Quantum phase transition in the Hubbard model on the honeycomb lattice

Jakub Imriška[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 apply the dynamical cluster approximation, an extension of the dynamical mean-field approximation, on the Hubbard model on the honeycomb lattice and investigate the quantum phase transition. Our results are compatible with the direct quantum phase transition from the paramagnetic semimetal to the antiferromagnetic insulator, without the hypothesized intermediate spin-liquid phase [1], and in agreement with the finite size simulations [2, 3] and a recent DCA study of the extended Hubbard model [8]. Performing simulations both in the paramagnetic and in the sublattice symmetry broken (i.e. allowing an antiferromagnetic ordering) regime, we are able to extrapolate the critical interaction U/t and find the single particle gap above the critical interaction.

DCA method

We use dynamical cluster approximation (**DCA**) [5], a cluster extension of the dynamical mean-field theory (DMFT) [4].

It is *exact* in the:

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

(as DMFT)

- limit of infinite cluster

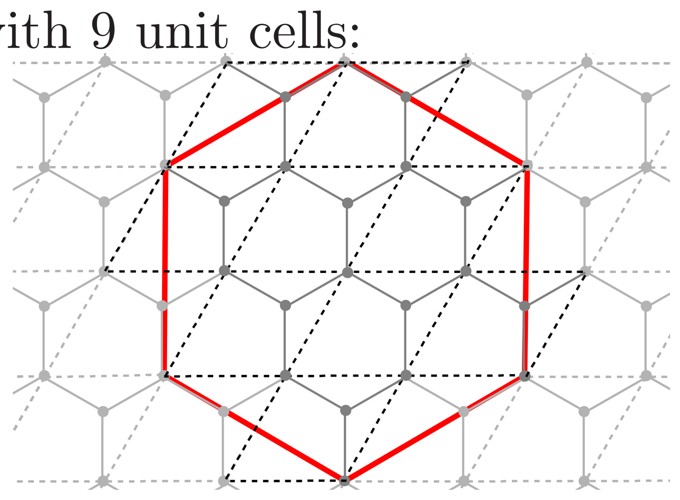
The lattice problem is selfconsistently mapped onto an impurity (=cluster) with periodic boundary conditions and additional noninteracting bath.

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

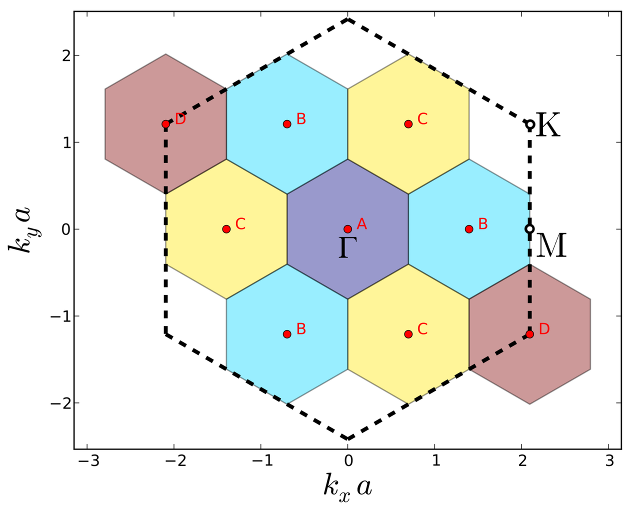
DCA: mapping in the reciprocal space of the cluster, approximation $\Sigma^{\text{lat}}(\mathbf{k}) \approx \Sigma^{\text{imp}}(\mathbf{K})$ (constant over patch)

Cluster with 9 unit cells:

realspace



reciprocal space



DMFT: selfconsistency condition

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

DCA: selfconsistency condition for L-cell cluster

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

Task is solved iteratively:

impurity solver: $G^{\text{imp}}(\mathbf{K})$

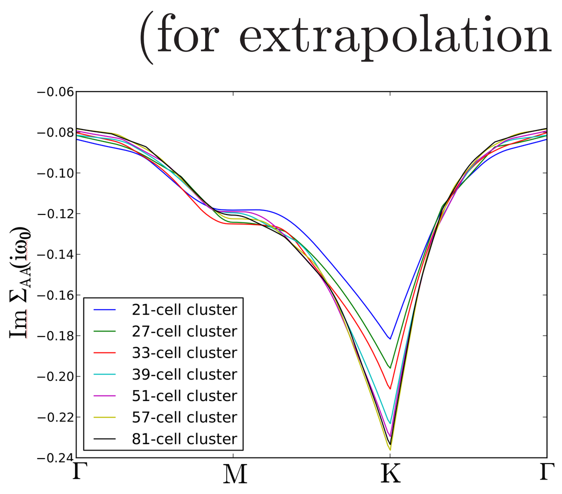
$G_0^{\text{imp}}(\mathbf{K}) = [\bar{G}(\mathbf{K})^{-1} + \Sigma(\mathbf{K})]^{-1}$ $\qquad \Sigma(\mathbf{K}) = [G_0^{\text{imp}}(\mathbf{K})^{-1} - G^{\text{imp}}(\mathbf{K})^{-1}]$

