Discriminating AF signatures in ultracold fermions using tunable dimensionality and geometric frustration

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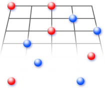
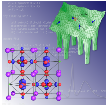
[Gorelik et al., Phys. Rev. A **85**, 061602(R) (2012)]

[Chang et al., arXiv:1306.4687, to appear in Phys. Rev. B]



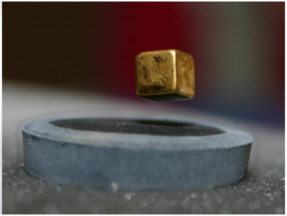
TR 49: *Condensed matter systems with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

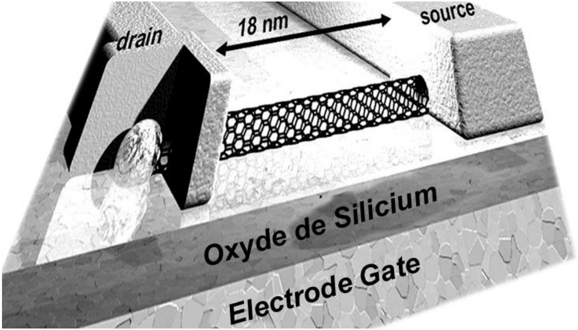
FOR 1346
LDA+DMFT
Augsburg *et al.*



Motivation: materials science, correlation phenomena

When and why are materials metallic, colored, magnetic, superconducting?





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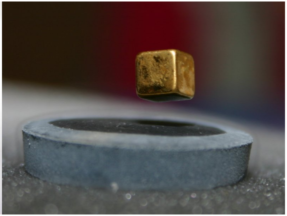
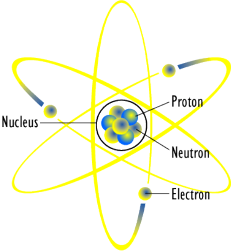
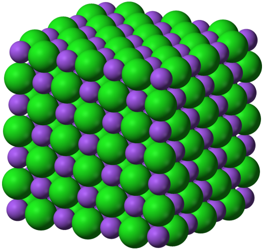


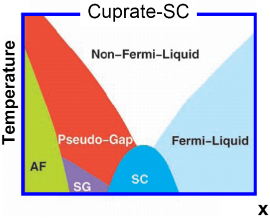
Structure: atoms (nuclei + electrons) in periodic arrangement



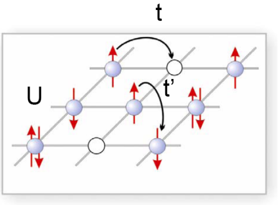


Motivation: Ultracold lattice fermions as quantum simulators?

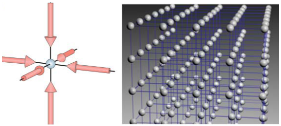
Correlated materials



Fermionic Hubbard model



Ultracold fermions on optical lattices



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

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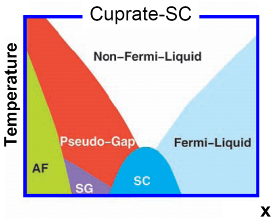

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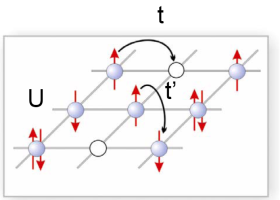

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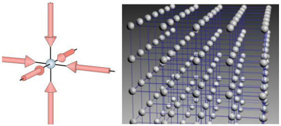


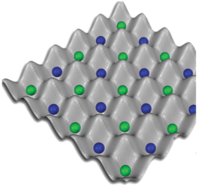
$\mathcal{O}(10^5)$ atoms

Ultracold fermions on optical lattices can realize Hubbard model (plus X)

- ⇝ reproduce known physics ⇝ verify models for correlated materials
- ⇝ access new regimes and properties (e.g., time resolution)

tunable parameters

- ⇝ "play" with models, switch features continuously
  - ⇝ understanding of phenomena



Our focus: antiferromagnetism (AF)

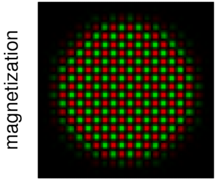
Specifics of ultracold fermions on optical lattices

1) Finite systems ($\lesssim 10^5$ fermions), trapping potential

$\rightsquigarrow$ Numerics expensive, e.g. using RDMFT

$\rightsquigarrow$ AF core radius (at best) only 10-20 lattice spacings

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



2) Tunable hopping and interactions (+ degeneracy)

3) Tunable anisotropy $\rightsquigarrow$ switch dimensionality

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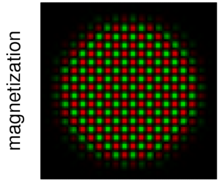

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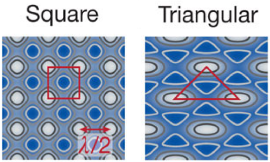
4) Tunable frustration (and dimerization)



5) Temperature in trap unknown, but loading $\sim$ adiabatic

$\rightsquigarrow$ use *entropy* as thermal parameter

Characteristics of AF in finite systems? Impact of dimensionality and frustration?

Outline

Dimensionality of (finite) lattice models

Probes of AF correlations and entropy in unfrustrated lattices

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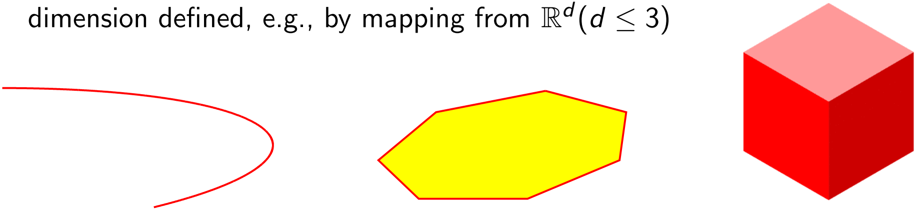
Summary

Poster by E. Gorelik:

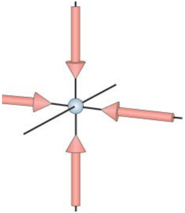
AF in honeycomb $\leftrightarrow$ square $\leftrightarrow$ dimerized lattice

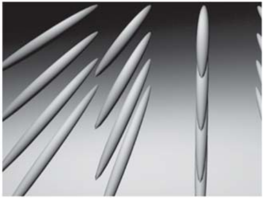
spin correlations near localized impurities (larger U, reduced t)

