Néel transition temperatures for the Hubbard model on layered honeycomb lattice

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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

} as DMFT

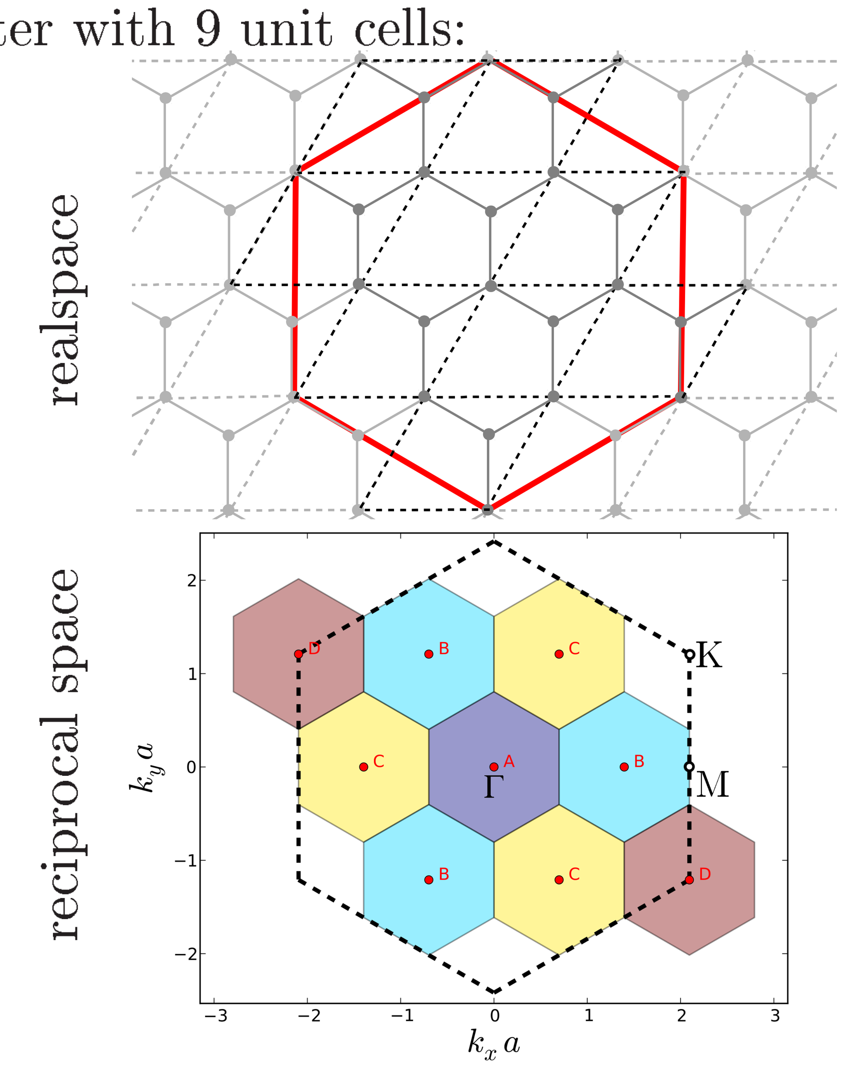
- limit of infinite cluster

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

DMFT: infinite coordination number
$\Rightarrow$ purely local (**k**-independent) selfenergy
$\Rightarrow$ approximation $\Sigma^{\rm lat}(\mathbf{k}) \approx \Sigma^{\rm imp}$
(constant over Brillouin zone)

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

Cluster with 9 unit cells:



DCA features:

- mean-field character if correlation length $\xi \gtrsim L^{1/d}$ (close to phase transitions of 2$^{\rm nd}$ kind)
- asymptotics: $\Sigma = \Sigma_L^{\rm DCA} + O\left(L^{-2/d}\right)$ (for extrapolation with cluster size L)

