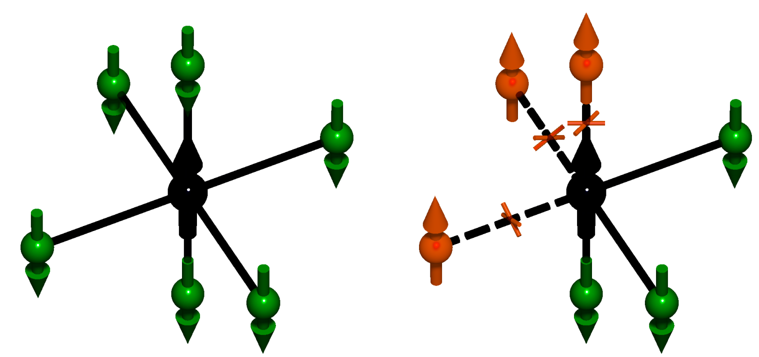
- argument for $D_{\mathrm{AF}}/D_{\mathrm{para}} \xrightarrow{U\to\infty} 2$ is independent of dimension



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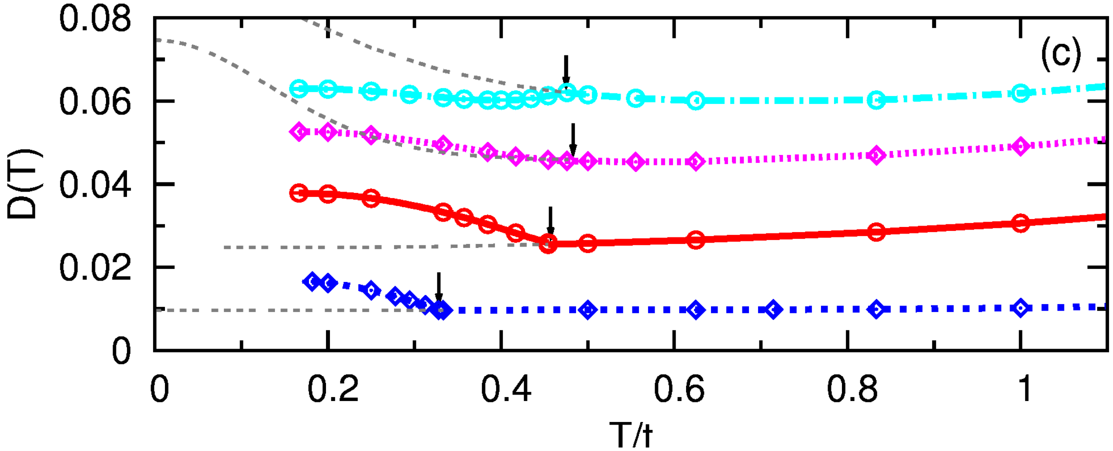

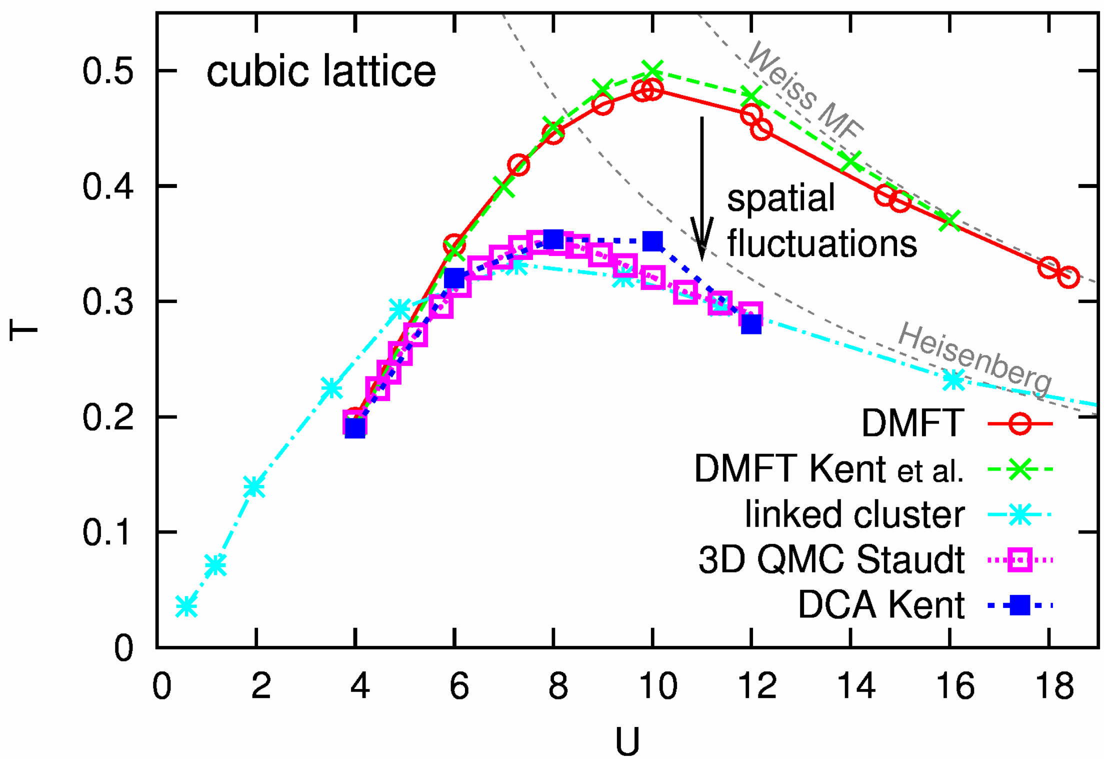

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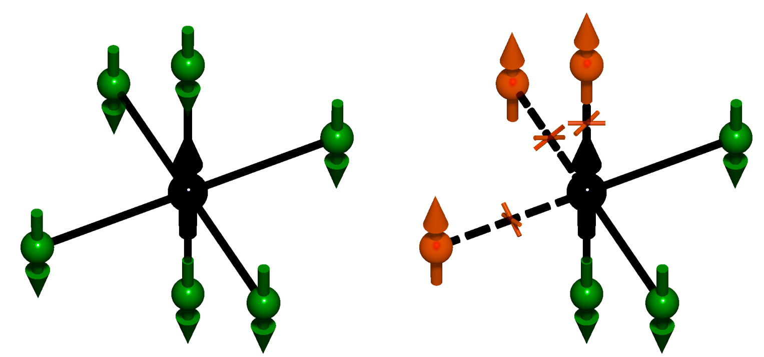
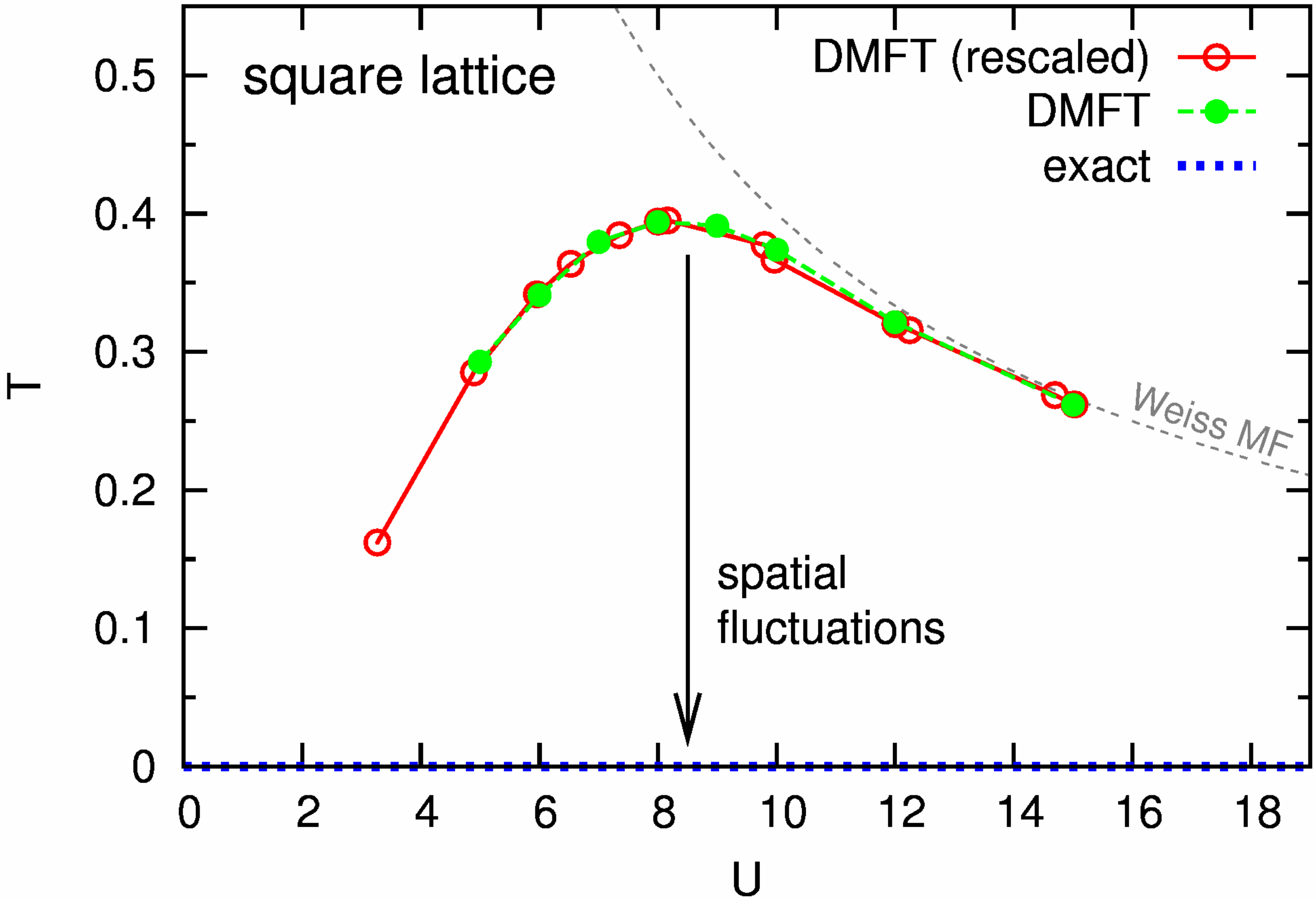