1) Lines, surfaces, bodies (mathematical objects in $\mathbb{R}^3$):
dimension defined, e.g., by mapping from $\mathbb{R}^d (d \leq 3)$



2) Continuum systems with finite widths - compare scales

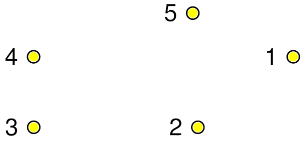




Dimensionality of finite-size systems: lattice case

General Hubbard model (N sites, $t_{ij} = t_{ji}$)

$$H = \sum_{i,j=1}^{N} \sum_{\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i=1}^{N} U_i\, n_{i\uparrow} n_{i\downarrow}$$



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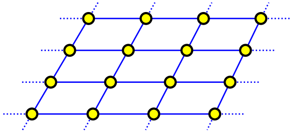
Familiar case: • sites form (infinite) mathematical lattice, with basis vectors $\boldsymbol{\tau}_\alpha$ $(1 \leq \alpha \leq d)$

• regular hopping: $t_{ij} \equiv t_{\boldsymbol{\tau}}$ (where $\boldsymbol{\tau} = \mathbf{r}_i - \mathbf{r}_j$)

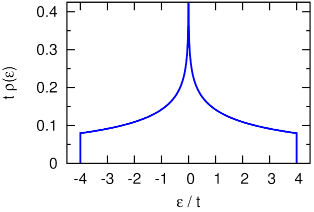
Example: square lattice



Clear: $d = 2$

Important property: noninteracting density of states (DOS) $\rho(\epsilon)$

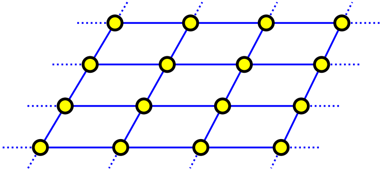
impact of cutoff?



Dimensionality of finite-size systems: lattice case

Consider 4x4 lattice with PBC's

– clearly two-dimensional character!?



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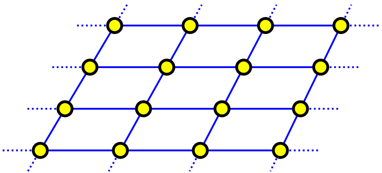
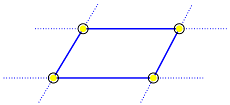


Hint: 2x2 lattice



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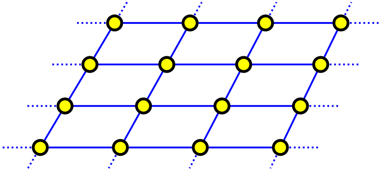

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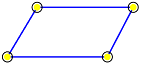

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$\rightsquigarrow d = 1$ ($\rightsquigarrow$ BA)

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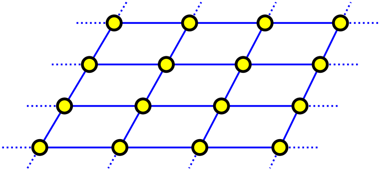

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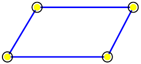

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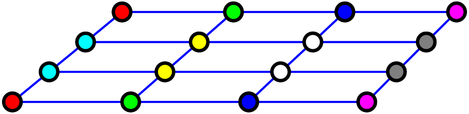

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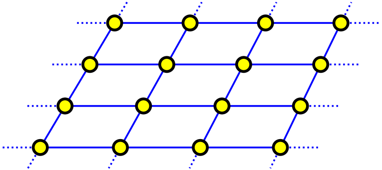

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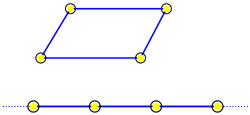

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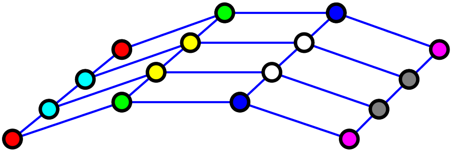

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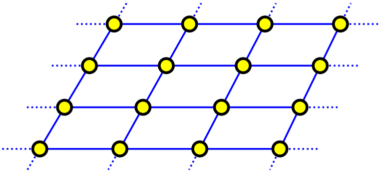

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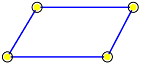

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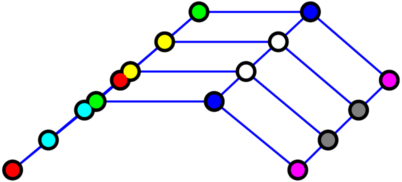

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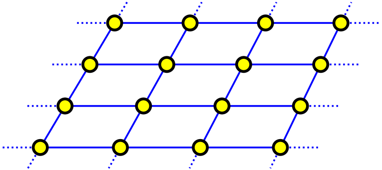

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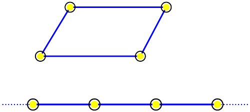

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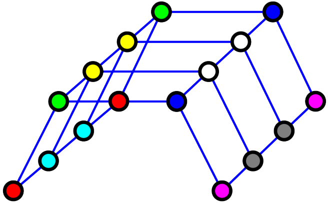

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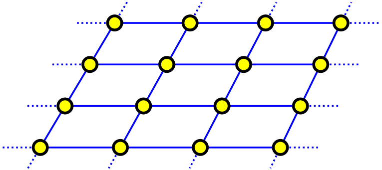

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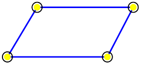

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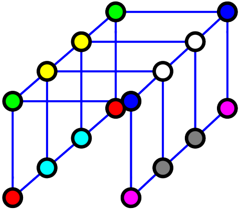

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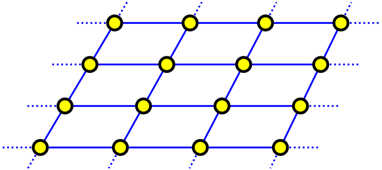

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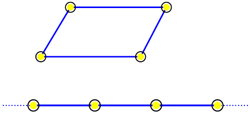

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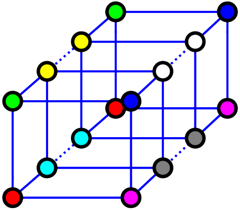

1. transform to tube
2. reinsert "horizontal" PBC's
3. split in two 2x2x2 cubes (one inverted)
4. consider "front-back" PBC's $\rightsquigarrow$ like colors linked - 4th dimension

Dimensionality of finite-size systems: lattice case

Message so far: dimensionality of small lattice systems is ambiguous

More general claim: fermion can "feel" dimensionality only by "exploring" large spatial regions (low entropy $\rightsquigarrow$ coherence)

So which lattice properties are always important?