$\bar{G}(\mathbf{K}) = \int_{\mathbf{K}\text{-patch}} [G_0(\mathbf{k})^{-1} - \Sigma(\mathbf{K})^{-1}]$

The impurity solver used: continuous time auxiliary field quantum Monte Carlo impurity solver (CT-AUX) [6, 7]

DCA features:

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



← $T = 0.1t$, $U = 4t$
← PM simulation
← natural neighbor interpolation (only to display)

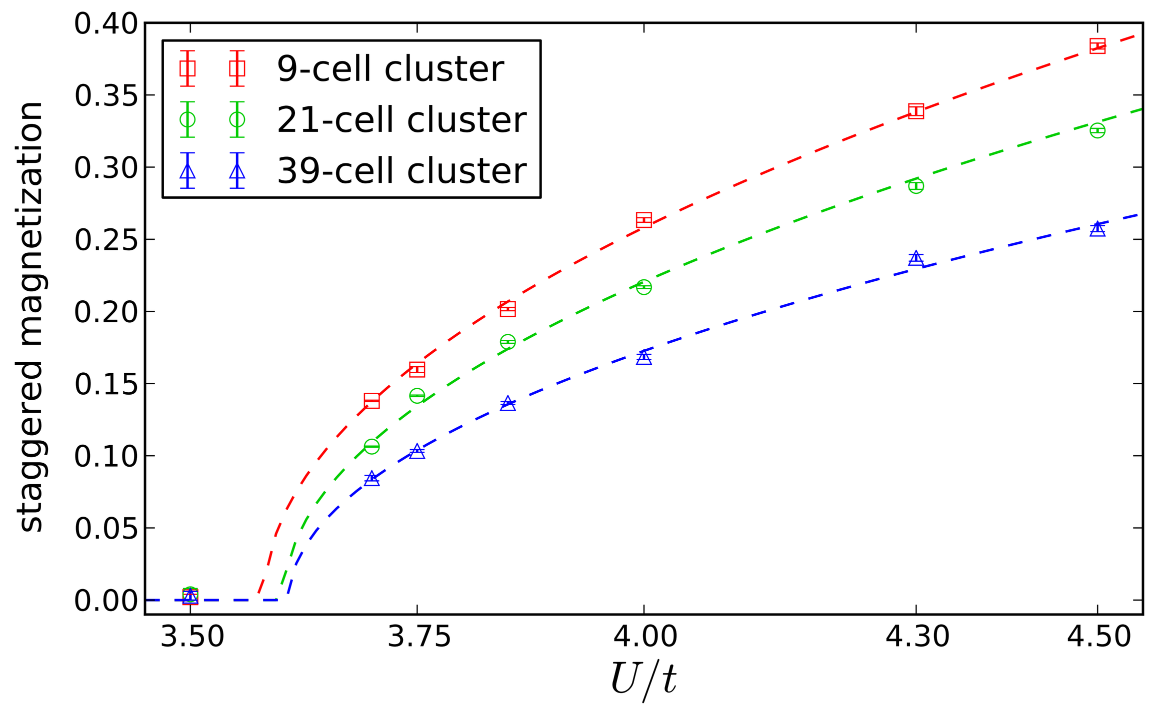
Model

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

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

Paramagnetic semimetal at $U = 0$ (tight-binding model for graphene); gap vanishes at K-points.
Mermin–Wagner–Hohenberg theorem: long-range (AF) ordering possible only at $T = 0$.
The model is sign-problem-free at half filling, where it was studied by projective MC [1, 2, 3].

Simulation allowing antiferromagnetic (AF) ordering



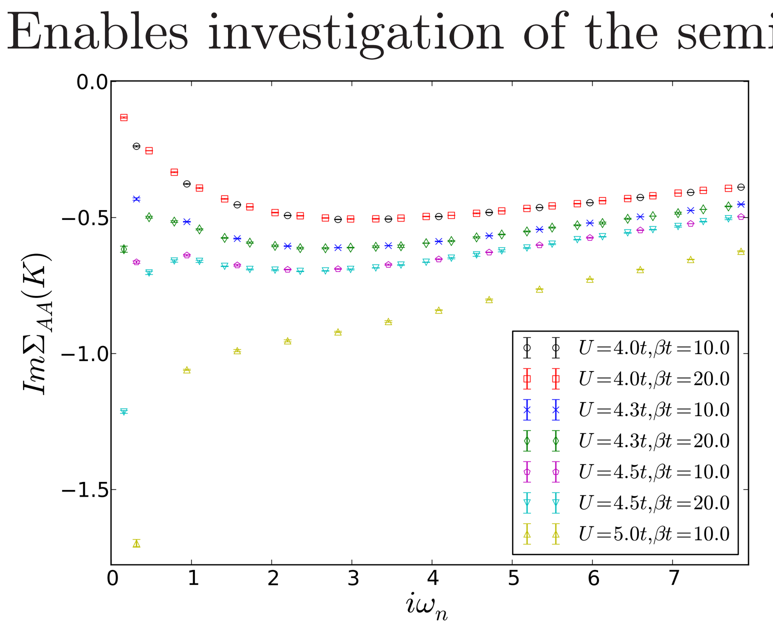
← simulation at $T = 0.05t$
← well fitted using the mean-field critical exponent $\beta = 0.5$

