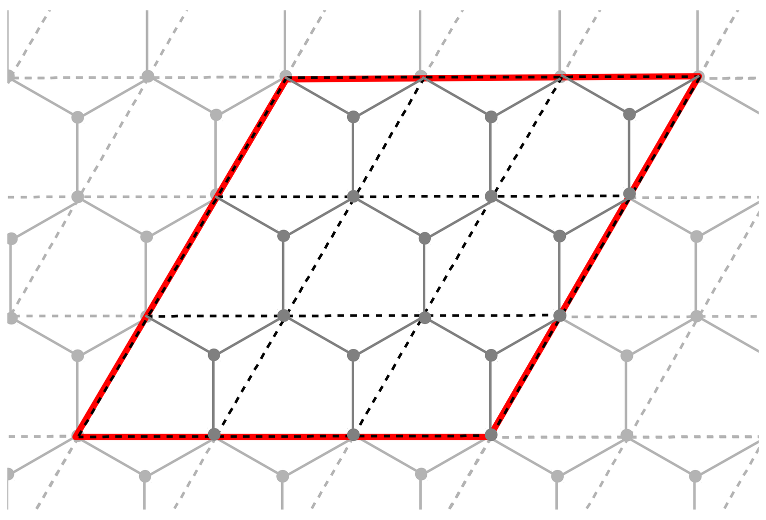
Anisotropy-driven enhancement of spin correlations

Jakub Imriška[1], Lei Wang[1], Emanuel Gull[2], and Matthias Troyer[1]
[1]Institut für theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland [2]University of Michigan, Ann Arbor, MI 48109, USA

We study the Hubbard model on different lattices - coupled 1D chains, coupled 2D layers made of square lattice, layered honeycomb lattice - and investigate the thermodynamic properties by the dynamical cluster approximation. We find that the short-range spin correlations are significantly enhanced for the anisotropic models in the direction with stronger tunneling amplitudes when compared to the isotropic 3D cubic system. Our results provide a thermometer for the quantum simulation experiment of ultracold fermions in an optical lattice and allow an quantitative estimate of the excess entropy during the lattice loading. We furthermore investigate the dependence of the critical temperature (entropy) at the Néel transition on anisotropy and lattice geometry.

DCA method

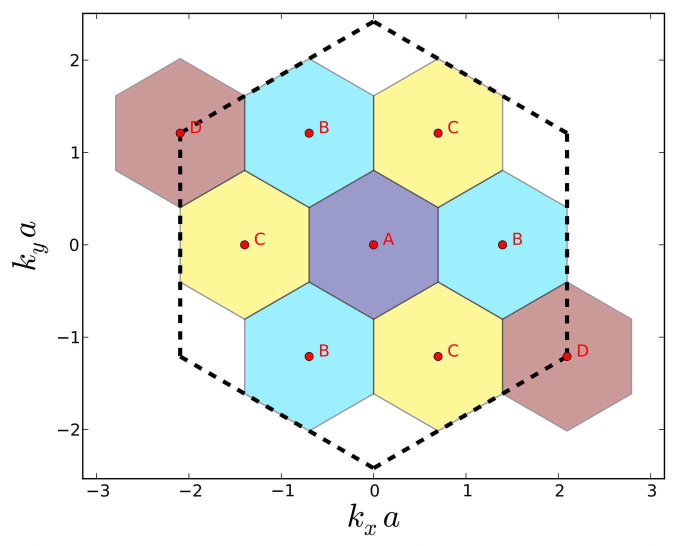
The method of choice is the dynamical cluster approximation (DCA) [2], a cluster extension of the dynamical mean-field theory (DMFT) [1]. The lattice problem is self-consistently mapped onto an impurity (=cluster) with periodic boundary conditions and additional non-interacting bath.



Cluster with 9 unit cells of the hexagonal lattice in the realspace.

The DMFT provides exact solution of the Hubbard model in an infinite dimensional system – in that case the self-energy is purely local (→ i.e. **k**-independent). That motivates the (only) approximation in any DMFT method: equality of the impurity and lattice self-energy – in particular for DCA we require

$$\Sigma^{\mathrm{imp}}(\mathbf{K}) \approx \Sigma^{\mathrm{lat}}(\mathbf{k}) \qquad \text{(constant over patch).}$$

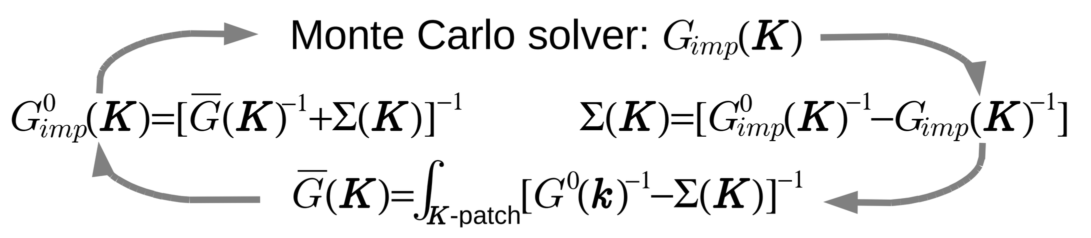


9-unit-cells cluster on the hexagonal lattice in reciprocal space, with hexagonal patches.