and independ. of long-range order

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

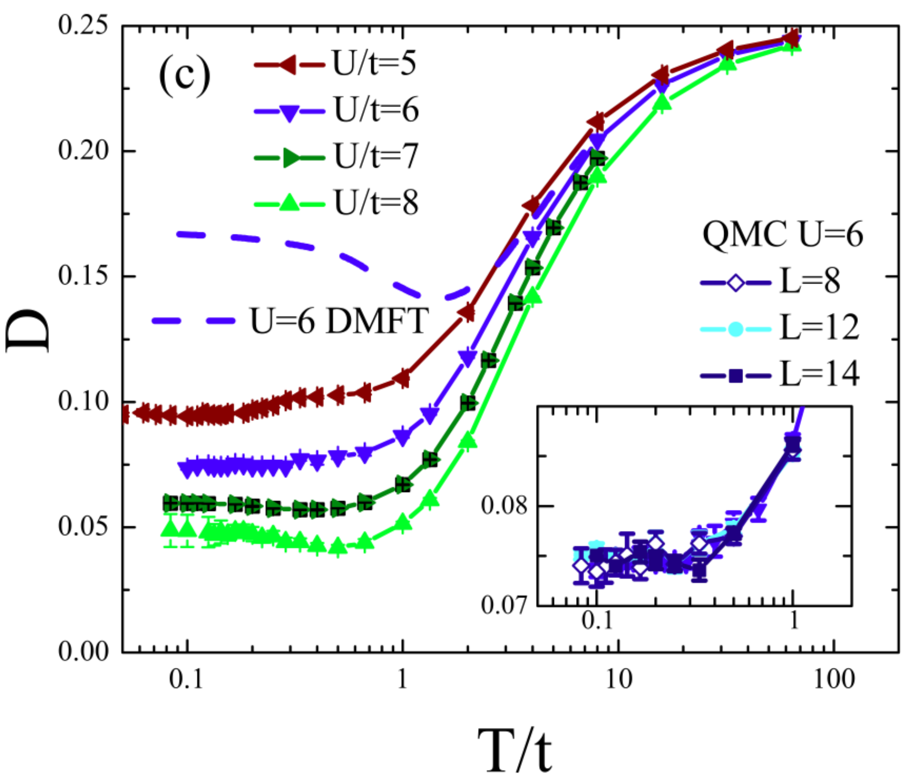


Will any enhancement of D at low T remain? At which temperature scale?

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

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)



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

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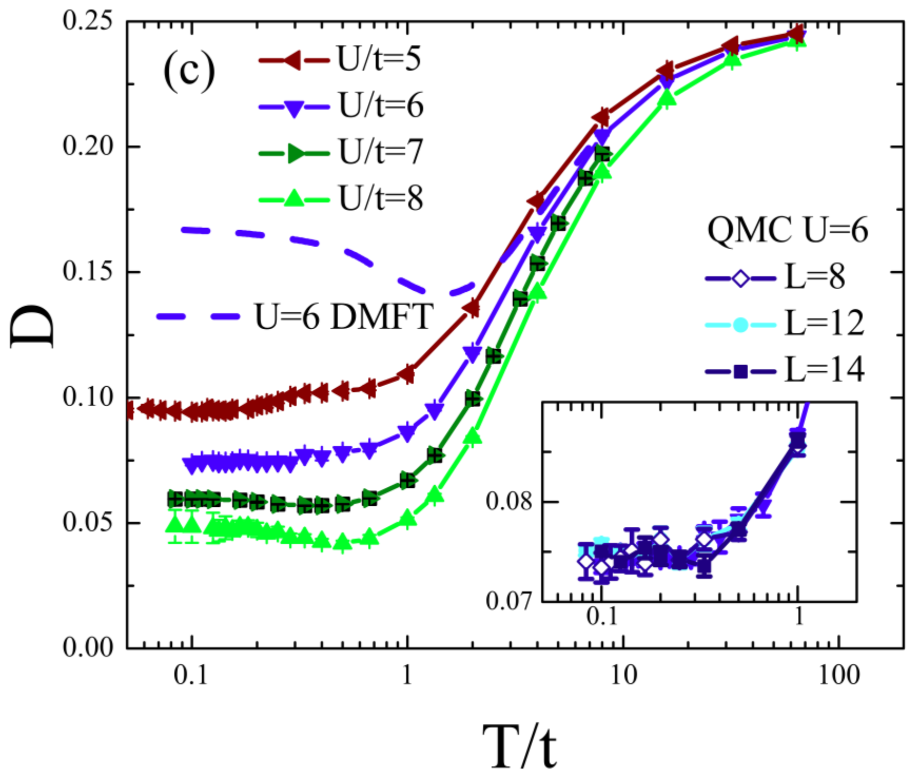
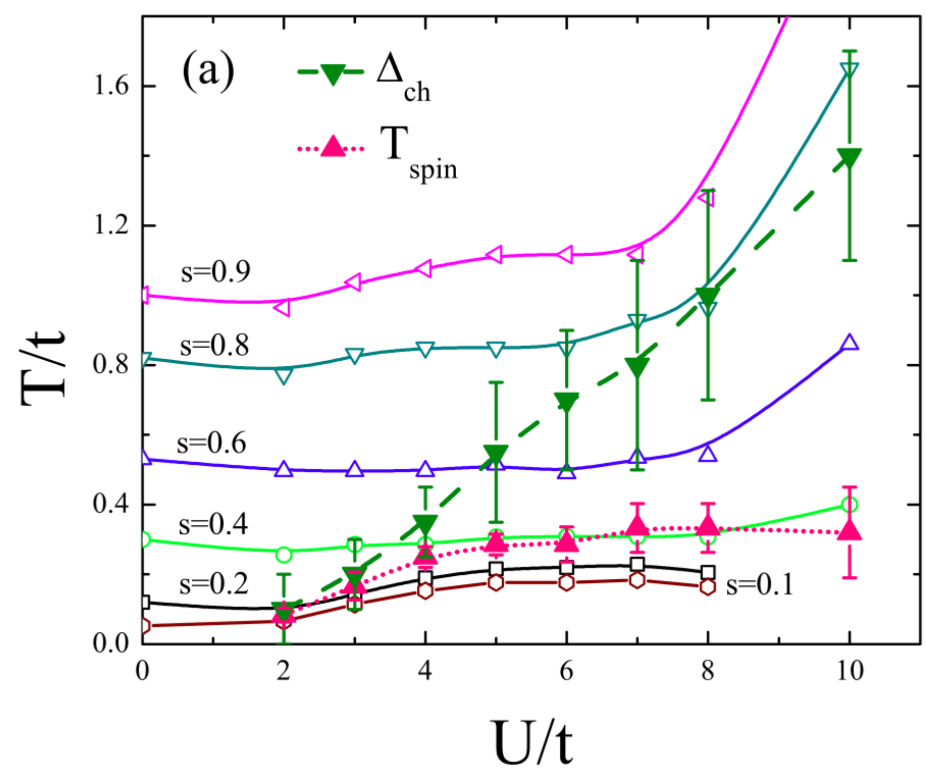
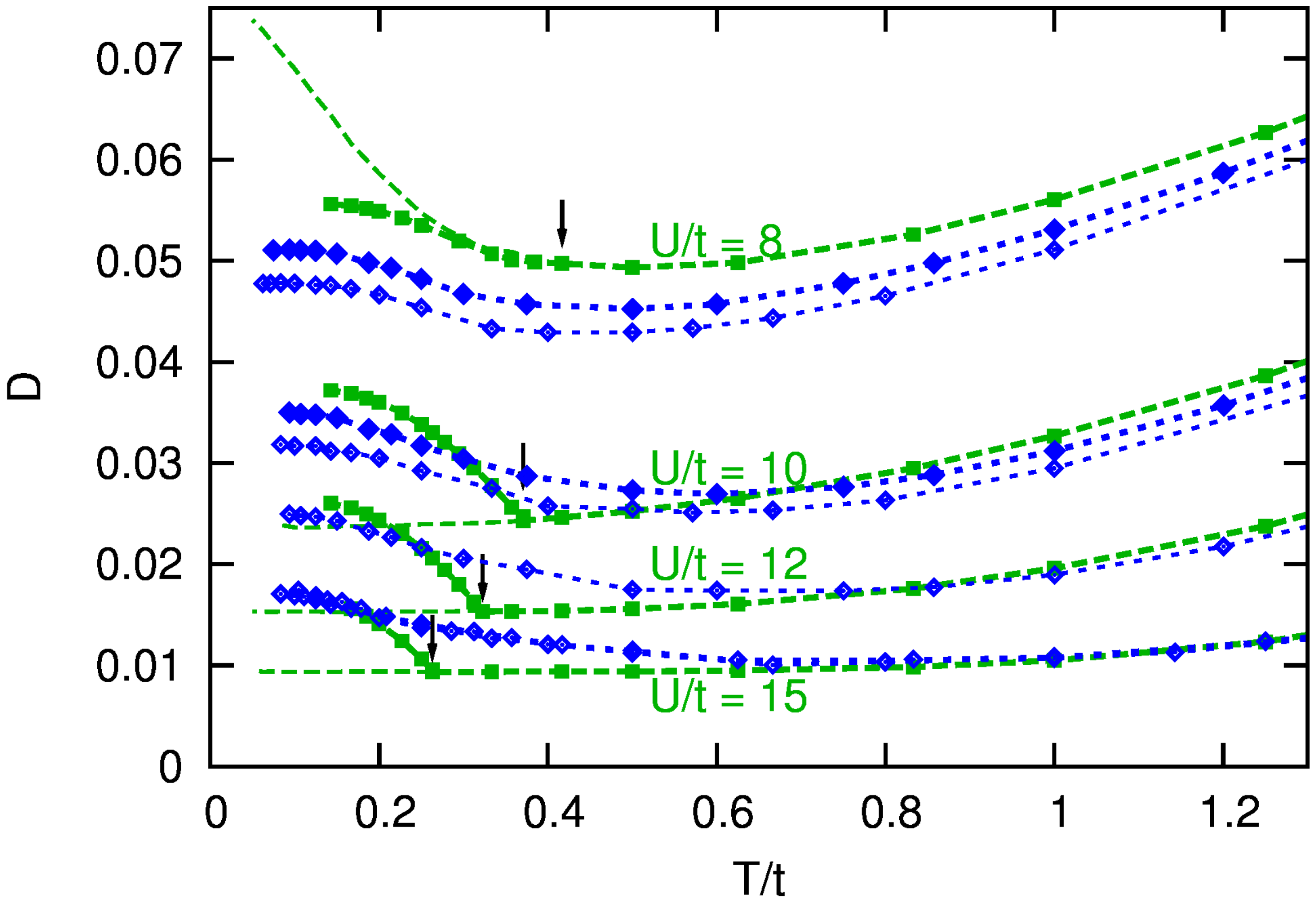