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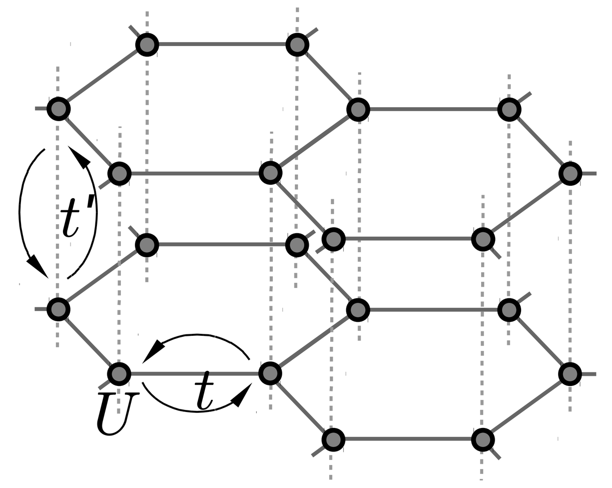
Model

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

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



Assuming $t' \leq t$.

Motivated by [7].

Technical details

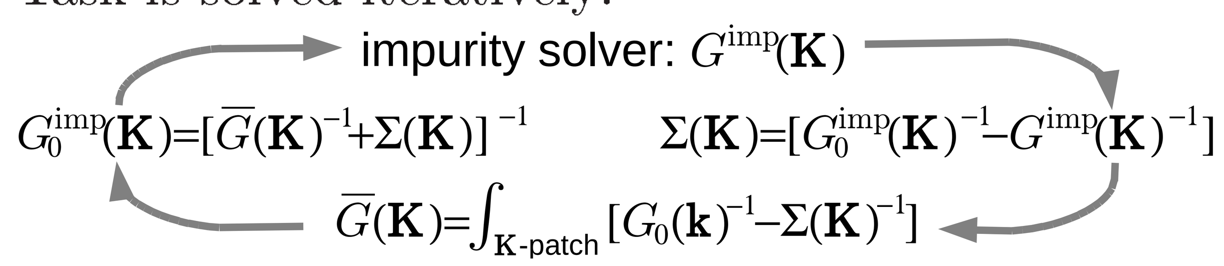
DMFT: selfconsistency condition

$$G^{\rm imp} = G^{\rm lat}_{\rm local} \equiv \frac{1}{\Omega}\int_{\rm Brillouin\ zone} \mathrm{d}\mathbf{k}\, G^{\rm lat}(\mathbf{k})$$

DCA: selfconsistency condition for L-cell cluster

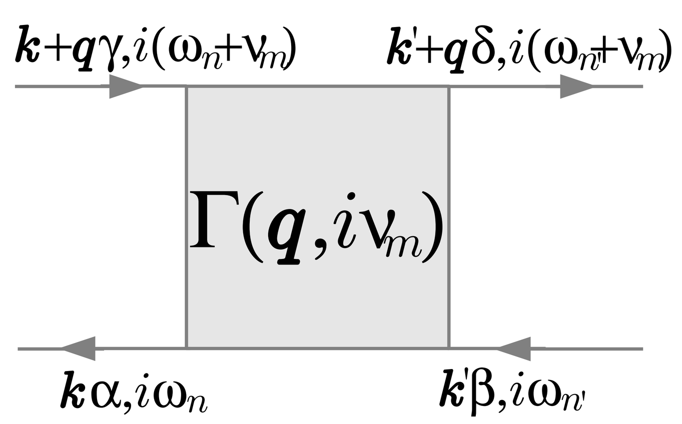
$$G^{\rm imp}(\mathbf{K}) = \frac{L}{\Omega}\int_{\mathbf{K}\text{-patch}} \mathrm{d}\mathbf{k}\, G^{\rm lat}(\mathbf{k})$$

Task is solved iteratively:



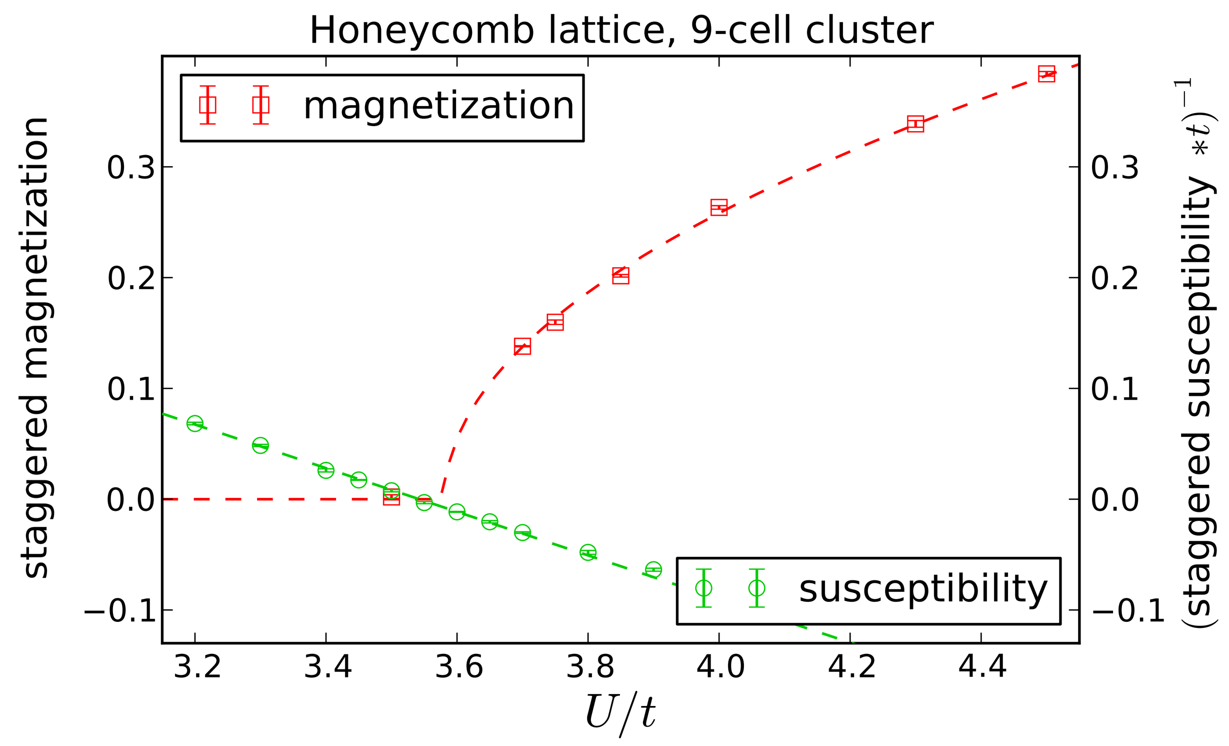
The impurity solver used: continuous time auxiliary field quantum Monte Carlo impurity solver (CT-AUX) [3, 4]

The lattice susceptibility is obtained based on approximation $\Gamma^{\rm lat} \approx \Gamma^{\rm imp}$ for the ireducible vertex.



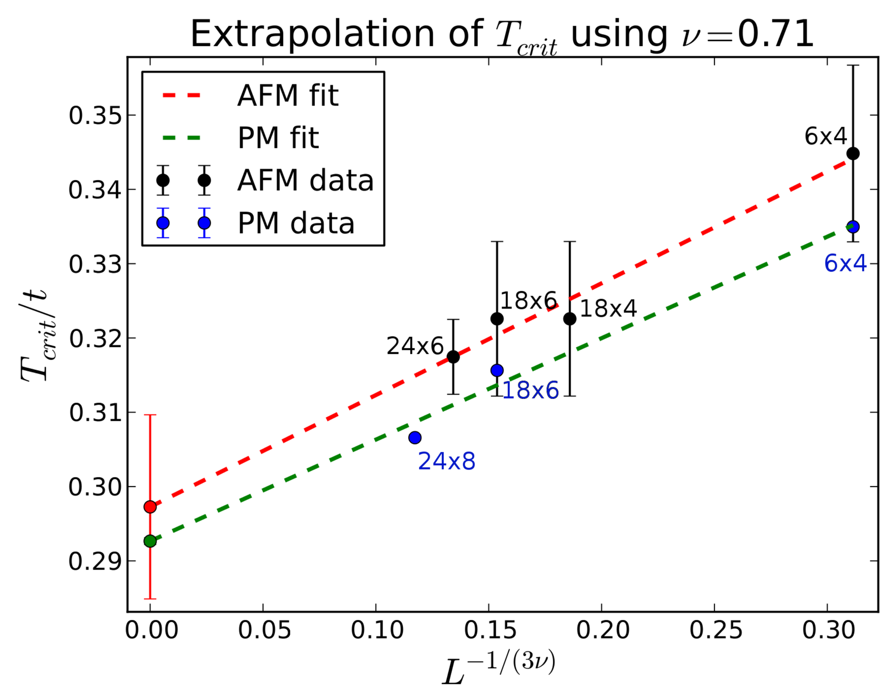
Bethe–Salpeter equation is used to obtain $\Gamma^{\rm imp}$ and to get the lattice susceptibility.