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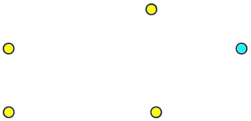

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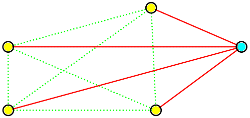

Relevant measure: 2nd moment of local DOS

$$\langle \epsilon^2 \rangle_i \equiv \int_{-\infty}^{\infty} d\epsilon \, \epsilon^2 \, \rho_i(\epsilon) = \sum_j t_{ij}^2$$

uniform case $\rightsquigarrow$ energy scale $\sqrt{\langle \epsilon^2 \rangle} = \sqrt{Z}\, t$

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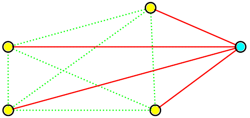

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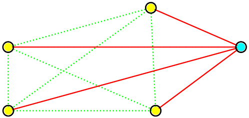

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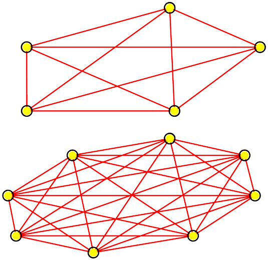
3) Is lattice bipartite (hopping from "A" site to "B" site)? $\rightsquigarrow$ AF order

Dimensionality of finite-size systems: lattice case

Example: fully connected lattice ($Z = N - 1$, non-bipartite, d undefined)

$\rightsquigarrow$ paramagnetic DMFT physics



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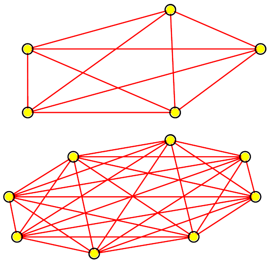
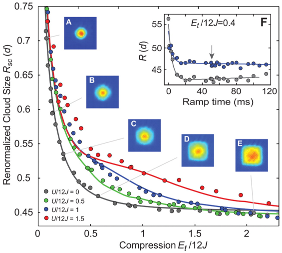
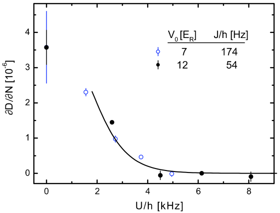




[Schneider et al, Science (2008)]



[Jördens et al., Nature (2008)]

Dimensionality of finite-size systems: lattice case

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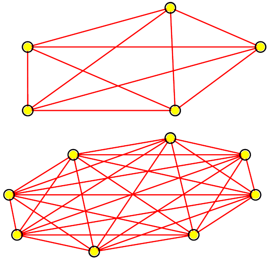

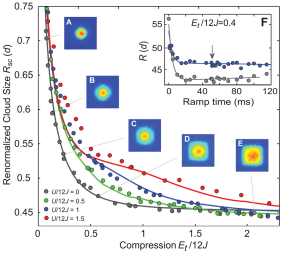

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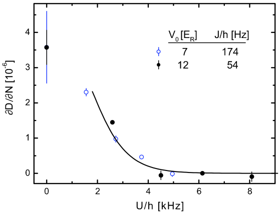
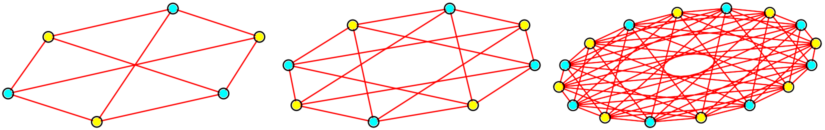


[Jördens et al., Nature (2008)]

Variation: bipartite maximally connected lattice $\rightsquigarrow$ AF DMFT physics



Universal probes for antiferromagnetic correlations and entropy in cold fermions on optical lattices

E. Gorelik, D. Rost, T. Paiva, R. Scalettar, A. Klümper, and N. Blümer

Phys. Rev. A **85**, 061602(R) (2012)

Motivation for the project

◦ How to detect AF order/correlations?

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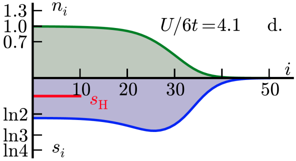
- Which entropy range is needed/interesting?



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

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- ◦ How to detect AF order/correlations?
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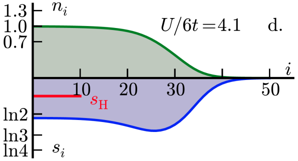

[Jördens et al., PRL **104**, 180401 (2010)]

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

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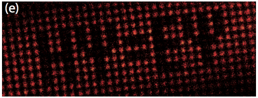
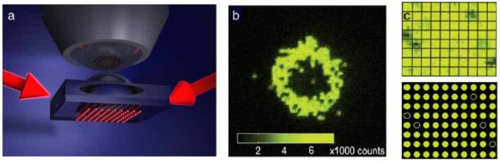
Mermin-Wagner: LRO $\leftrightarrow d = 3$

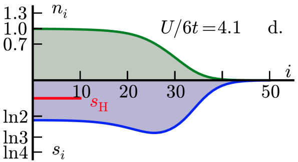
Experimental advantage of 2 dimensions:
single-site resolution



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



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



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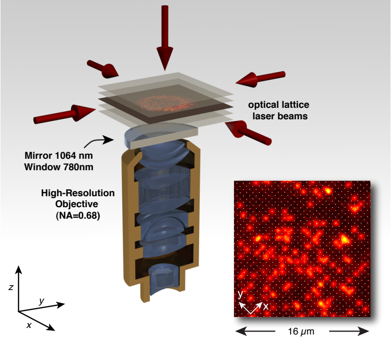
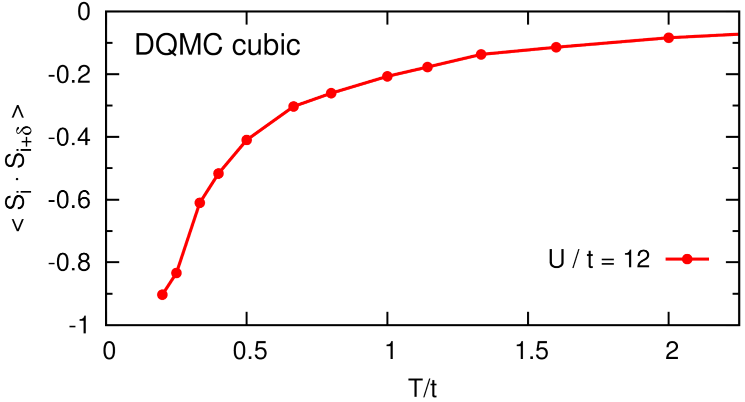