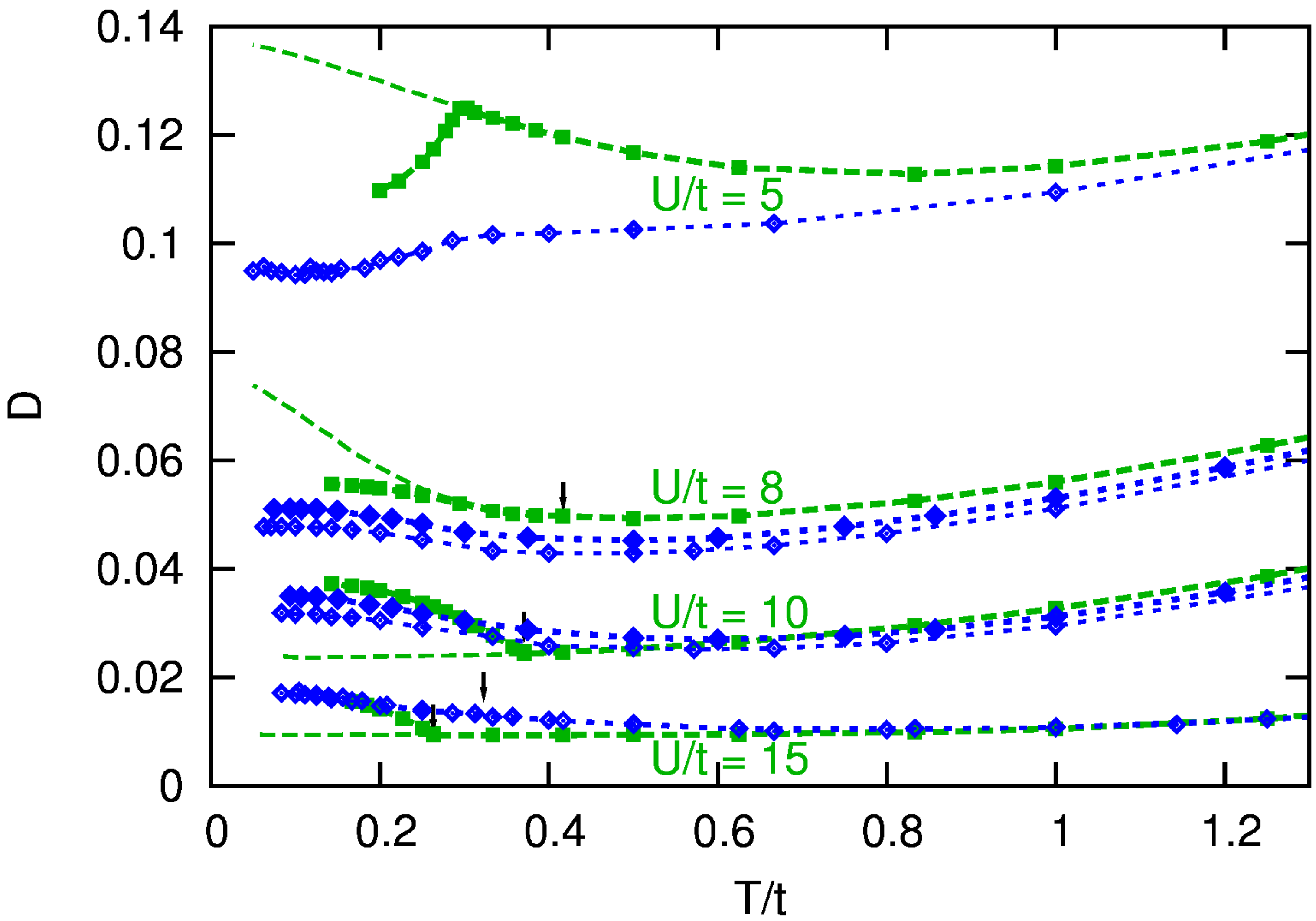
Comparison DMFT – direct QMC for the 2d square lattice ($n = 1$)



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

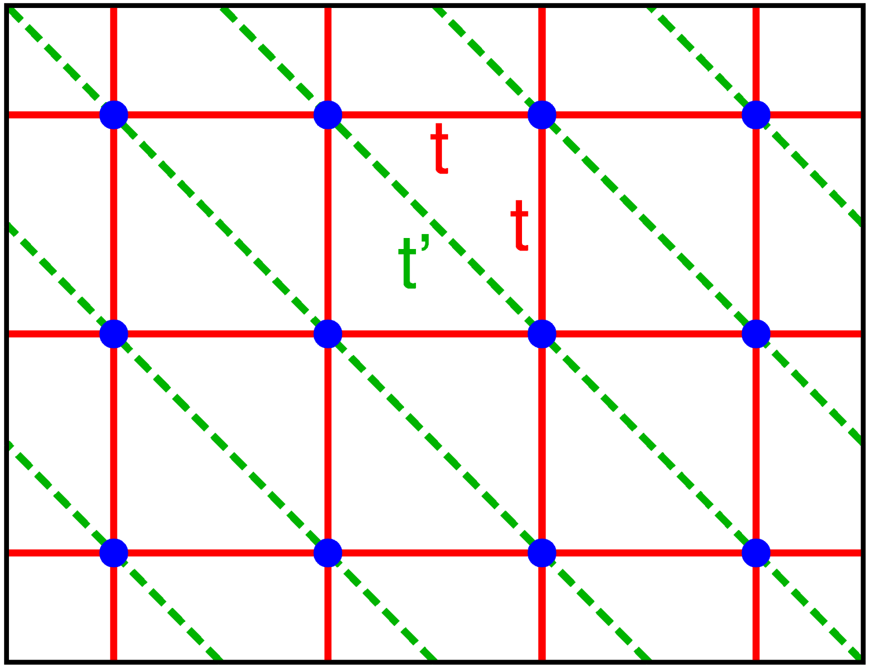
Even the low -T suppression of D at small U corresponds with direct QMC:



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:



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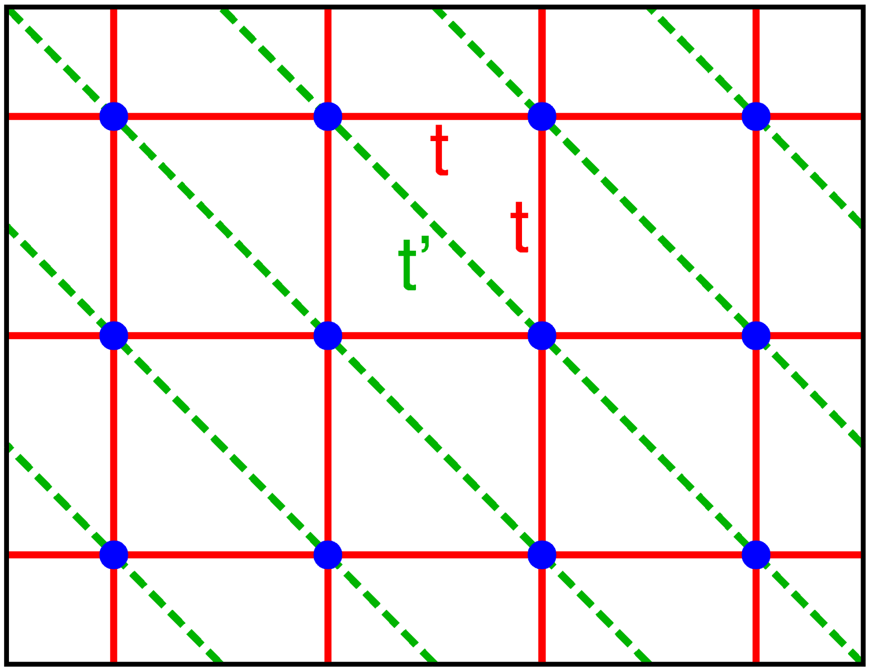

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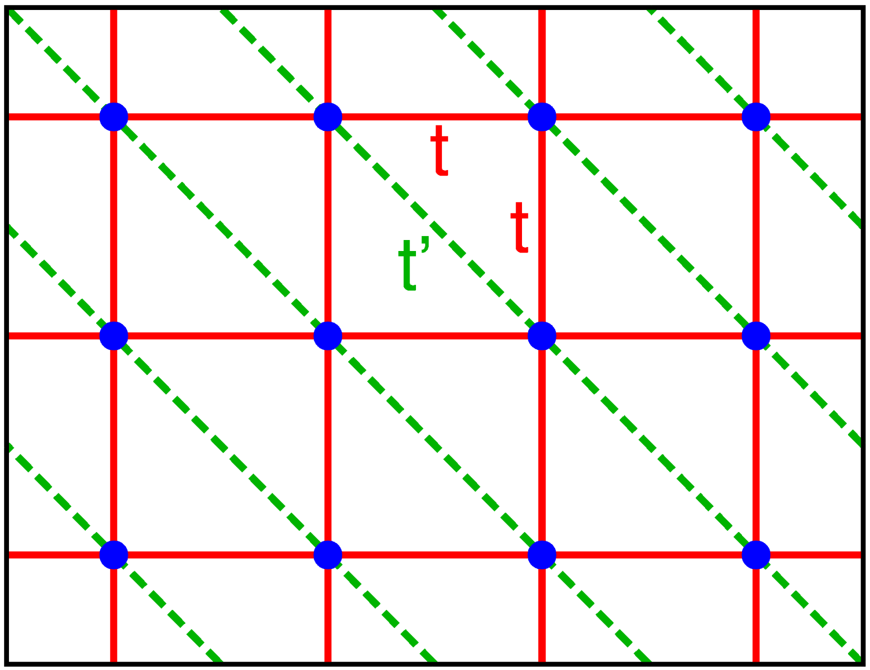

Problem: t' also changes bandwidth

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

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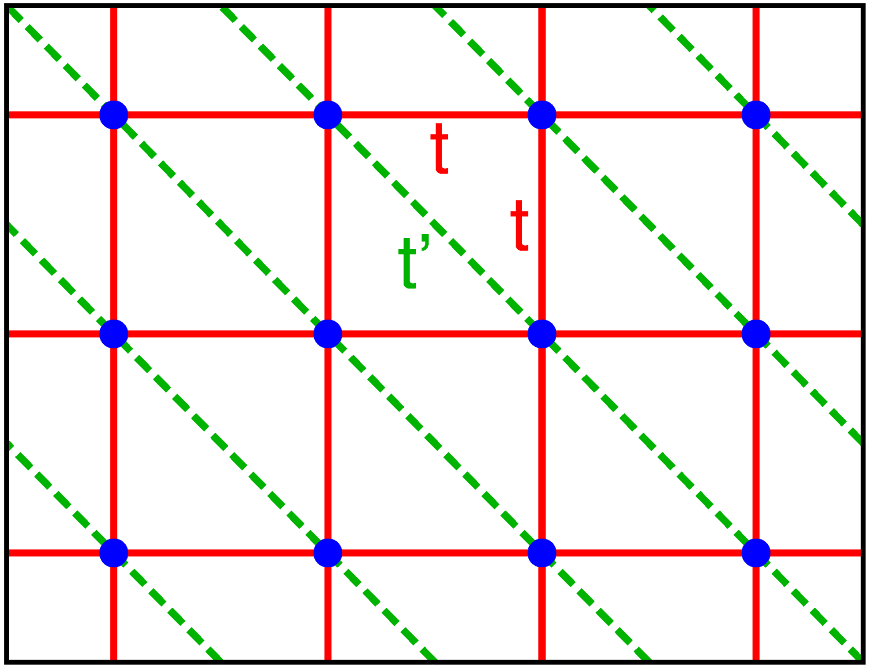