The mapping is determined by the selfconsistency condition

$$G^{\mathrm{imp}}(\mathbf{K}) = \frac{1}{\Omega}\int_{\mathbf{K}\text{-patch}} \mathrm{d}\mathbf{k}\, G^{\mathrm{lat}}(\mathbf{k}).$$

The impurity solver for the DCA calculations used for this work was the continuous time auxiliary field quantum Monte Carlo impurity solver (CT-AUX) [3] [4].



Iterative solution scheme

The DCA method is a controllable approximation and it becomes exact in the limit of infinite cluster size. The mean-field character remains in the vicinity of the phase transitions of 2nd kind, where the correlation length is larger than the cluster size and thus it cannot be captured by the impurity. Away from the phase transitions the observables may be extrapolated to the thermodynamic limit using the known asymptotical behavior.

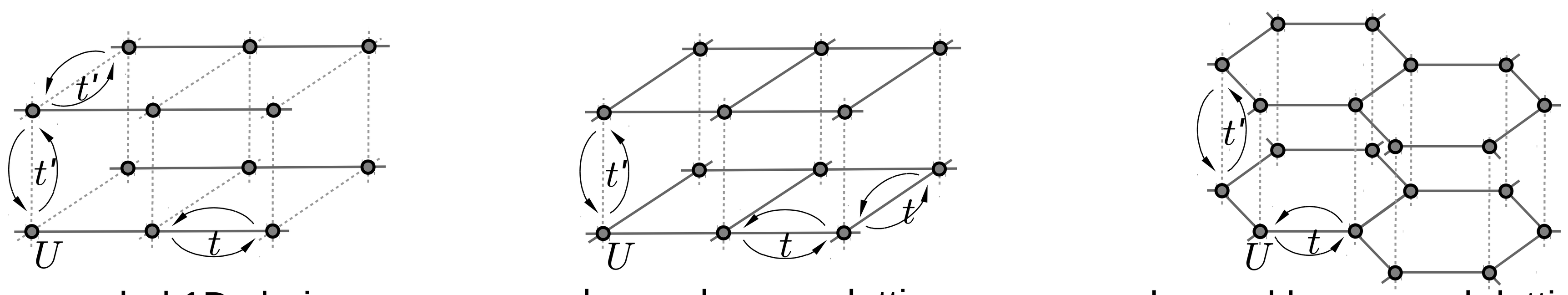
A way to measure the susceptibility and to find the phase transition is usage of the pairing matrix formalism with an additional approximation on the vertex function,

$$\Gamma^{\mathrm{imp}}(\mathbf{Q}m, \mathbf{K}n, \mathbf{K}'n') \approx \Gamma^{\mathrm{lat}}(\mathbf{Q}m, \mathbf{k}n, \mathbf{k}'n').$$

Model

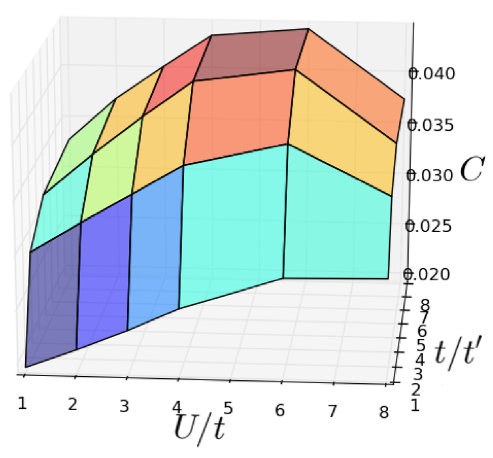
We study the anisotropic Hubard model on 3-dimensional lattices described by the Hamiltonian

$$\hat{H} = -\sum_{\langle i,j\rangle,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_{i,\sigma}\hat{n}_{i\sigma}.$$



coupled 1D chains ($t' \leq t$) — layered square lattice ($t' \leq t$) — layered honeycomb lattice ($t' \leq t$)