[Sherson et al., Nature **467**, 68 (2010)]

Current experimental focus: nearest-neighbor spin correlation function

Modulation spectroscopy, super-lattice approach



Note: strong (universal) high-temperature tails, monotonous

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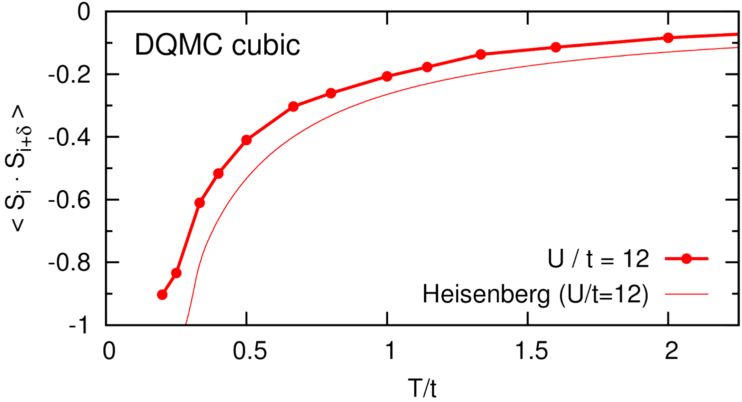

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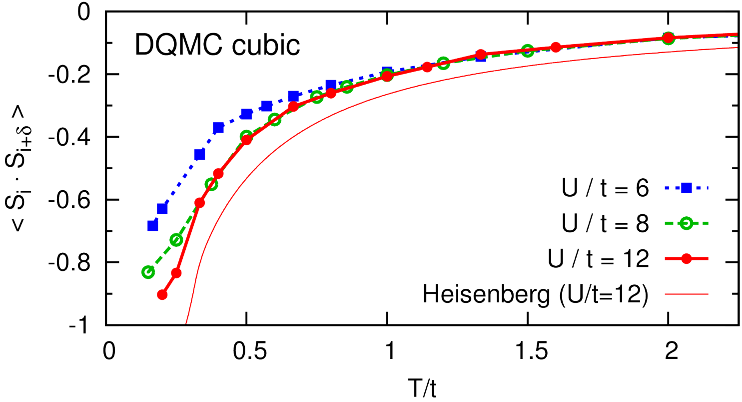

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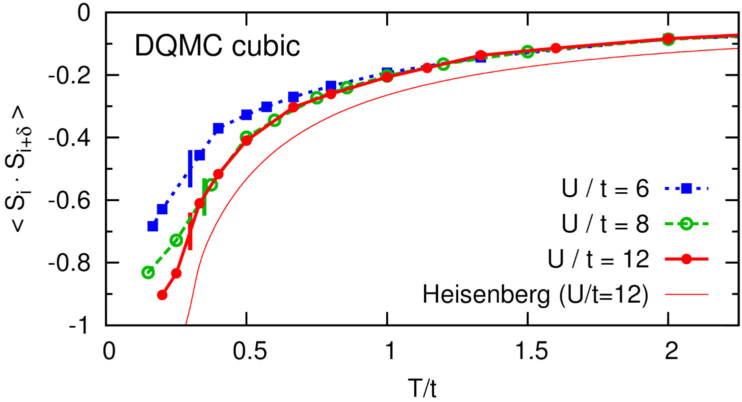

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No distinct features at Néel temperature ($\approx 0.3t$)

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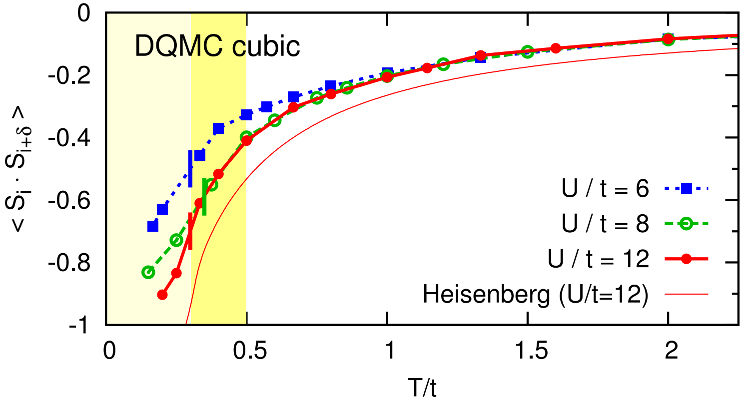

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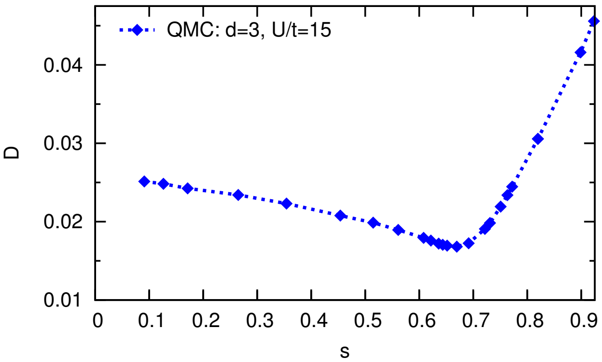
No distinct features at Néel temperature ($\approx 0.3t$)

Interesting spin physics above T_N, not visible in NN correlations

Double occupancy as a universal measure of AF correlations + entropy



Exact determinantal QMC:
AF enhances D at low-s

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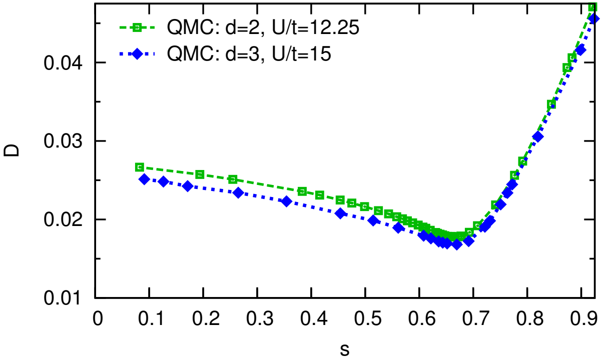