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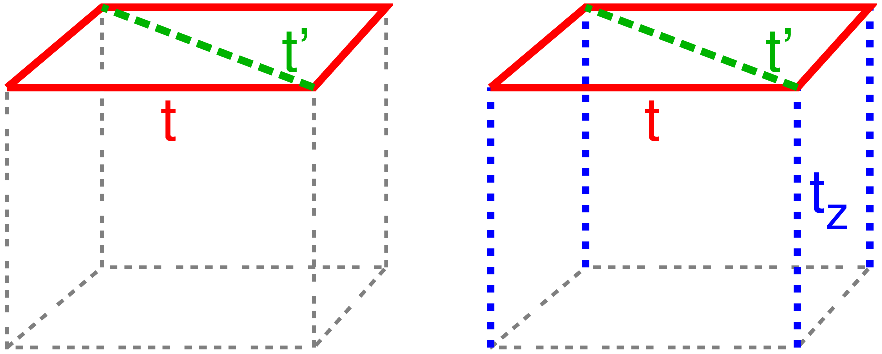
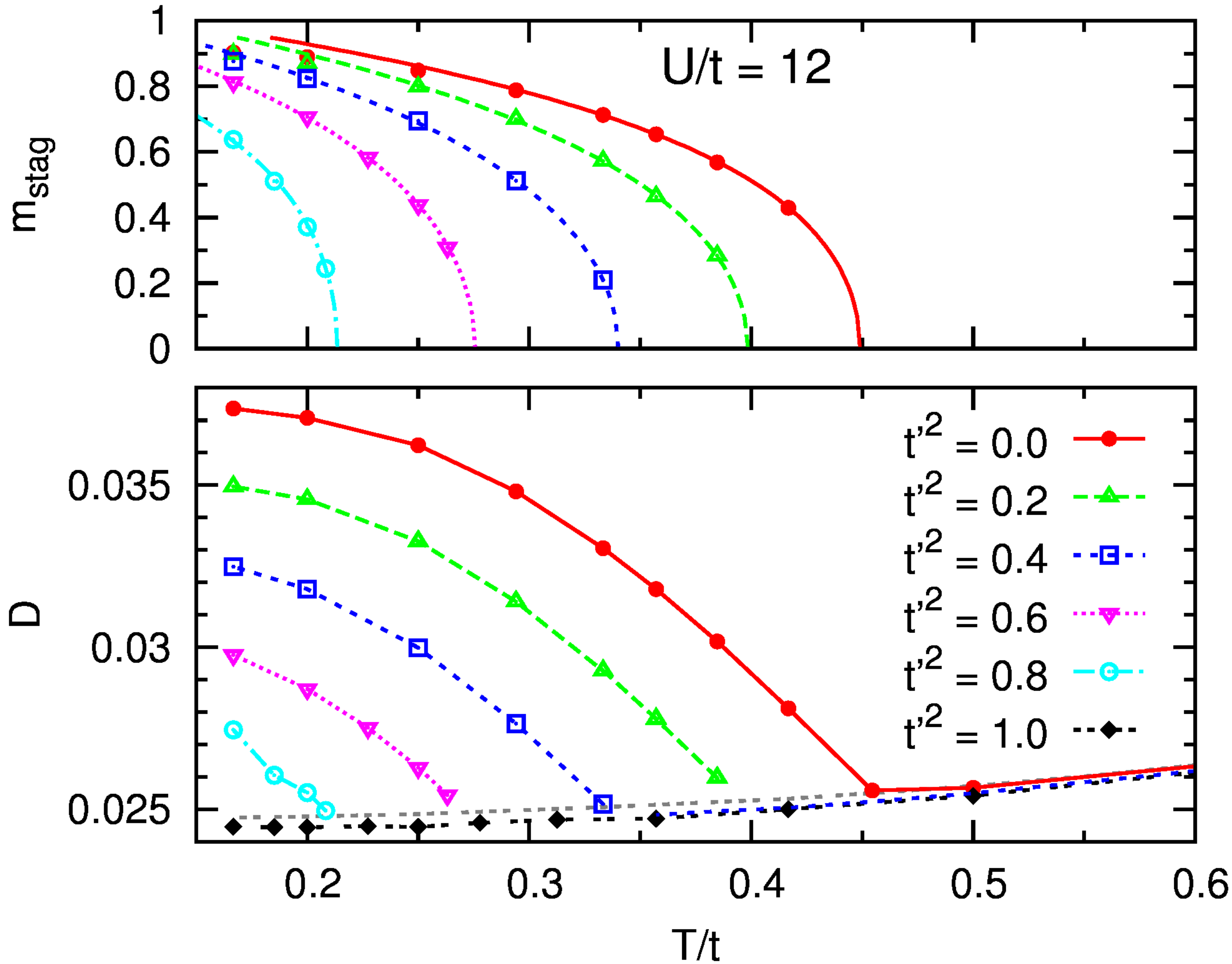
$$\langle \epsilon^2 \rangle \equiv \int_{-\infty}^{\infty} d\epsilon \, \epsilon^2 \rho_0(\epsilon) = 4t^2 + 2t'^2$$

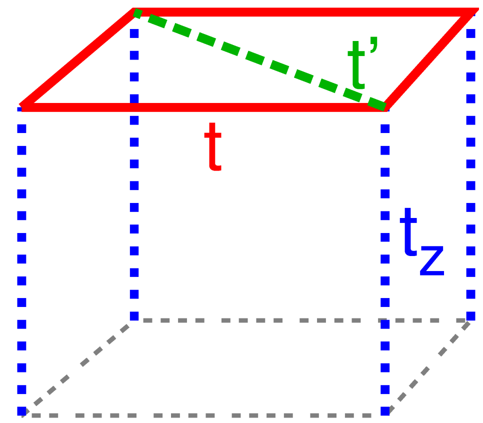
Solution: add third dimension
and hopping t_z between planes



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

Tuning the frustration from the cubic to the triangular lattice

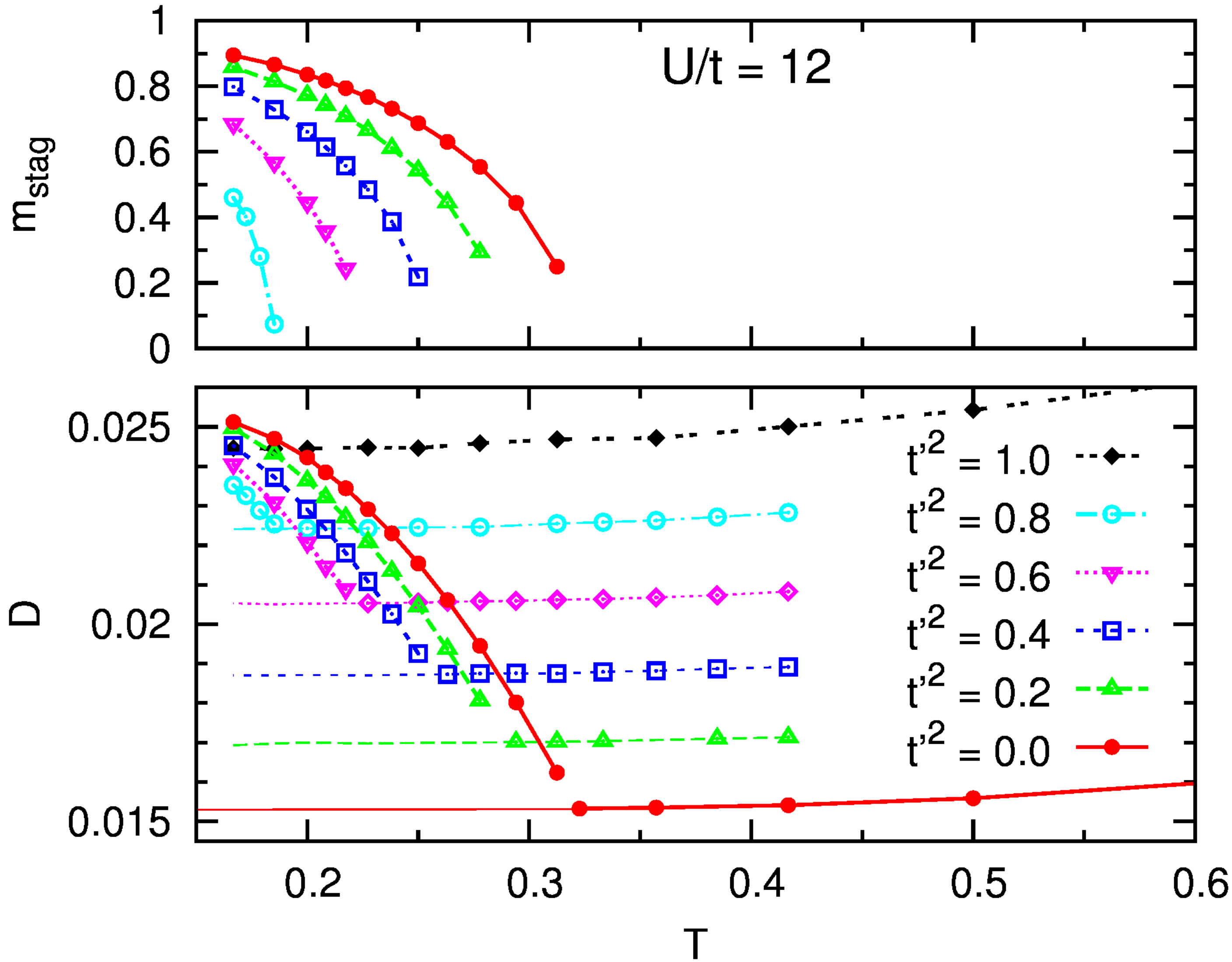


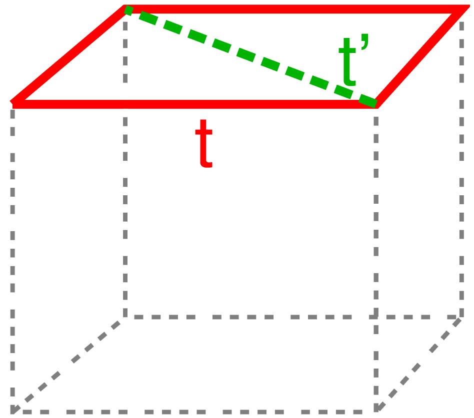


D suppressed before AF breaks down

paramagnetic phase hardly affected by t'