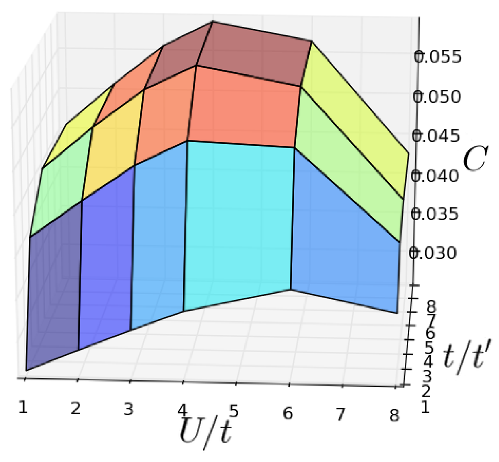
Short-range spin-spin correlations $C = -2\left\langle S^z_{\mathbf{r}} S^z_{\mathbf{r}+\mathbf{\Delta}}\right\rangle$

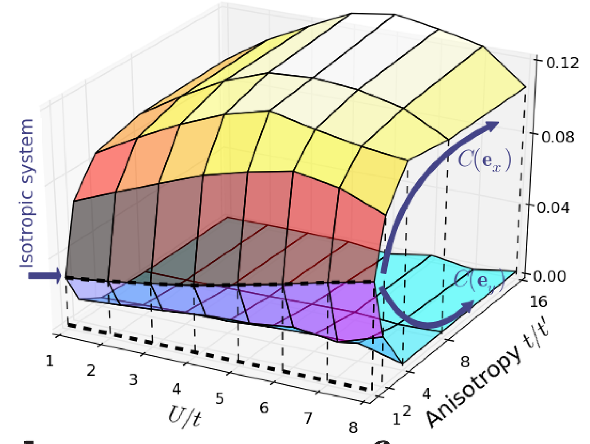


Layered lattices at $S/N = 0.8$ at half filling

← layered square

layered honeycomb →





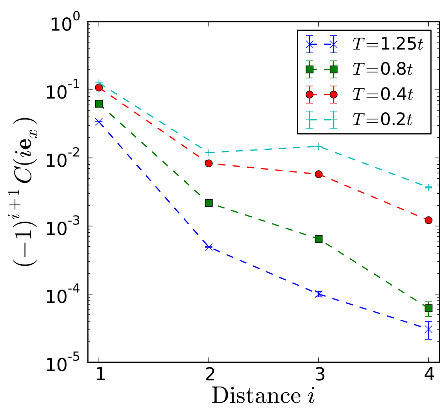
Coupled 1D chains at half filling [6]

← at temperature $T = t/2$

Upper sheet: in-chain direction

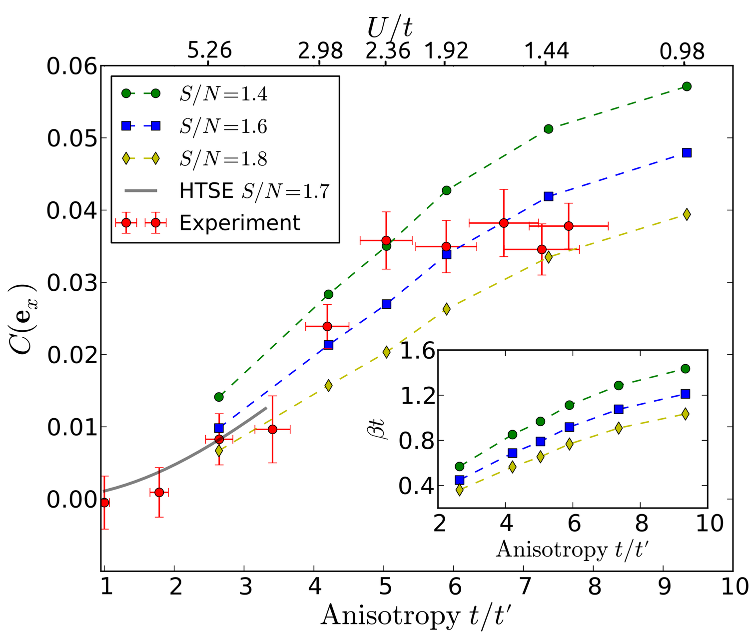
Lower sheet: ⊥ direction

$U = 1.44t$, $t/t' = 7.36$ →



▶ **Enhancement of nearest-neighbor spin-spin correlation roughly proportional to the inverse coordination number ratio, counting hoppings t only.**

