# Anisotropic Hubbard model on a cubic lattice examined by the dynamical cluster approximation

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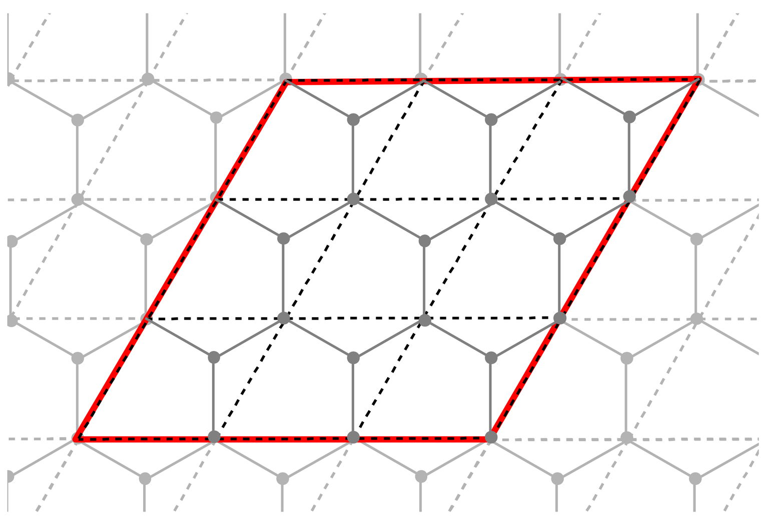
*Dynamical cluster approximation study shows that the short-range spin-spin correlation is enhanced with anisotropy in 3D Hubbard model. These results agree well with the experimentally observed nearest neighbor spin-spin correlation in a cold-atom realization of the anisotropic Hubbard model. Since the Néel temperature decreases rapidly with anisotropy, the highly anisotropic Hubbard model is not favorable for realization of the antiferromagnetic long-range order.*

## DCA method

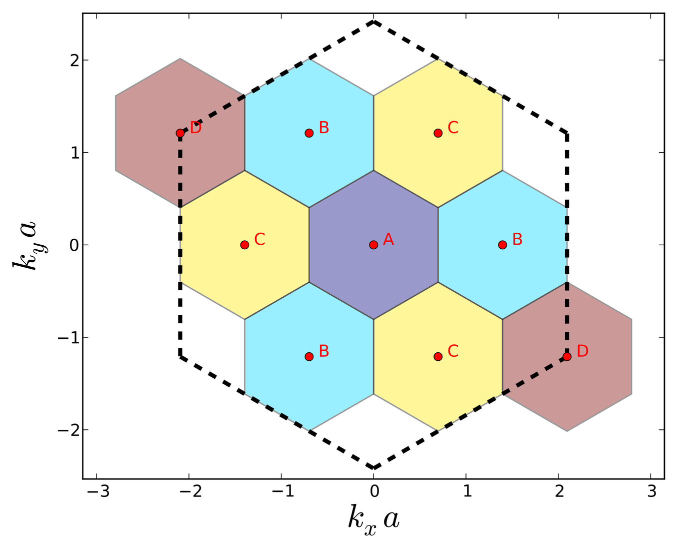
The method of choice is the dynamical cluster approximation (DCA) [2], a cluster extension of the dynamical mean-field theory [1]. The lattice problem is selfconsistently mapped onto an impurity (=cluster) with periodic boundary conditions and additional non-interacting bath.



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

If the interaction consists of onsite only terms, the selfenergy is a much more local quantity in realspace than the Green's function – therefore we approximate the lattice selfenergy by the impurity selfenergy; in DCA this is done in the reciprocal space (=grained **K**-space) of the impurity,

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

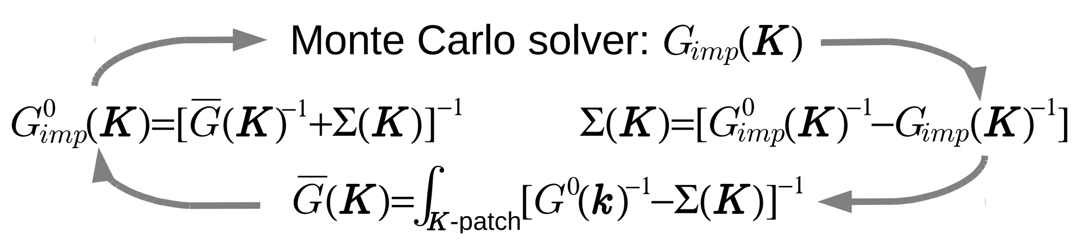



*9-unit-cells cluster on the hexagonal lattice in reciprocal space, with hexagonal patches.*

The mapping is determined by the selfconsistency condition

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

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].




The DCA method is a controllable approximation as 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 scaling.