- mean-field allows (unphysical) ordering at $T > 0$
- spontaneous magnetization at U^L_{crit}:

$$L^{1/2} \sim \xi(U^L_{\text{crit}}(T), T)$$

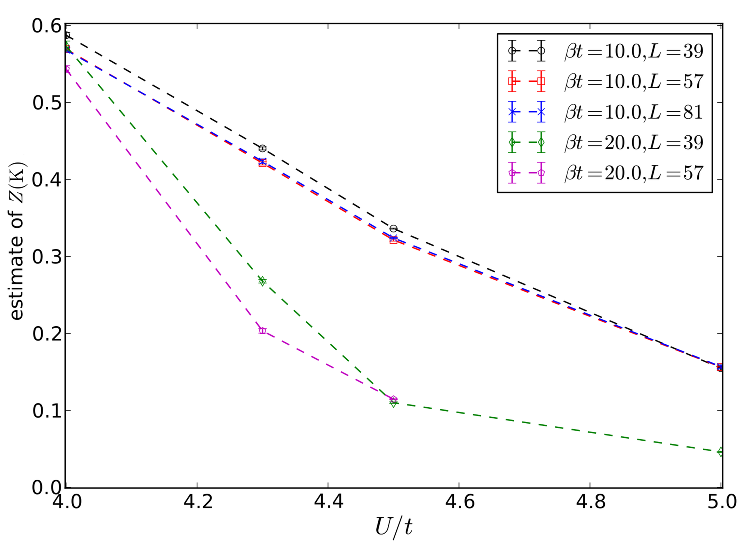
Simulation within the paramagnetic (PM) regime

Enforcing PM prevents (unphysical) AF ordering at $T > 0$.
Enables investigation of the semimetal to insulator transition.



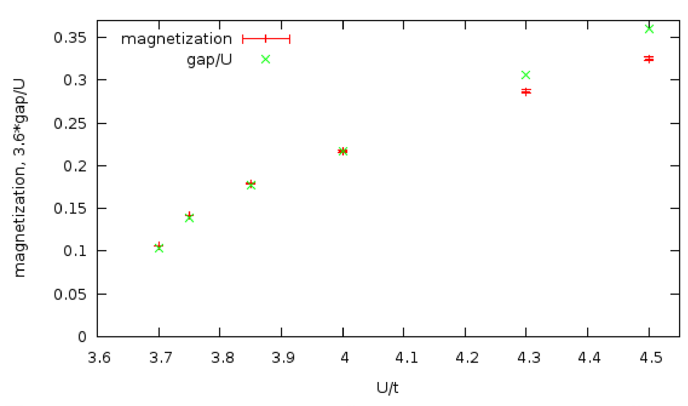
← simulation using 57-cell cluster
← pole emerges in the selfenergy at the Dirac point K
$\Rightarrow$ insulator for $U \geq 4.3t$

estimate of quasiparticle weight
$Z(K) \approx \left(1 - \frac{\Im\Sigma_{AA}(K, i\omega_0)}{\omega_0}\right)^{-1}$ →



Single particle gap Δ_{sp} at the Dirac K-point could be obtained via fitting of the $G(K, \tau; T = 0.05t)$ close to $\tau = \beta/2$ for $U \geq 4.3t$ (reliably as $\Delta_{sp} \gg T$); within error bar consistent with [3].
Gap verified by simulations away from half filling: clear evidence by $n(\mu; U, T)$ at $U = 5t$, $T = 0.05t$.

Conclusions and comparison with other studies



← single particle gap Δ_{sp}/U obtained in the AF simulation by fitting of $G(K, \tau; T = 0.05t, L = 21)$ shows same functional form as the staggered magnetization up to $U = 4t$
← quantitatively different from [3] (mean-field regime)

Long-range ordering precedes the potential semimetal-to-insulator transition, contrary to the finding in [1], and in agreement with [2, 3]. We cannot provide as precise estimate of U_{crit} as in [2, 3], with $U_{\text{crit}}/t \in (3.8, 3.9)$ and $U_{\text{crit}} = 3.78t$, resp.
Discrepancy in the selfenergy (existence of pole at $\omega = 0$) with respect to [8] for $T = 0.05t$, $L = 12$, $U \approx 4.4t$, which may originate from bath discretization in the impurity solver employed in [8].

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