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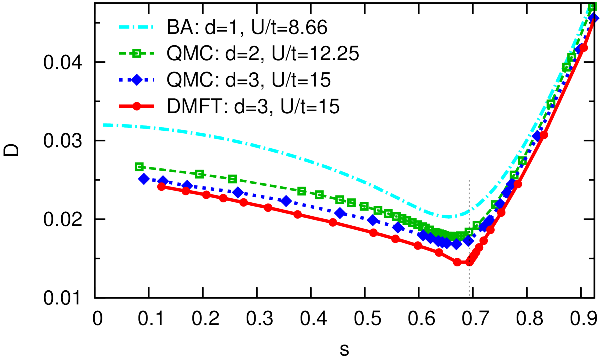

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Universal minimum at
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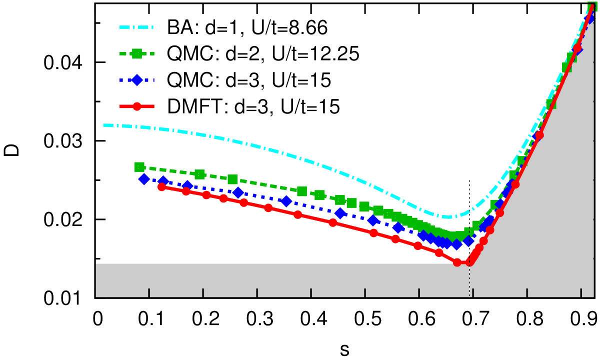

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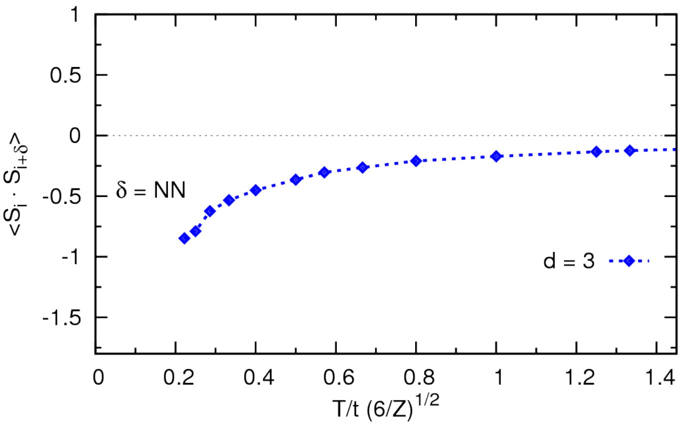
AF enhancement of D is larger in lower dimensions:

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

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

Spin correlation functions: what range is needed?

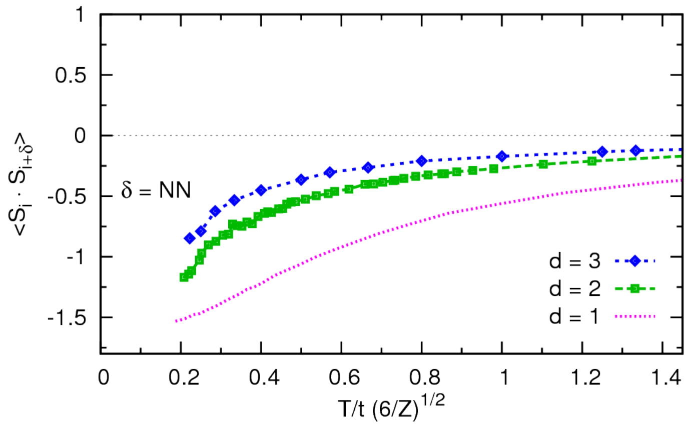
NN spin correlations: high-T tails



Spin correlation functions: what range is needed?

NN spin correlations: high-T tails, similar for $d = 2, 3$

increase with lowering d



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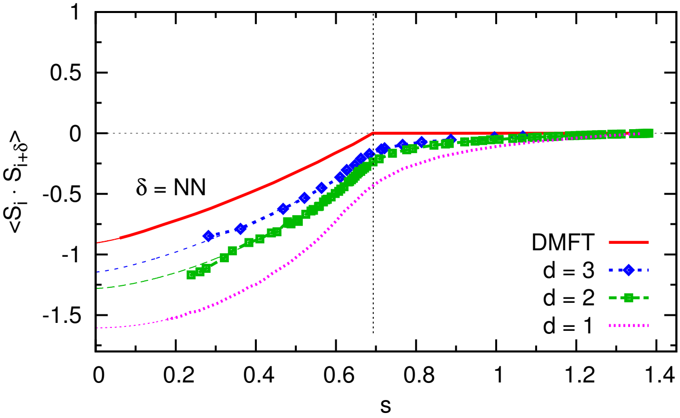

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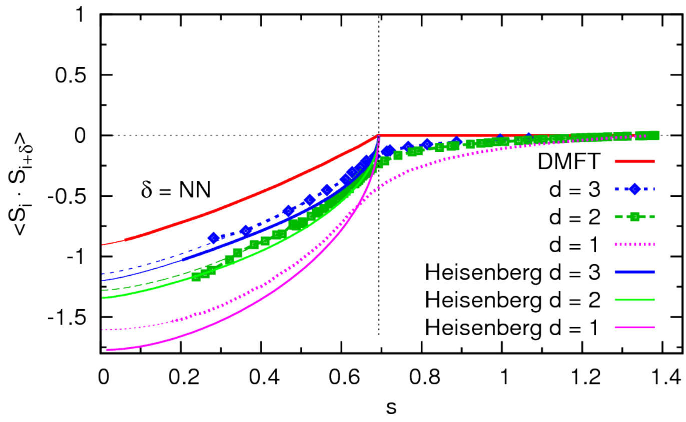

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Dimensional
crossover
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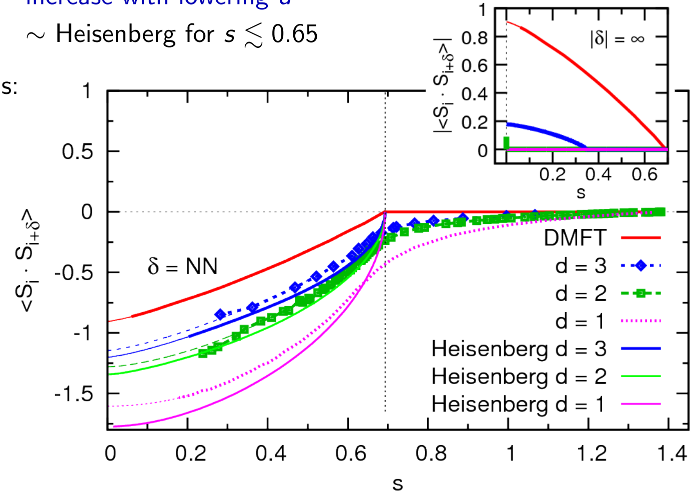