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,

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

## Introduction

The interest on the anisotropic Hubbard model was raised by an experimental measurement of the short-range magnetic correlation in a cold atoms experiment [5] done in an anisotropic realization of the Hubbard model. Several question have arised:

- What is the role of the anisotropy in the enhanced spin-spin correlation?
- What is the nature of the state realized in the experiment? How long-ranged is the spin-spin correlation?
- Is to possible to come closer to the true (antiferromagnetic) ordering within the cold atoms in the anisotropic set-up than in the isotropic case?

## Model

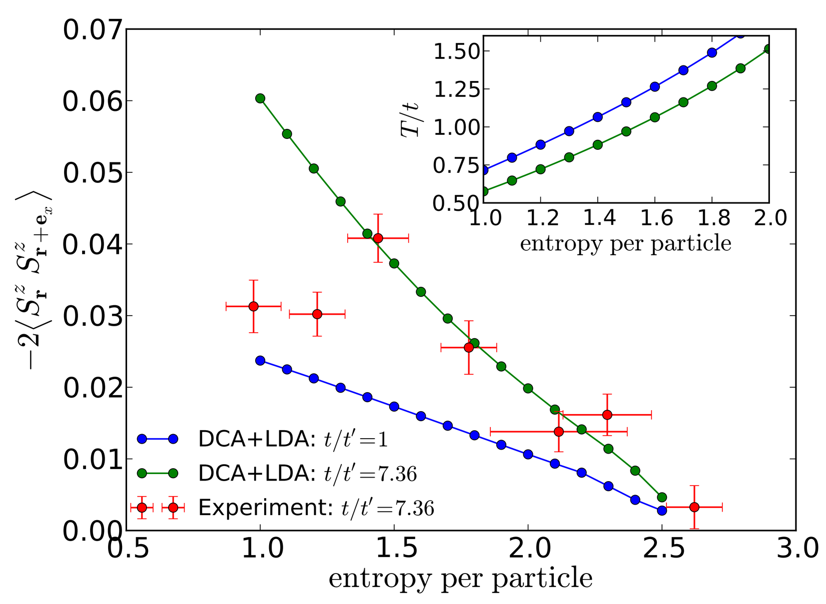
We study the anisotropic Hubard model on a cubic lattice described by the Hamiltonian

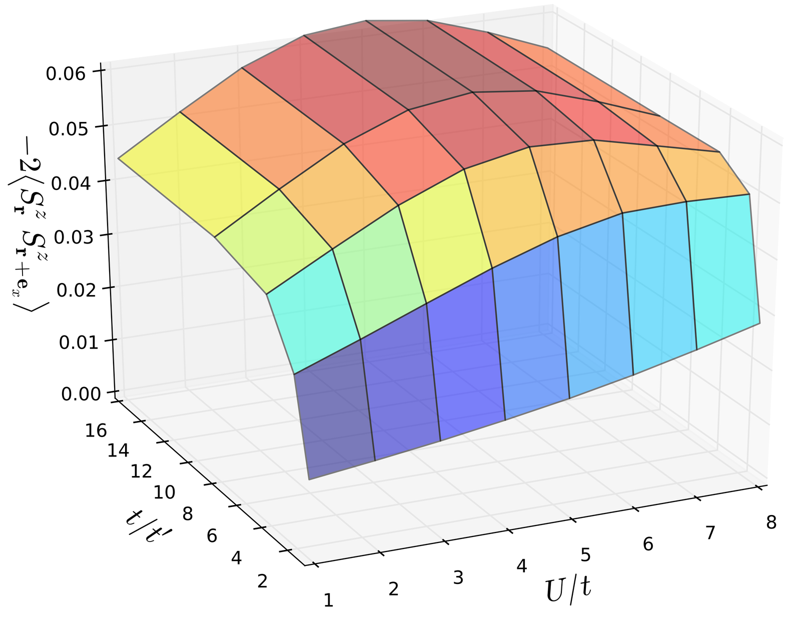
$$\hat{H} = U\sum_{\mathbf{r}} \hat{n}_{\mathbf{r}\uparrow}\hat{n}_{\mathbf{r}\downarrow} - \mu\sum_{\mathbf{r},\sigma}\hat{n}_{\mathbf{r}\sigma} - t\sum_{\mathbf{r},\sigma}\left(\hat{c}^\dagger_{\mathbf{r}+\mathbf{e}_x\sigma}\hat{c}_{\mathbf{r}\sigma} + h.c.\right) - t'\sum_{\mathbf{r},\sigma}\left(\hat{c}^\dagger_{\mathbf{r}+\mathbf{e}_y\sigma}\hat{c}_{\mathbf{r}\sigma} + \hat{c}^\dagger_{\mathbf{r}+\mathbf{e}_z\sigma}\hat{c}_{\mathbf{r}\sigma} + h.c.\right),$$

where $\hat{c}^\dagger_{\mathbf{r}\sigma}$ creates a fermion at lattice point $\mathbf{r}$ with spin $\sigma \in \{\uparrow,\downarrow\}$; $\hat{n}_{\mathbf{r}\sigma} \equiv \hat{c}^\dagger_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}\sigma}$; the lattice constant is 1; $\mathbf{e}_i$ denotes the unit vector. We study $t' \le t$ only: from the isotropic cubic lattice to the weakly coupled 1-D chains.