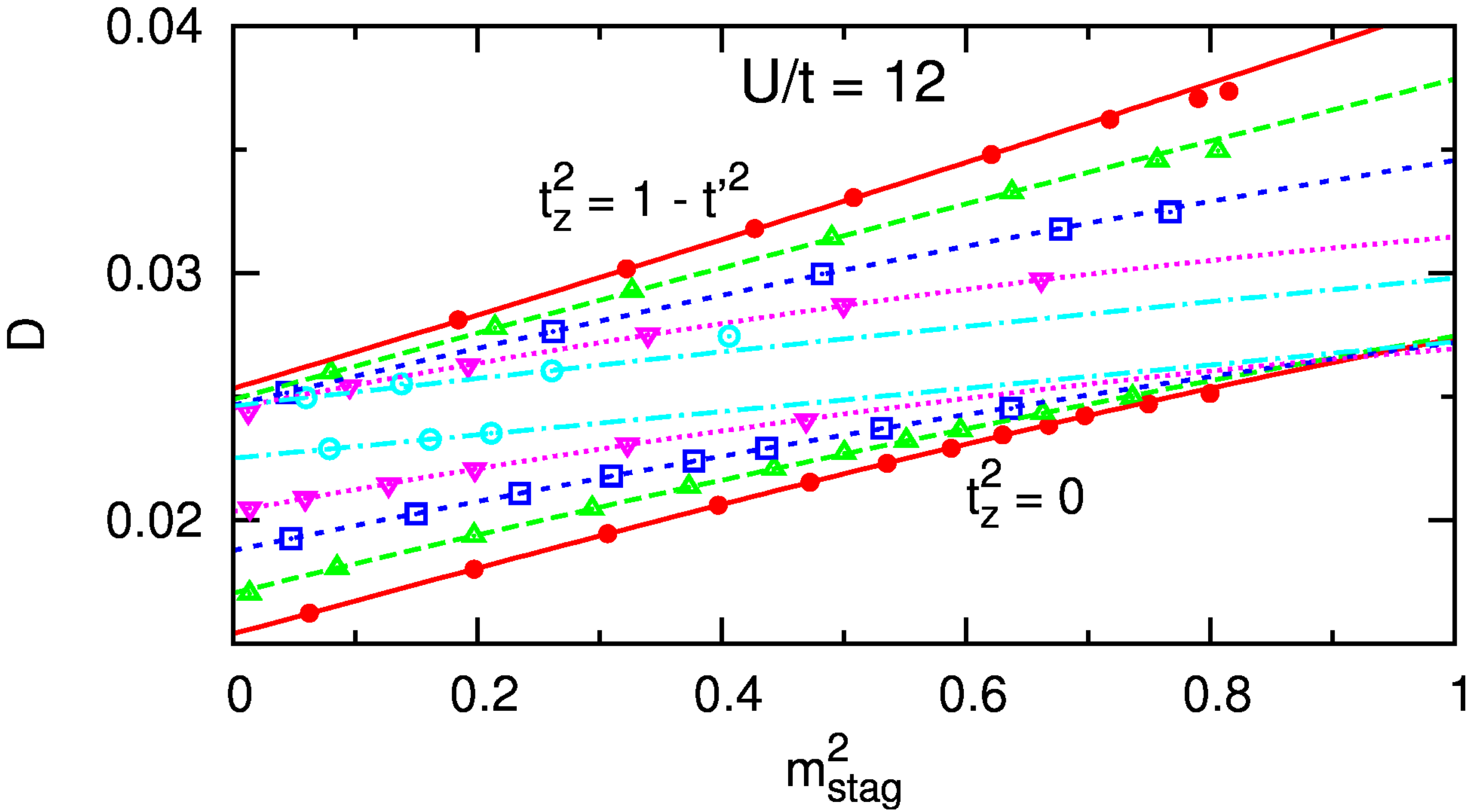
Tuning the frustration from the square to the triangular lattice





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

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

*Related proposal: measure $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ via D creation rate in modulation spectroscopy

[Jordens et al., Nature **455**, 204 (2008); Sensarma, Pekker, Lukin, Demler, PRL **103**, 035303 (2009)]

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)

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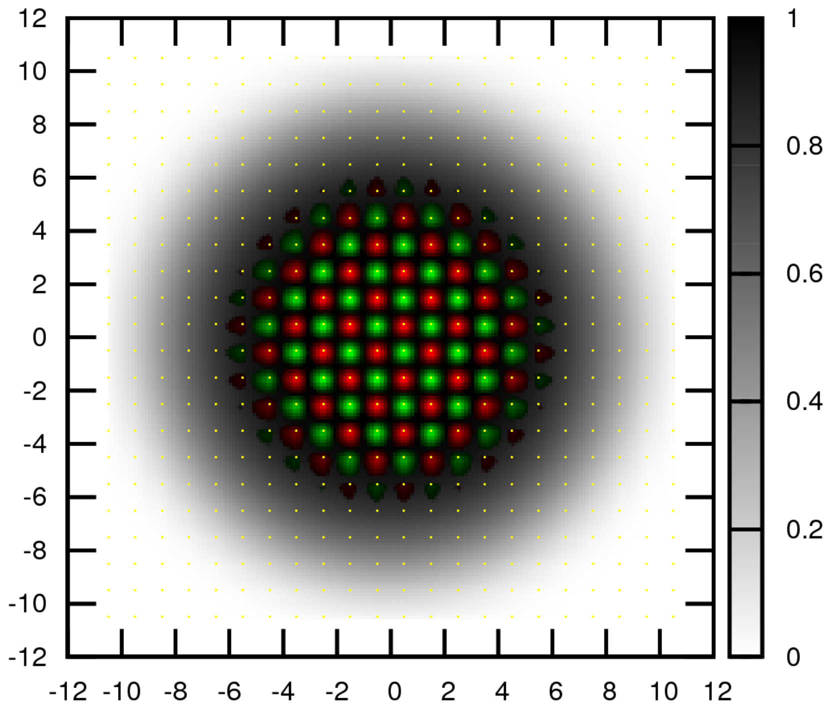
Practical (dense inversion, fully parallel): $\lesssim$ 10000 sites $\rightsquigarrow$ need smart strategies



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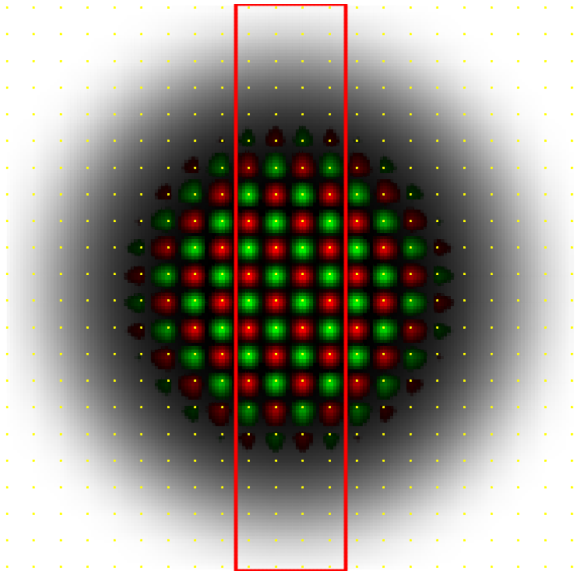

