We study the Hubbard model on a layered honeycomb lattice for different interlayer couplings and interaction strengths. We provide estimates of the Néel transition temperature based on the dynamical cluster approximation. The lattice susceptibility is obtained based on the approximation of the irreducible lattice vertex by the irreducible cluster impurity vertex. The approach leads to consistent results with the direct measurement of the order parameter when allowing for the symmetry breaking.

**DCA METHOD**

We use dynamical cluster approximation (DCA) [2], a cluster extension of the dynamical mean-field theory (DMFT) [1]. It is exact in the:

- non-interacting case
- atomic limit
- limit of infinite coordination number
- limit of infinite cluster

The lattice problem is self-consistently mapped onto an impurity (=cluster) with periodic boundary conditions and additional noninteracting bath.

DMFT: infinite coordination number

⇒ purely local (k-independent) selfenergy

⇒ approximation \( \Sigma^{\text{lat}}(k) \approx \Sigma^{\text{imp}}(k) \) (constant over Brillouin zone)

DCA: mapping in the reciprocal space of the cluster, approximation \( \Sigma^{\text{lat}}(k) \approx \Sigma^{\text{imp}}(K) \) (constant over patch)

Cluster with 9 unit cells:

![Honeycomb lattice, 9-cell cluster diagram]

**MODEL**

We study the Hubbard model on a layered honeycomb lattice described by the Hamiltonian

\[
H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}.
\]

Assuming \( t' \leq t \), Motivated by [7].

**TECHNICAL DETAILS**

DMFT: selfconsistency condition

\[
G^{\text{imp}} = \frac{1}{N} \sum_{k} \frac{1}{G^{\text{lat}}(\mathbf{k})} dk G^{\text{lat}}(\mathbf{k})
\]

DCA: selfconsistency condition for L-cell cluster

\[
G^{\text{imp}}(\mathbf{K}) = \frac{1}{L} \sum_{\mathbf{k} \in \text{Brillouin zone}} dk G^{\text{lat}}(\mathbf{k})
\]

Task is solved iteratively:

- impurity solver: \( G^{\text{imp}}(\mathbf{K}) \)
- \( G^{\text{imp}}(\mathbf{K}) = [G^{\text{lat}}(\mathbf{K})^{\dagger} + \Sigma^{\text{lat}}(\mathbf{K})]^{-1}
\]

The impurity solver used: continuous time auxiliary field quantum Monte Carlo impurity solver (CT-AUX) [8, 4].

The lattice susceptibility is obtained based on approximation \( \text{Im} G \approx G^{\text{imp}} \) for the irreducible vertex.

\[
\Gamma(q, \omega_n) = k' q \delta(q, \omega_n)
\]

Bethe–Salpeter equation is used to obtain \( \Sigma^{\text{imp}} \) and to get the lattice susceptibility.

**ESTIMATE OF \( T_{\text{crit}} \) FOR A GIVEN CLUSTER**

- simulation at \( T = 0.05t \) (ordering at \( T > 0 \) is artifact of mean-field)
- spontaneous magnetization at \( \xi \approx L^{1/2} \)
- well fitted using the mean-field critical exponents \( \beta = 0.5, \gamma = 1.0 \)
- \( \text{consistent} \) \( T_{\text{crit}} \) estimates
- \( T_{\text{crit}} \) for a given cluster

**EXTRAPOLATION OF \( T_{\text{crit}} \) FOR A LATTICE**

- layered honeycomb lattice with \( t = t' = 6t \)
- \( \nu \) for the universality class of 3D Heisenberg model
- \( T_{\text{crit}} \) for a given cluster

\[
T_{\text{crit}}(U, t) \propto \frac{U}{t} \epsilon_{\text{crit}}(U/t)
\]

\( \epsilon_{\text{crit}}(U/t) \) is consistent around \( U/t = 6 \rightarrow T_{\text{crit}} \) (cubic: around \( U = 8t \) [5])

In the anisotropic case the \( T_{\text{crit}} \) goes expectedly down.

**REFERENCES**