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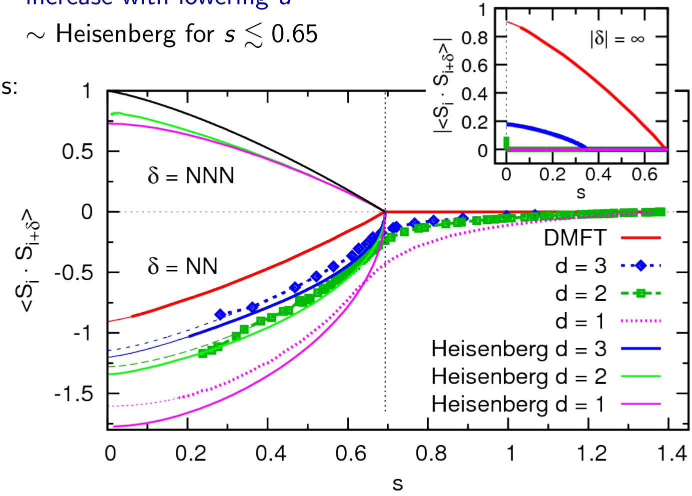

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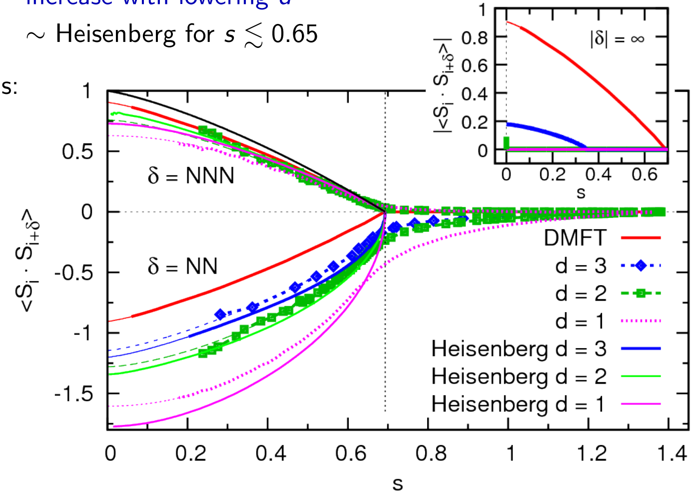

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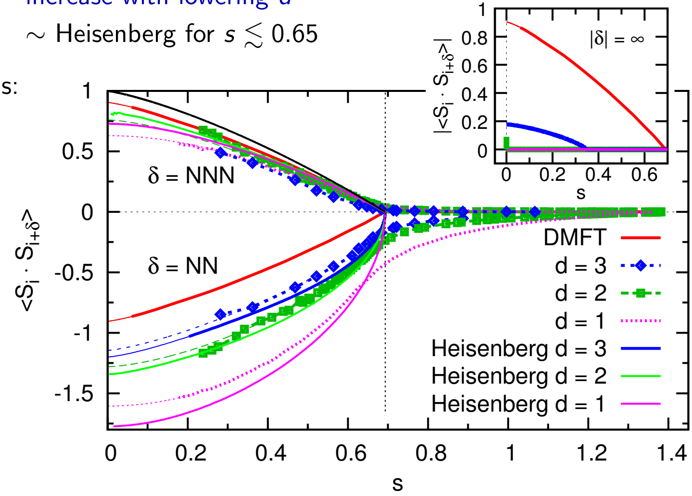
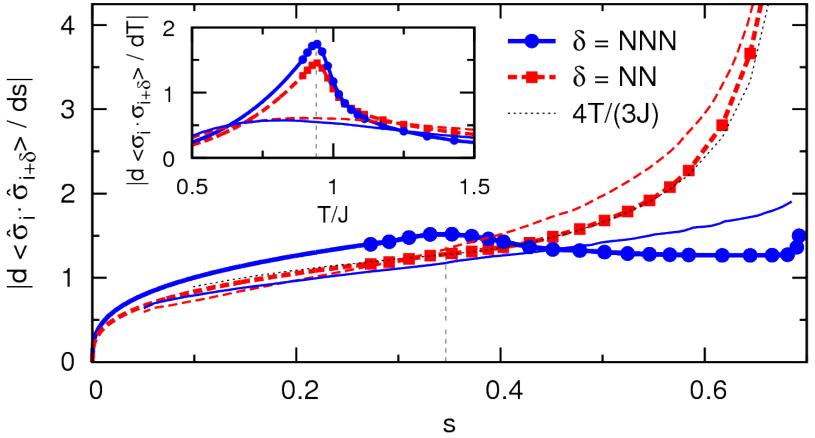


NNN spin correlation function signals: Heisenberg regime, low entropy

Spin correlation functions versus s: why no signature of T_N?

Heisenberg model: $d = 3$ (symbols), $d = 2$ (thin lines)



Use of entropy as thermal variable can hide important physics!

Discriminating antiferromagnetic signatures in ultracold fermions by tunable geometric frustration

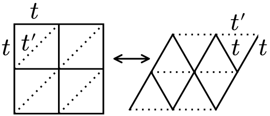
C.-C. Chang, R. T. Scalettar, E. V. Gorelik, and N. Blümer

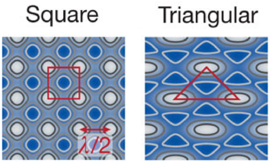
arXiv:1306.4687, to appear in Phys. Rev. B

Tunable geometric frustration

Interpolate between square and triangular lattice:

vary $\alpha = t'/t$





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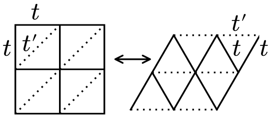

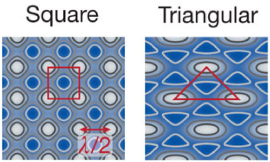

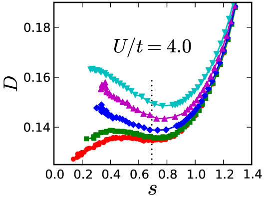

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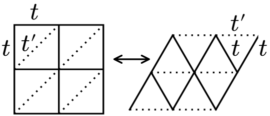

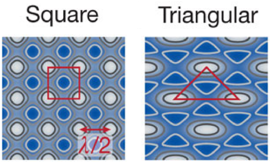

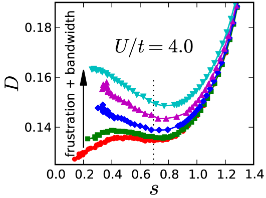

significant changes of D at all s due to bandwidth change!