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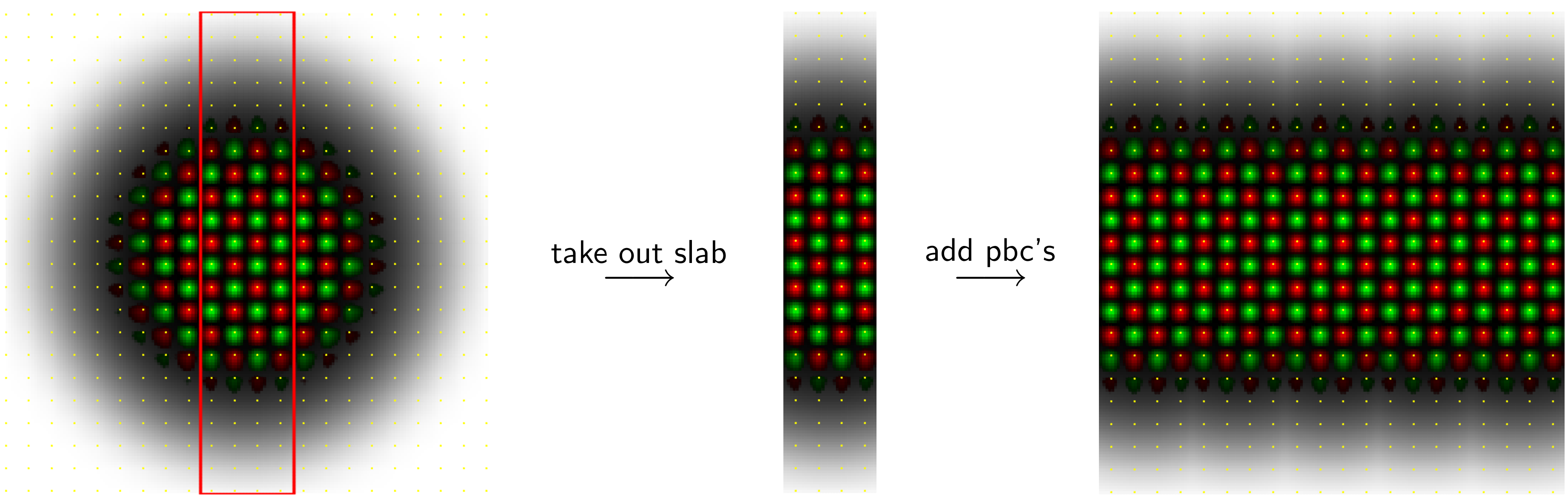
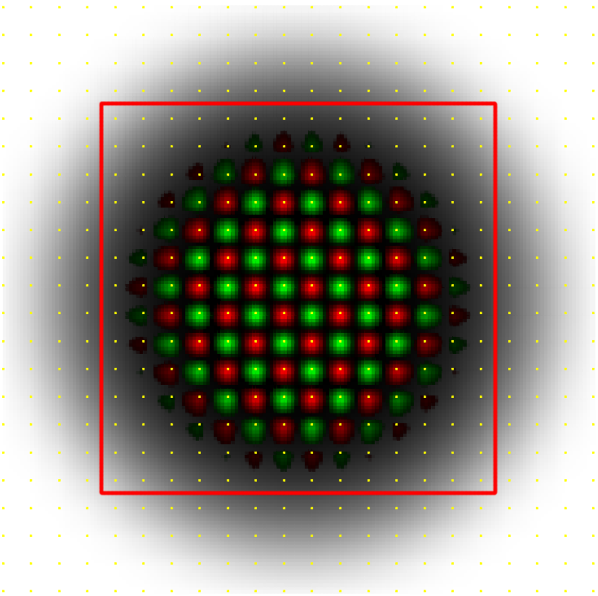
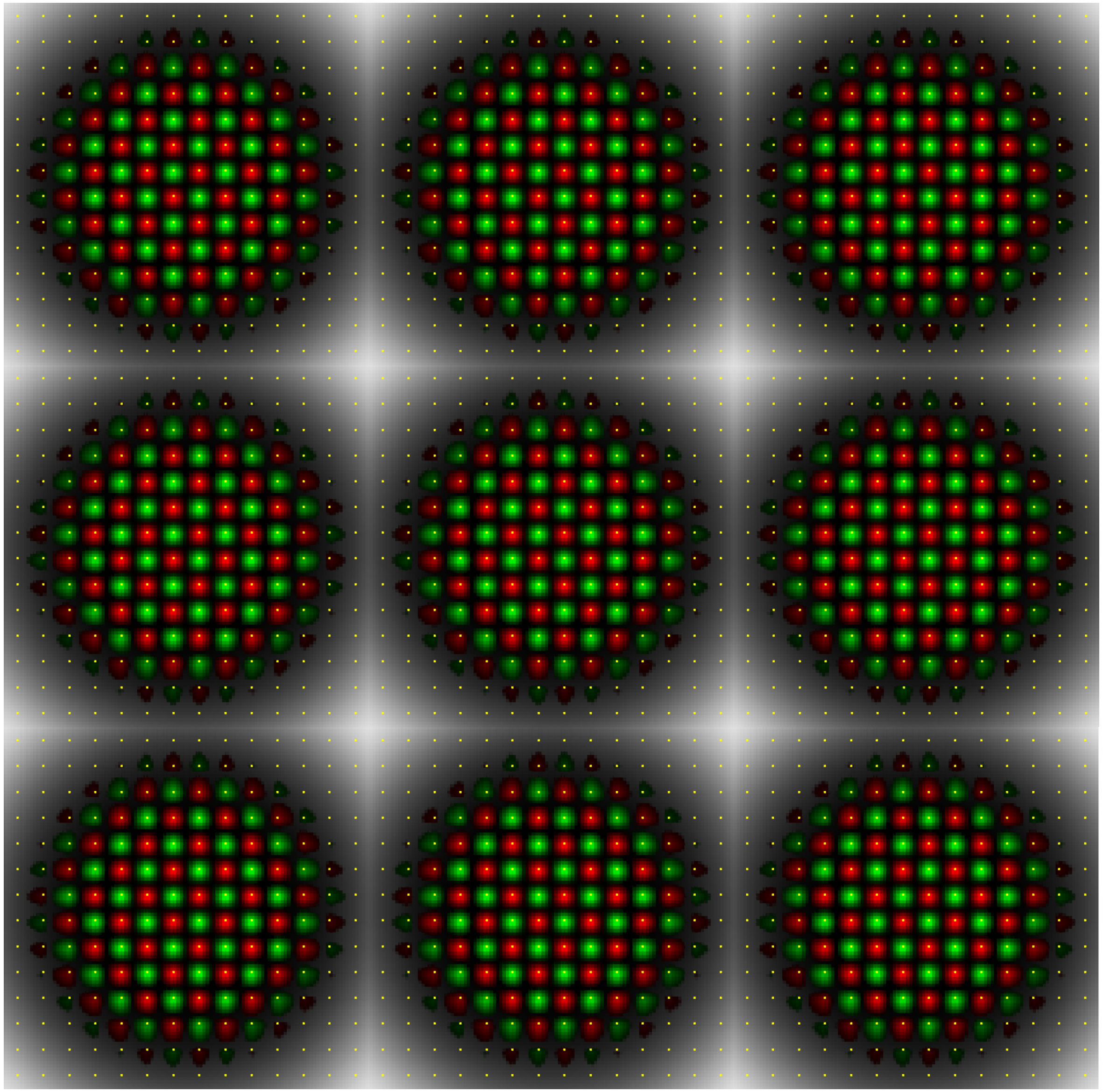


In practice: cylindrical potential (equivalent layers)

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

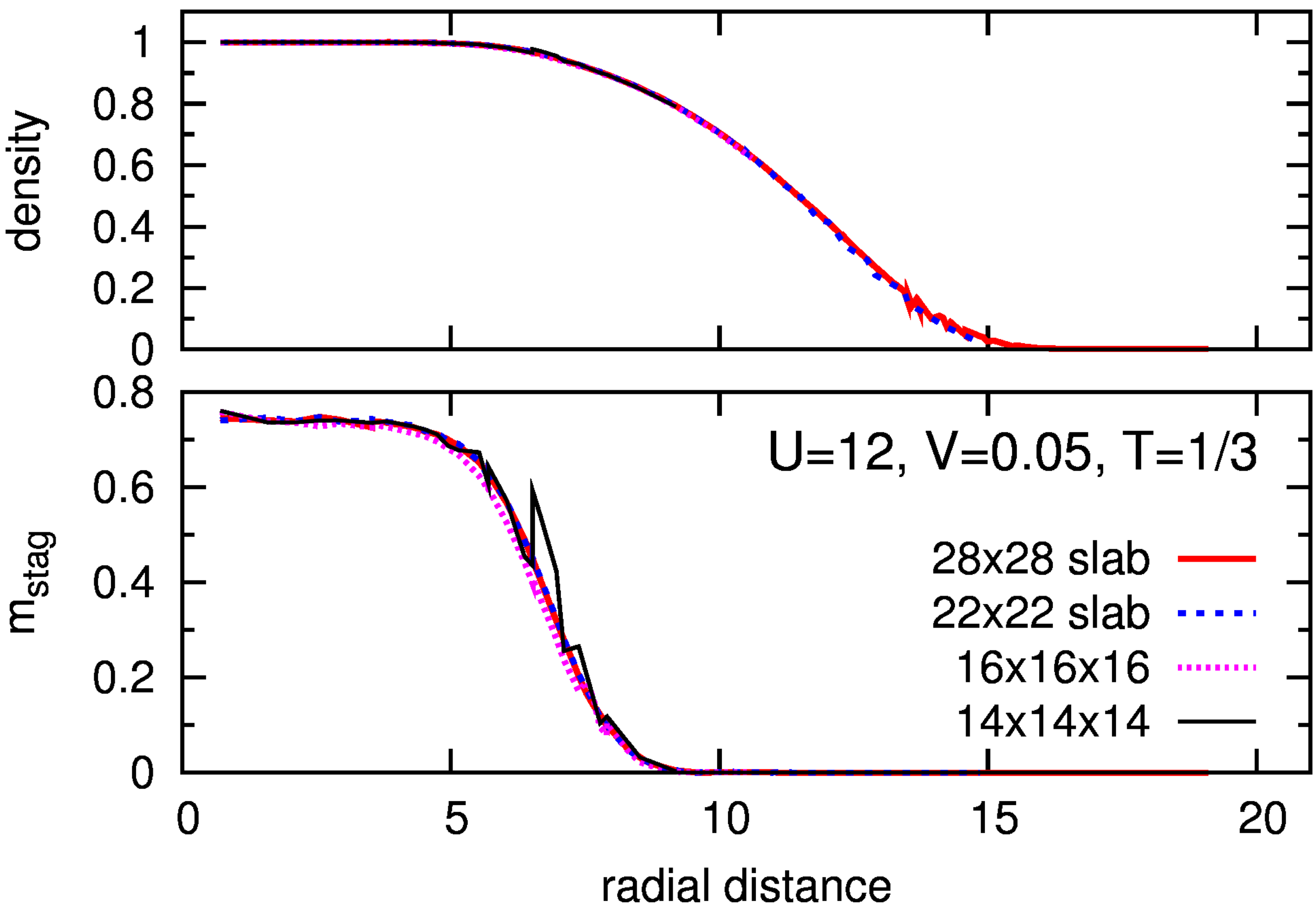


$\longrightarrow$



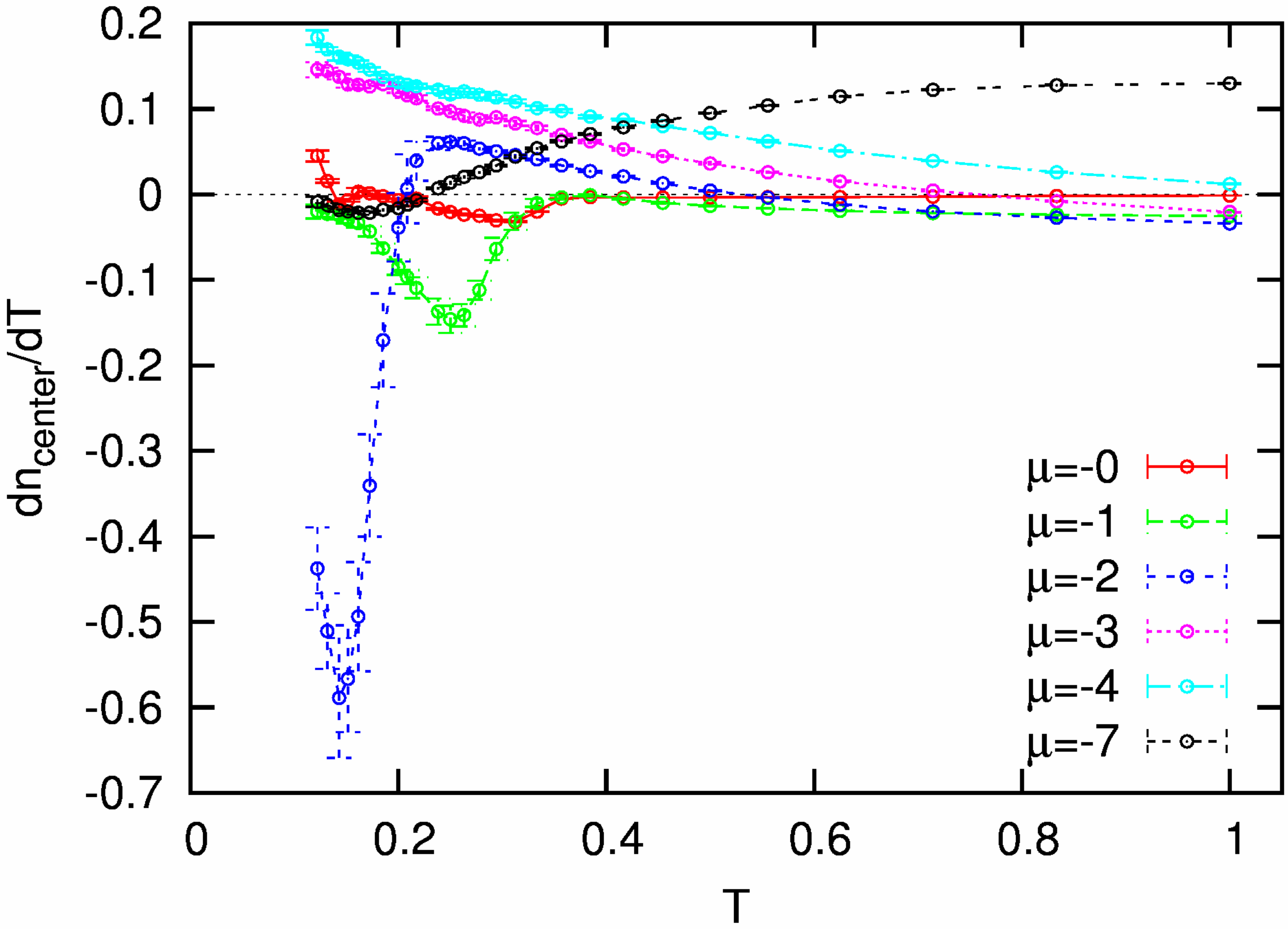
Most efficient: slab calculation focussing on AF core (with pbc)

