Correlations in the anisotropic Hubbard model

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Hubbard model:

- **repulsive interaction**  \( U > 0 \)
- **\( t_{ij} \)**: nearest neighbor hopping  \( t \) and  \( t' \) (\( t' \leq t \)),

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

- coupled 1D chains (\( t' \leq t \))
- layered square lattice (\( t' \leq t \))
- layered honeycomb lattice (\( t' \leq t \))
Static mean-field concept

Mean-field density $n_i$:

$$\hat{n}_i = n_i + (\hat{n}_i - n_i)$$

Neglect spatial & temporal fluctuations:

$$(n_i + \hat{\delta}_i)(n_j + \hat{\delta}_j) = n_in_j + n_i\hat{\delta}_j + n_j\hat{\delta}_j + \hat{\delta}_i\hat{\delta}_j$$

$$\mathcal{H}_{MF} = -\sum_{\langle i,j \rangle,\sigma} t_{ij} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + U \sum_{i,\sigma} n_{i\sigma} \hat{n}_{i\bar{\sigma}} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$

with condition $\langle \hat{n}_{i\sigma} \rangle = n_{i\sigma}$.

FM example: impurity with parameters $n_{\uparrow}, n_{\downarrow}$.

For classical models exact for $Z \rightarrow \infty$ ($dim \rightarrow \infty$).

Quantum models: variational approach.
Dynamical mean-field approximation/theory:

- Selfconsistent mapping of the problem: lattice $\mapsto$ impurity
- Constructed to be exact in $Z \to \infty$:
  - onsite interactions (Hubbard model)
  - $\Rightarrow$ selfenergy constant in reciprocal space (local in realspace)
- Physically motivated approximation:
  - lattice selfenergy $\approx$ impurity selfenergy
- DMFT selfconsistency condition:
  
  $$
  \frac{1}{\Omega_{BZ}} \int_{BZ} \, \text{d}k \ G_{\text{lat}}(k) = G_{\text{lat,local}} = G_{\text{imp}}
  $$

- Exact for $t_{ij} = 0$, $U = 0$ and $Z \to \infty$. 
Iterative solution scheme:

Monte Carlo solver: $G_{imp}$

$$G_{imp}^0 = \left[ \overline{G}^{-1} + \Sigma \right]^{-1}$$

$$\overline{G} = \int_{BZ} \left[ G^0(k)^{-1} - \Sigma \right]^{-1}$$

$$\Sigma = G_{imp}^{-1} - G_{imp}^{-1}$$

Interpretation of the impurity task with $G_{imp}^0(\tau)$:

Impurity problem solved by perturbation theory in interactions, numerically (Monte Carlo) sampling over all contributing orders.

Anderson impurity model
Dynamical Cluster Approximation (DCA)

DCA: cluster extension of the DMFA (exact for infinite cluster)
9-cell cluster on hexagonal lattice
← realspace
reciprocal space →

- Mapping in reciprocal space:

\[
\frac{1}{\Omega_{patch}} \int_{\text{patch}} \, d\tilde{k} \, G_{\text{lat}}(K + \tilde{k}) = G_{\text{imp}}(K) \quad (1)
\]

- Selfconsistency: \( \Sigma^{\text{lat}}(K + \tilde{k}, i\omega_n) \approx \Sigma^{\text{imp}}(K, i\omega_n) \)
- Solution scheme: iterative as for DMFT, for each \( K \)-point
Nearest-neighbor spincorrelations

Spincorrelations $C = -2 \langle \hat{S}_i^z \hat{S}_j^z \rangle$

Coupled 1D chains
at temperature $T = t/2$
at half filling

Upper sheet: in-chain direction
Lower sheet: $\perp$ direction

Layered lattices
at $S/N = 0.8$
at half filling
← layered square
layered honeycomb →

$T \sim t, \ T \gg t' \Rightarrow C \propto (\text{coordination \ # \ of \ hoppings \ } t)^{-1}$

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Coupled 1D chains: comparison with experiment

Experiment: cold atoms in optical lattice [Science 340, 1307 (2013)]
Numerics: extrapolated DCA + local density approximation

Main plot: coupled 1D chains, $U/t = 1.4375$, $t/t' = 7.36$

Ref.: PRL 112, 115301 (2014)
Consistent with Mermin–Wagner–Hohenberg theorem in the limit $t / t' \to \infty$; large anisotropy disables long-range order.

Optimal $U/t$ changes with anisotropy.

Highest $S_{\text{crit}}/N$ for isotropic cubic lattice.

**Critical entropy per particle for half filled coupled 1D chains**

![Graph showing critical entropy per particle for half filled coupled 1D chains]
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