$\alpha = 0.0$	$\alpha = 0.6$
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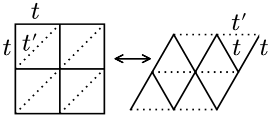
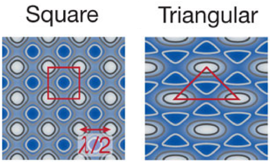
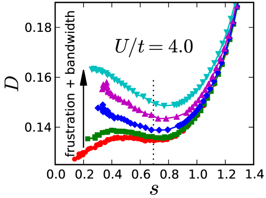


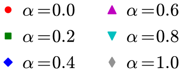




significant changes of D at all s due to bandwidth change!

Eliminate bandwidth effects:

scale with $t_\alpha = t\sqrt{Z_\alpha/Z_0}$; $Z_\alpha = 4 + 2\alpha^2$



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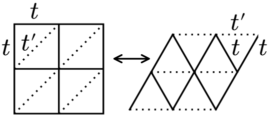

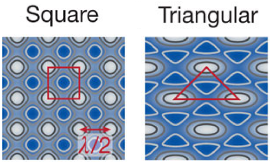

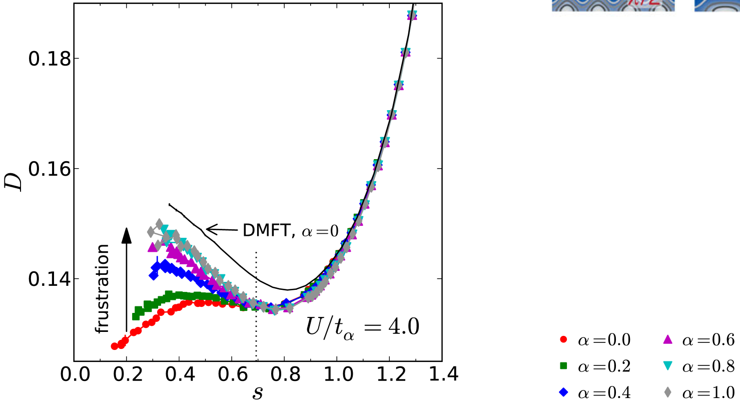

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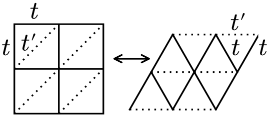

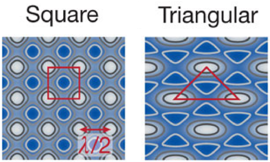

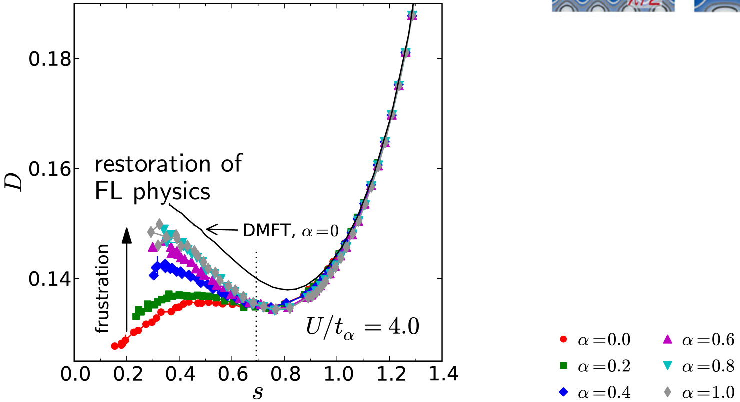

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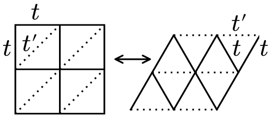
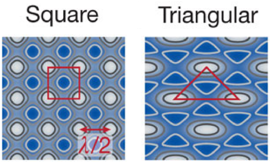
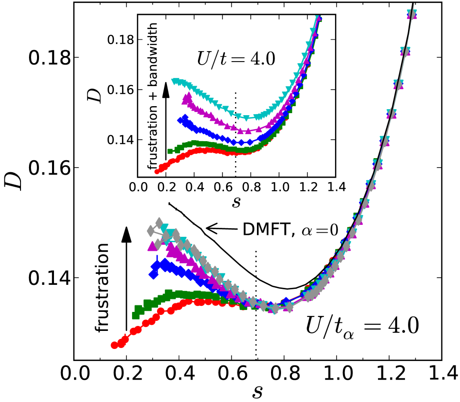
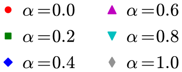


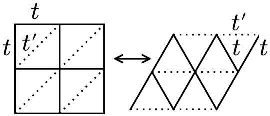


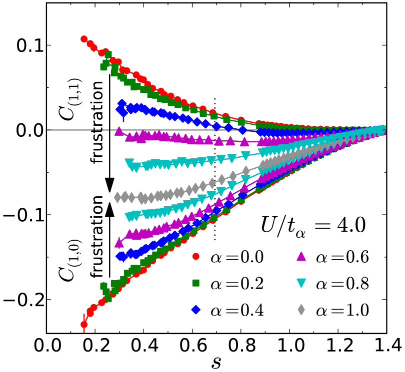




Tunable geometric frustration: weak coupling

Short range correlation functions

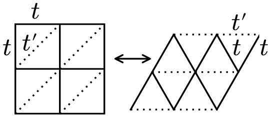


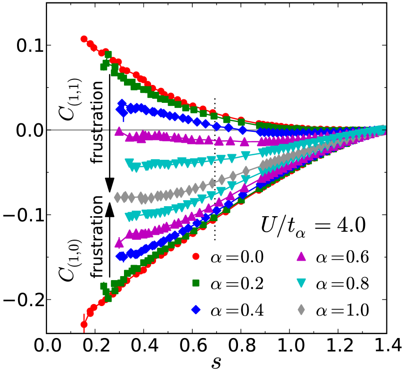


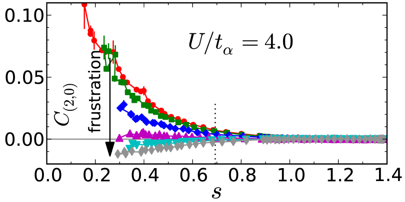
- robust evolution of $C_{(1,0)}$ and $C_{(1,1)}$ with α
- at $\alpha = 1$ $C_{(1,0)} \equiv C_{(1,1)}$