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



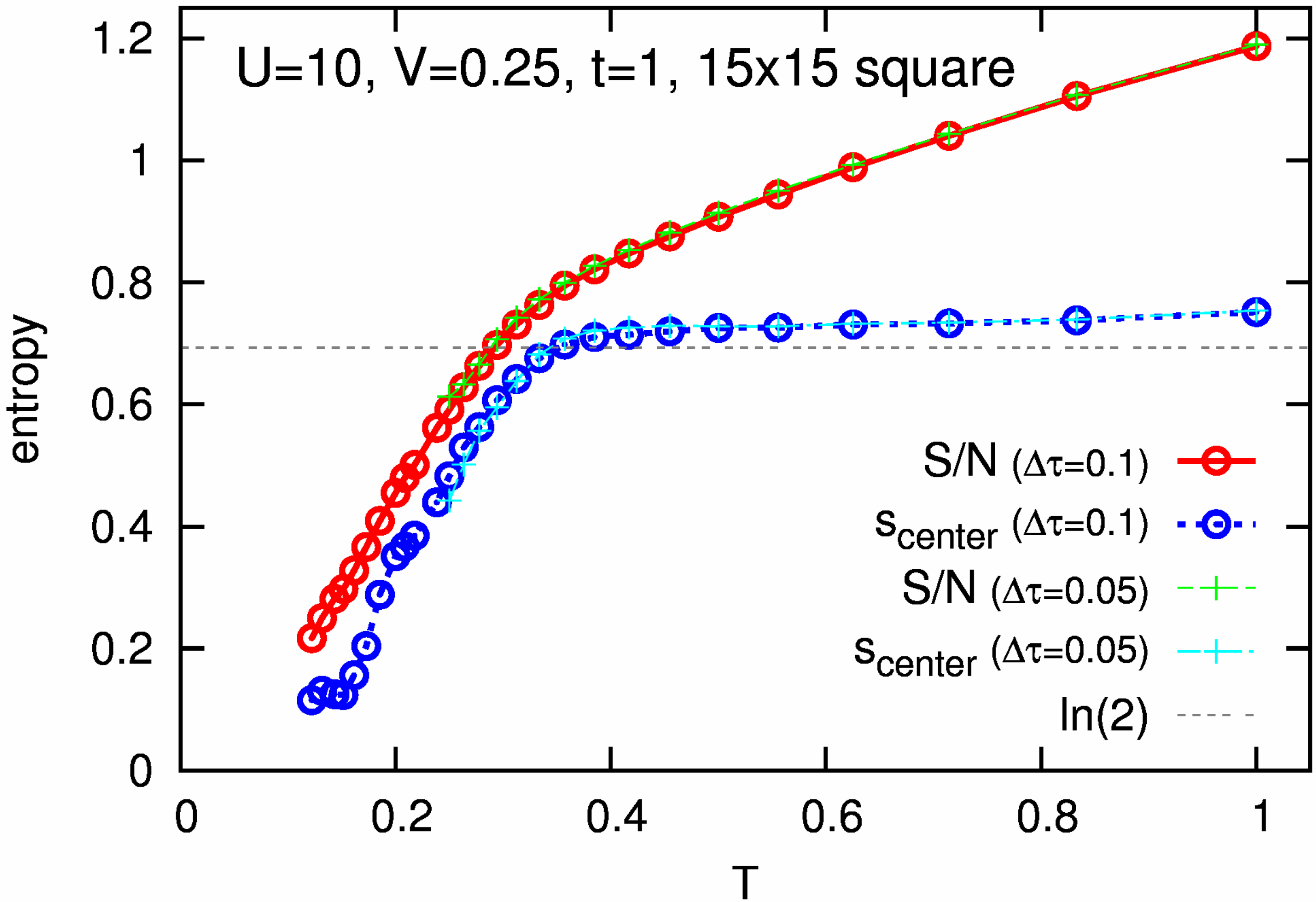
Significant deviations only if core touches boundaries!

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

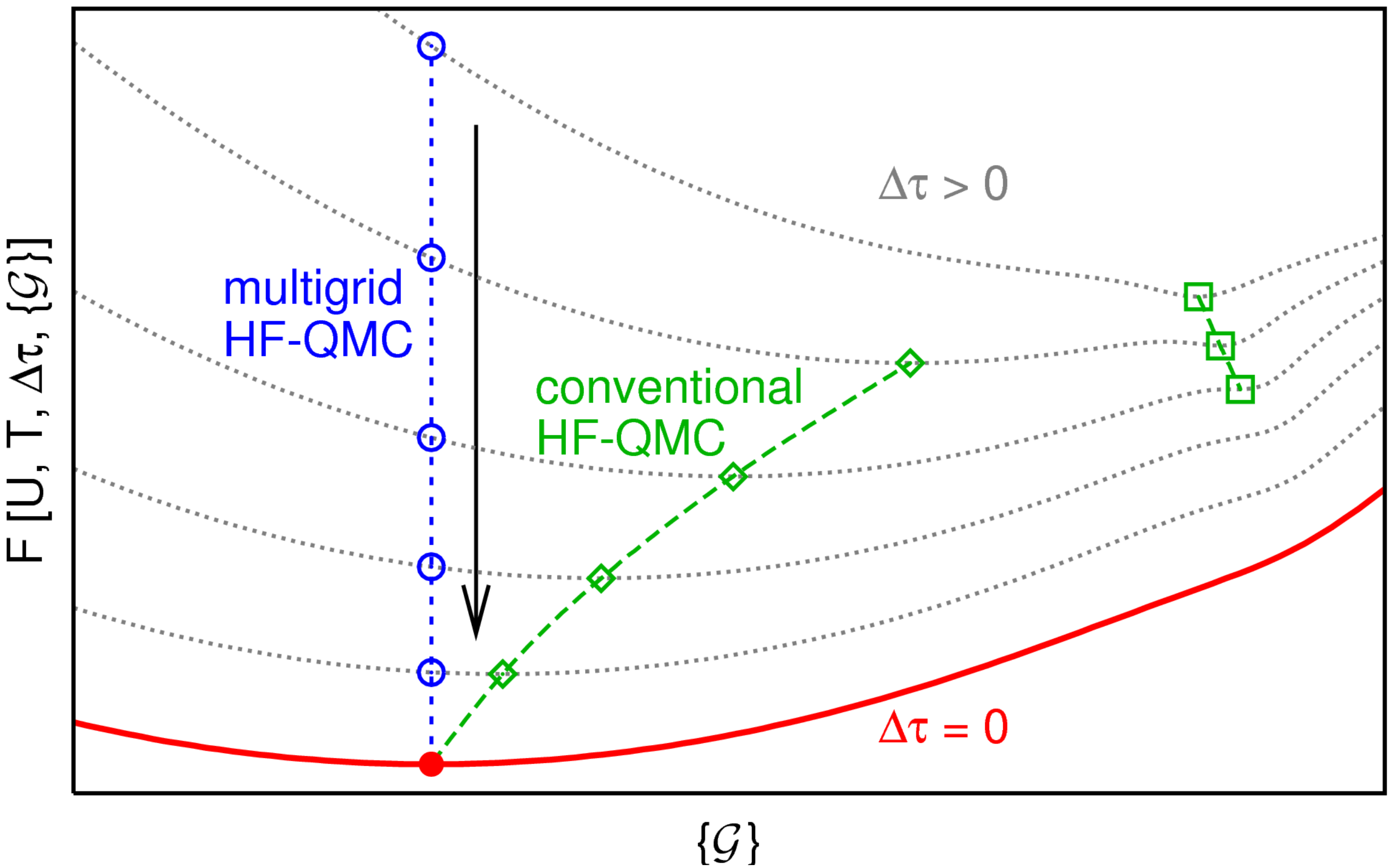
Strong negative peak at Neel temperature ($\rightsquigarrow$ need fine integration grid)