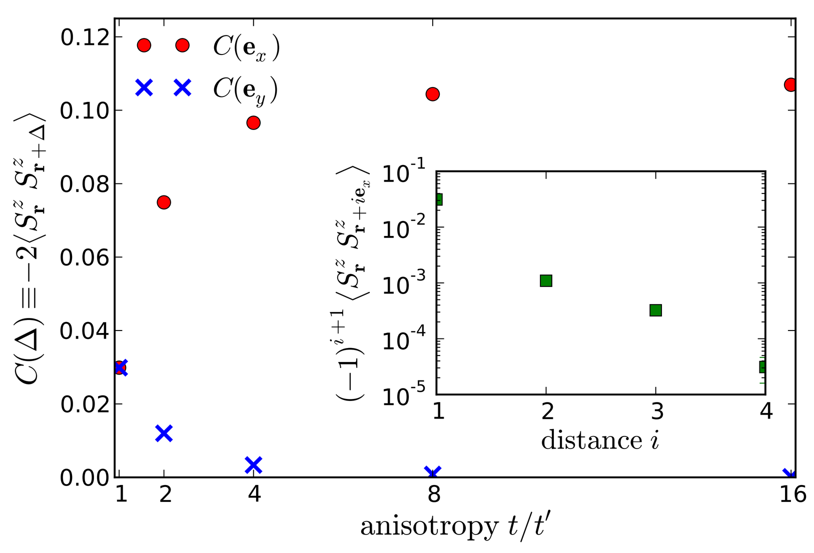
## Anisotropic Hubbard Model

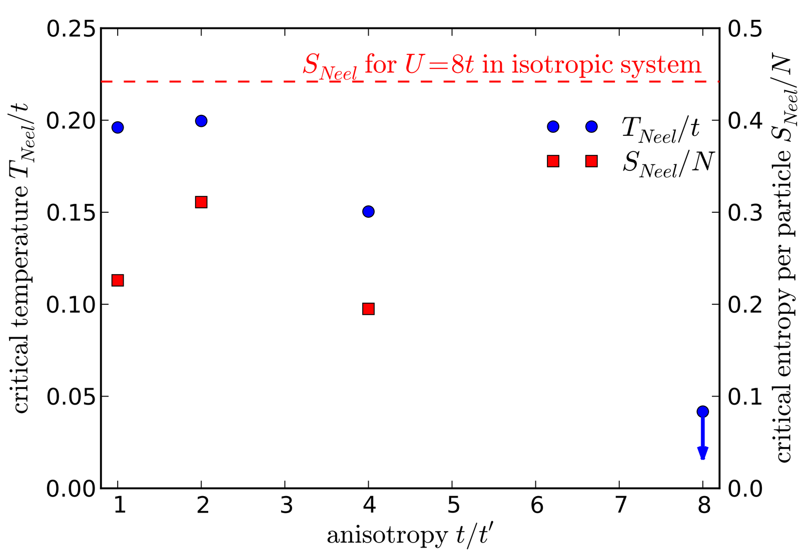
Using DCA we have found the equation of states and the spin-spin correlation $\langle S^z_{\mathbf{r}} S^z_{\mathbf{r}+\mathbf{\Delta}}\rangle$, done extrapolation to the thermodynamic limit and used that within the local density approximation to find the trap-averaged quantities comparable with experimentally obtained data.




*Left: Comparison of the experimentally obtained data with our numerical analysis data; $U = 1.4375t$.*
*Right: Spin-spin correlation at half-filling, in a homogeneous system, at $T = t/2$.*




*Left: Spin-spin correlation along $x$ and perpendicular to it; $U = 2t$, $T = t/2$, at half-filling.*
*Inset: $T = 0.8t$, $U = 1.44t$, half-filled.*
*Right: The $T_{Neel}$ and $s_{Neel}$ for a homogeneous system at $U = 4t$ and at half-filling.*

Conclusions:

- The spin-spin correlation is enhanced significantly in the anisotropic case on the cost of the transverse spin-spin correlation – that has made it possible to detect it experimentally.
- The spin-spin correlation is in the realized state very short-ranged, with exponential decay and strongly suppressed transverse spin-spin correlation.
- The entropy per particle to reach the ordered phase is for the slightly anisotropic system higher than in the isotropic case for fixed $U = 4t$. However the optimally chosen isotropic system with $U = 8t$ has the critical entropy even higher.

## References

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