Comparison with experiment [5] utilizing LDA



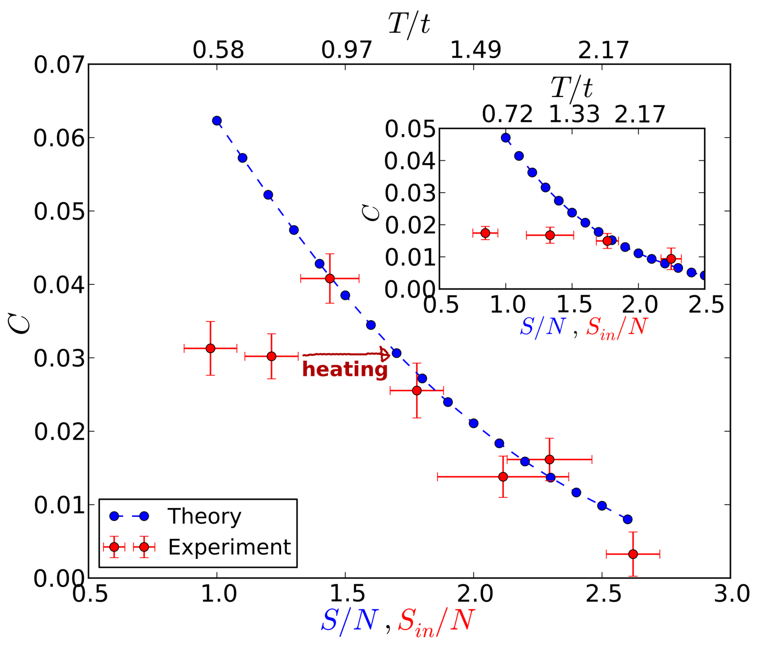
Coupled 1D chains: comparison with experiment [6]

← **Thermometer:** $C \to T/t$

Estimate of heating → during the lattice loading

Main: $U = 1.44t$, $t/t' = 7.36$

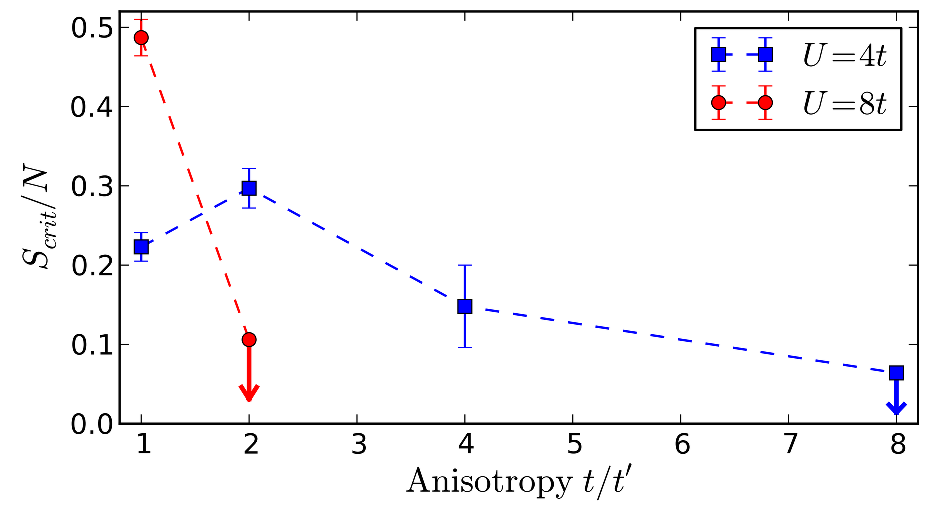
Inset: $U = 2.98t$, $t/t' = 4.21$



Long-range antiferromagnetic order at half filling

lattice	t/t'	U/t	S_{crit}/N
layered square	2.0	6.0	0.45(3)
layered square	2.0	8.0	0.37(12)
layered honeycomb	1.0	8.0	< 0.49

coupled 1D chains [6] →



▶ **Cubic lattice is in terms of highest S_{crit}/N optimal.**

References

[1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg: *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions*, Rev. Mod. Phys. **68**, 13 (1996)

[2] M. Jarrell, Th. Maier, C. Huscroft, and S. Moukouri: *Quantum Monte Carlo algorithm for nonlocal corrections to the dynamical mean-field approximation*, Phys. Rev. B **64**, 195130 (2001)

[3] E. Gull, P. Werner, O. Parcollet, and M. Troyer: *Continuous-time auxiliary field Monte Carlo for quantum impurity models*, EPL 82 No 5 (June 2008) 57003

[4] E. Gull, P. Staar, S. Fuchs, P. Nukala, M. S. Summers, T. Pruschke, T. C. Schulthess, and T. Maier: *Submatrix updates for the continuous-time auxiliary-field algorithm*, Phys. Rev. B **83**, 075122 (2011)

[5] D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger: *Short-Range Quantum Magnetism of Ultracold Fermions in an Optical Lattice*, *Science* 14 June 2013: **340** (6138), 1307-1310 (2013)

[6] J. Imriška, M. Iazzi, L. Wang, E. Gull, D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, M. Troyer: *Thermodynamics and Magnetic Properties of the Anisotropic 3D Hubbard Model*, Phys. Rev. Lett. **112**, 115301 (2014).