Tunable geometric frustration: weak coupling

Short range correlation functions

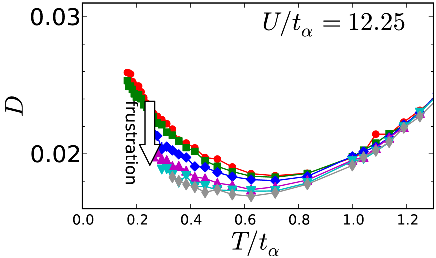






- robust evolution of $C_{(1,0)}$ and $C_{(1,1)}$ with α
- at $\alpha = 1$ $C_{(1,0)} \equiv C_{(1,1)}$
- sharp signature in $C_{(2,0)}$

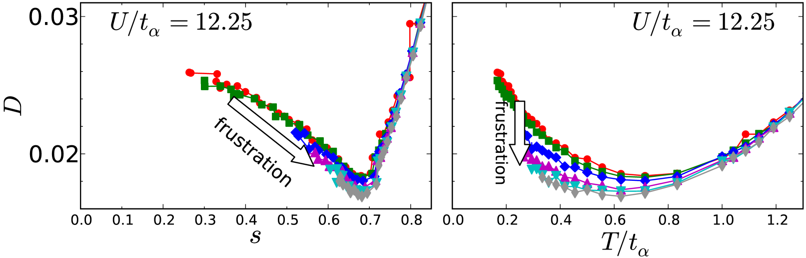
Tunable geometric frustration: intermediate and strong coupling



Strong coupling:

- elimination of low-T enchancement by frustration

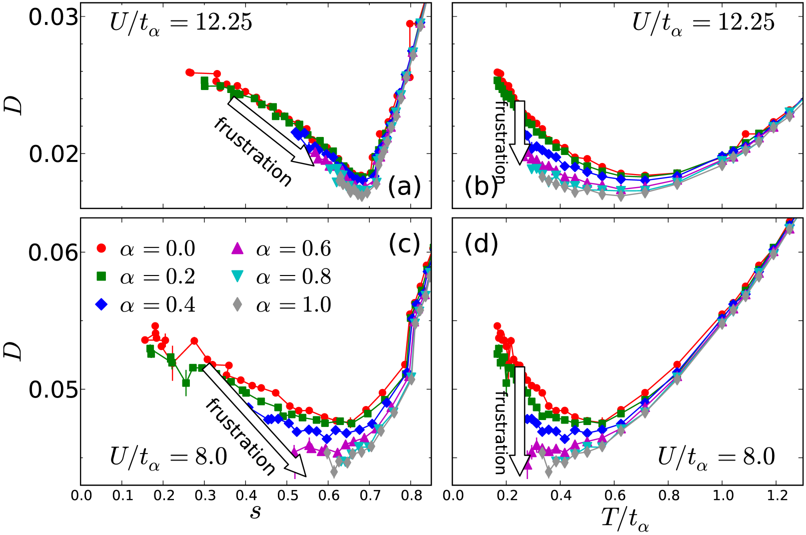
Tunable geometric frustration: intermediate and strong coupling



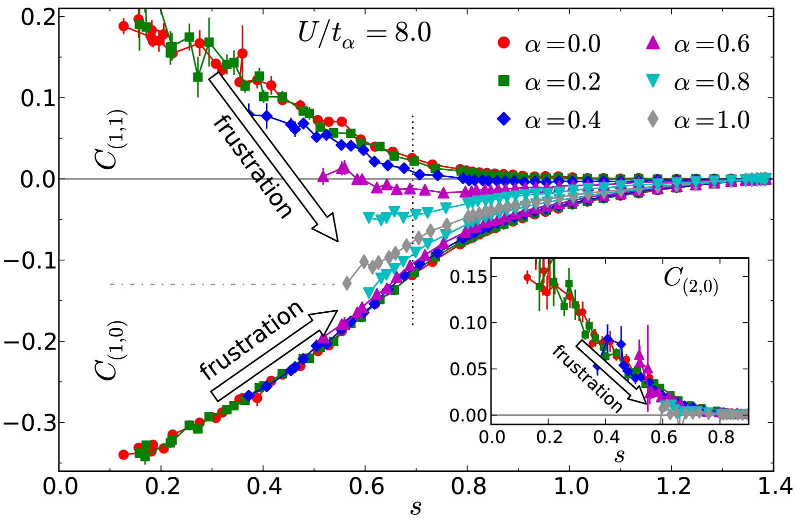
Strong coupling:

- elimination of low-T enchancement by frustration
- cancellation of α-effect in $D(s)$

Tunable geometric frustration: intermediate and strong coupling



Tunable geometric frustration: intermediate coupling

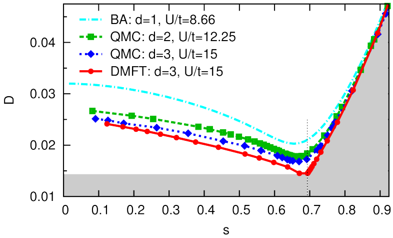


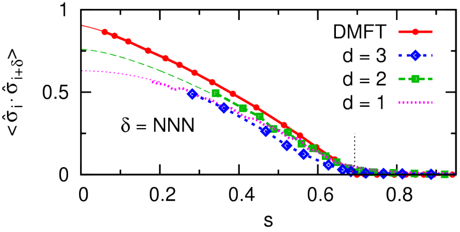
Summary

NN AF correlations LRO

NN AF correlations ↔ "finite-range antiferromagnetism" ↔ LRO

Universal characteristics, tuning of d ⇝ discriminate AF effects

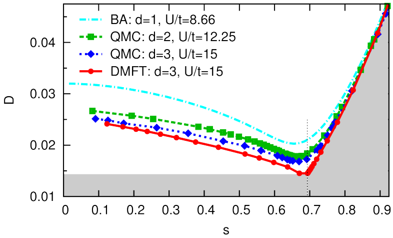


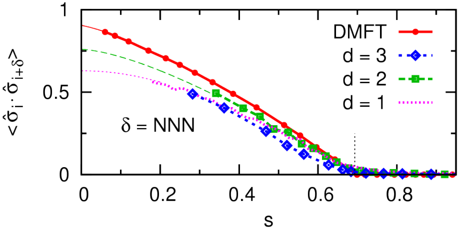


Summary

NN AF correlations $\leftrightarrow$ "finite-range antiferromagnetism" $\leftrightarrow$ LRO

Universal characteristics, tuning of d $\rightsquigarrow$ discriminate AF effects





Tunable frustration:

discriminate magnetic from nonmagnetic physics

[arXiv:1306.4687]