very small discretization dependence

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

Schematic comparison via generalized Ginzburg-Landau functionals



Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

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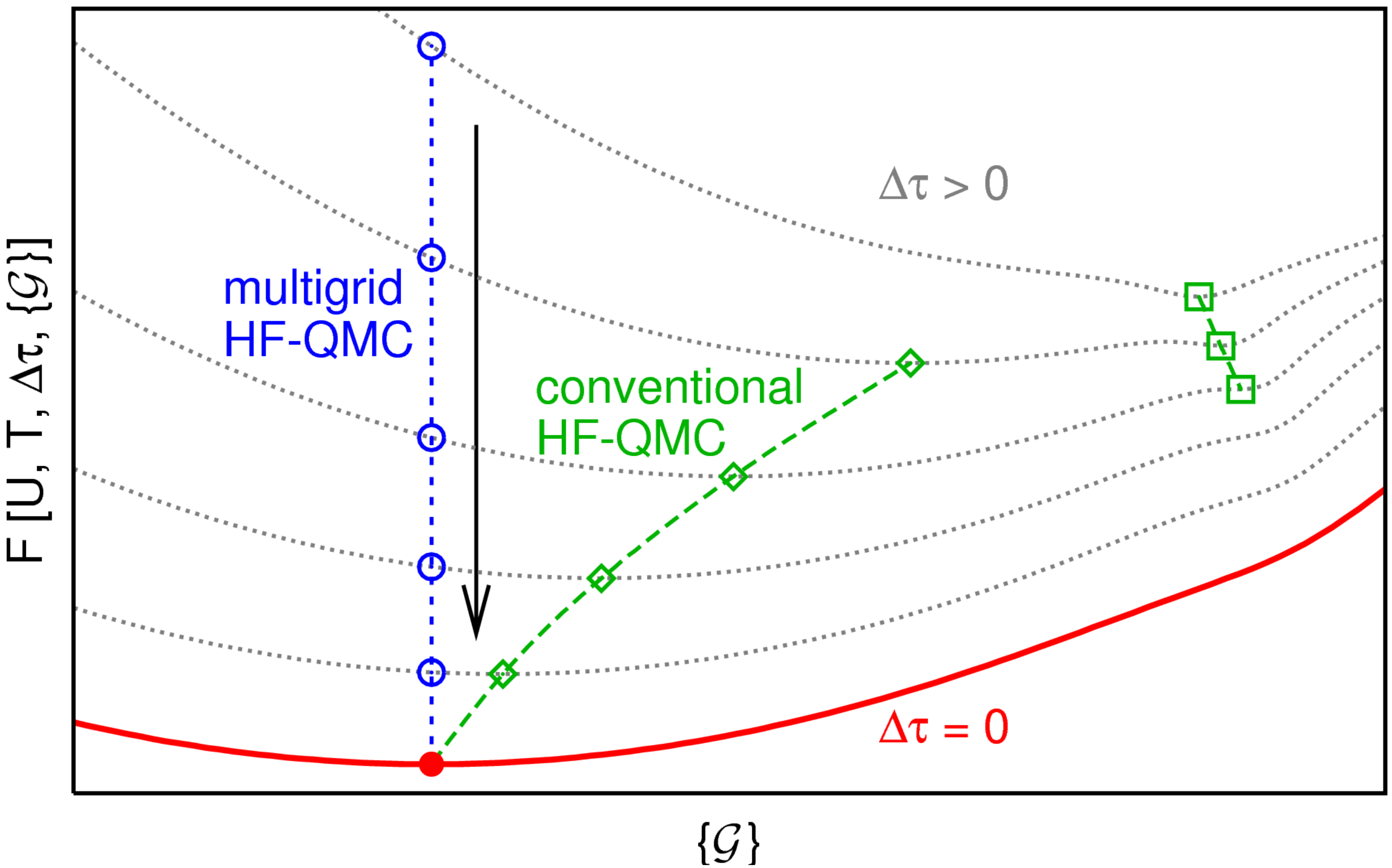
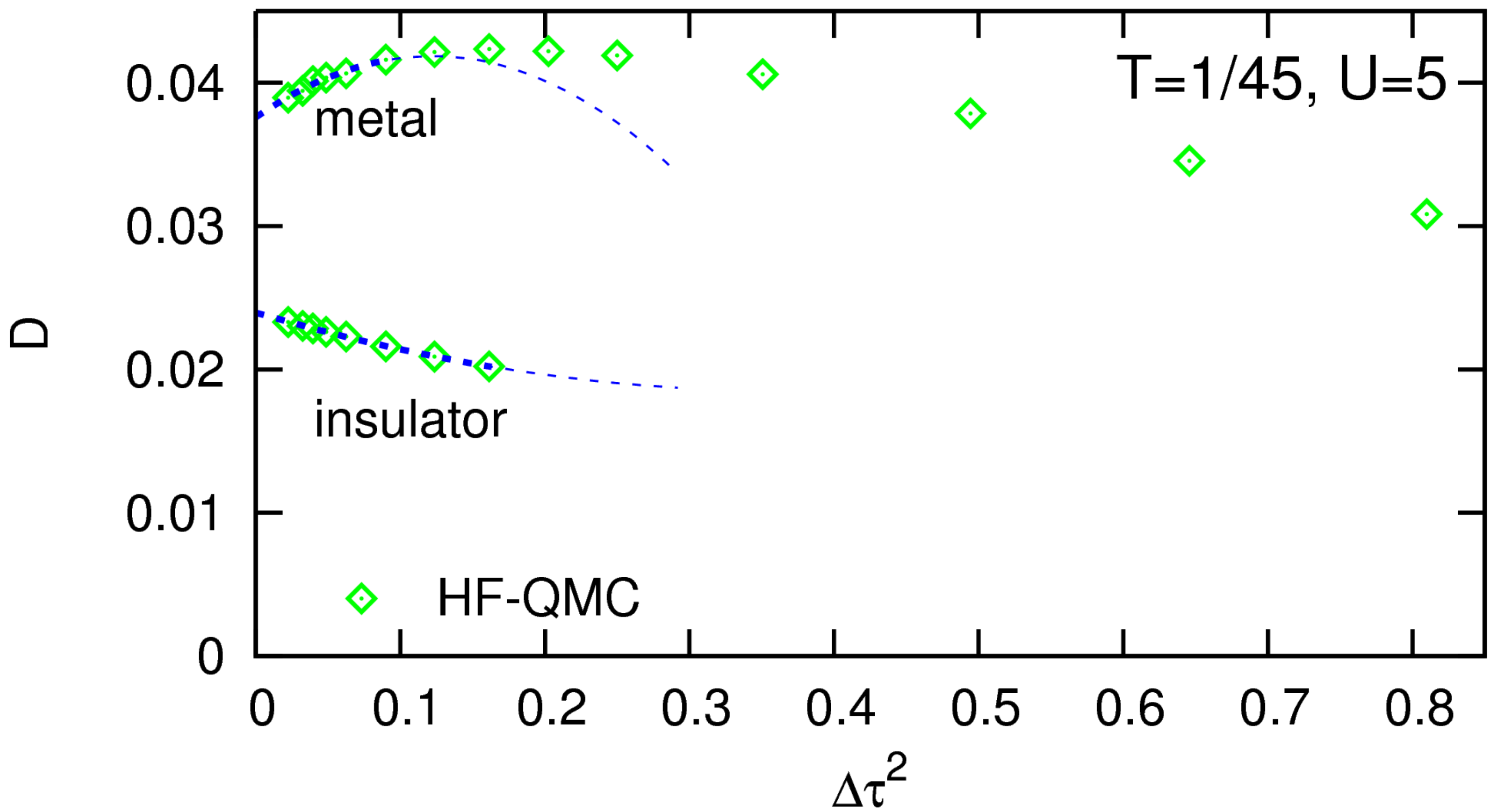


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

Implementation: Green function extrapolation, hierarchy of frequency scales

Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$

very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

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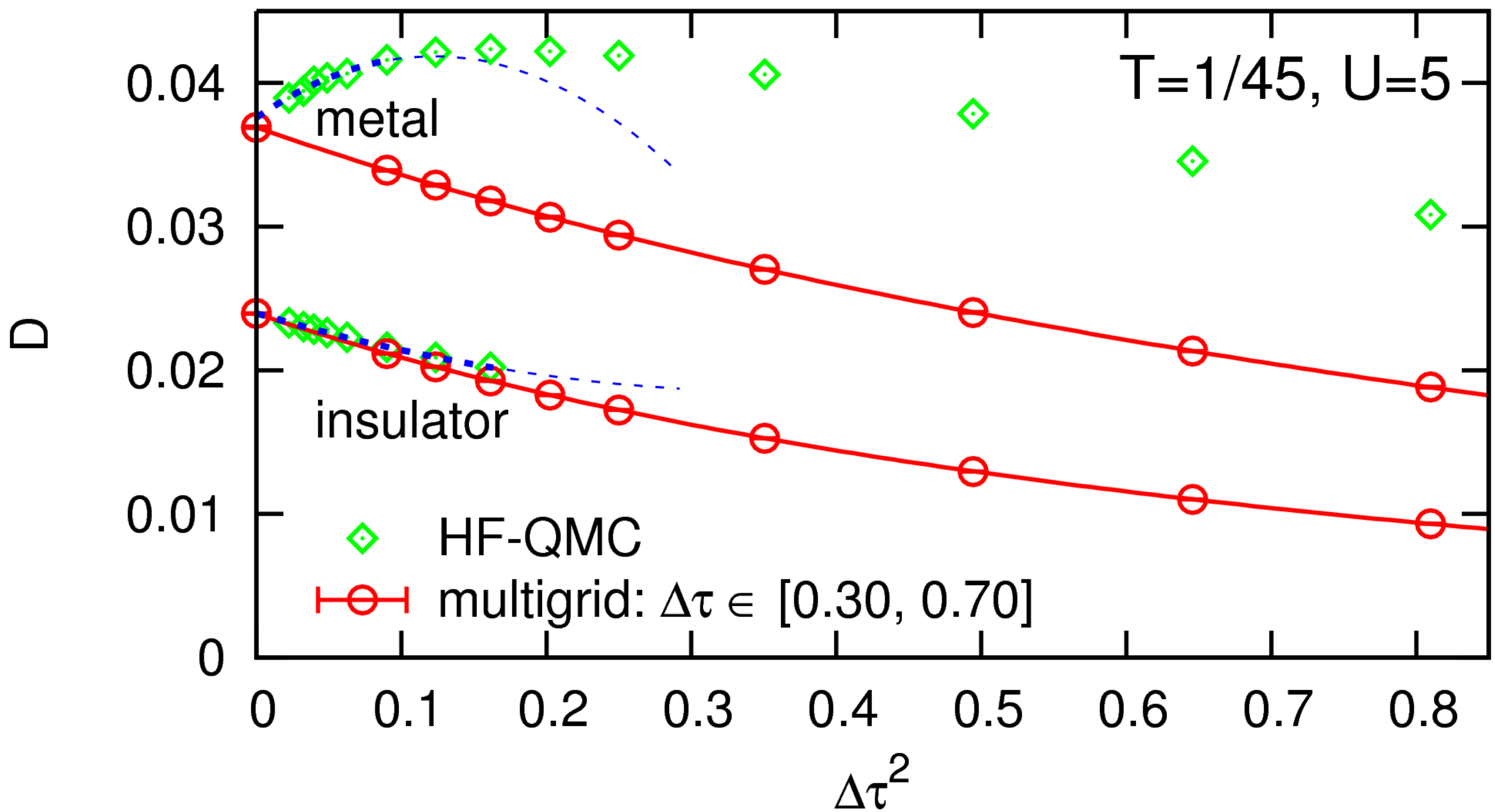

Conventional HF-QMC:	no insulating solution for $\Delta\tau \gtrsim 0.4$
	very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$
Multigrid HF-QMC:	vastly larger useful range of $\Delta\tau$