Estimate of $T_{\rm crit}$ for a given cluster



$\leftarrow$ simulation at $T = 0.05t$
(ordering at $T > 0$ is artifact of mean-field)
(spontaneous magnetization at $\xi \sim L^{1/2}$)
$\leftarrow$ well fitted using the mean-field critical exponents $\beta = 0.5$, $\gamma = 1.0$
$\leftarrow$ **consistent** $T_{\rm crit}$ estimates
$\leftarrow$ ω_n cut-off $N_\omega = 48$
(extrapolation in N_ω using 2$^{\rm nd}$ order high-frequency asymptotics; check possible by impurity based measurement $\langle \hat{m}(\tau)\hat{m}(\tau')\rangle$)

Extrapolation of $T_{\rm crit}$ for a lattice



$\leftarrow$ layered honeycomb lattice with $t = t'$, $U = 6t$
$\leftarrow$ ν for the universality class of 3D Heisenberg model
$\leftarrow$ AFM simulations suffer from critical slowing down (# of iterations explode $\Rightarrow$ only bounds found)
$\leftarrow$ PM simulations limited by memory $\propto L^2 T^{-2}$
$\leftarrow$ PM simulations performed using 4-site per cell ($\mathbf{q} = \mathbf{0}$) description, or more effectively by 2-site per cell ($\mathbf{q} = \pi\hat{\mathbf{e}}_z$)
$\leftarrow$ $N_\omega = 16$ (12 for largest cluster)

$T_{\rm crit}$ for the layered honeycomb lattice

U/t	t/t'	$T_{\rm crit}/t$	cluster
4.0	1.0	0.216(1)	6x4
6.0	1.0	0.297(12)	extr.
8.0	1.0	0.282(36)	extr.
6.0	2.0	0.251(16)	extr.
4.0	2.0	0.196(1)	18x2

Isotropic case:

- $T_{\rm crit}/t$ peaks around $U = 6t$ (cubic: around $U = 8t$ [5])
- $S_{\rm crit}(U = 6t) = 0.409(44)$
(cubic: $S_{\rm crit}(U = 8t) = 0.487(23)$ [6])

In the anisotropic case the $T_{\rm crit}/t$ goes expectedly down.

References

[1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg: Rev. Mod. Phys. **68**, 13 (1996)
[2] M. Jarrell, Th. Maier, C. Huscroft, and S. Moukouri: Phys. Rev. B **64**, 195130 (2001)
[3] E. Gull, P. Werner, O. Parcollet, and M. Troyer: 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: Phys. Rev. B **83**, 075122 (2011)
[5] S. Fuchs, E. Gull, L. Pollet, E. Burovski, E. Kozik, T. Pruschke, M. Troyer: Phys. Rev. Lett. **106**, 030401 (2011)
[6] J. Imriška, M. Iazzi, L. Wang, E. Gull, D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, M. Troyer: Phys. Rev. Lett. **112**, 115301 (2014)
[7] T. Uehlinger, G. Jotzu, M. Messer, D. Greif, W. Hofstetter, U. Bissbort, T. Esslinger: Phys. Rev. Lett. **111**, 185307 (2013)