Correlations in the anisotropic Hubbard model

Jakub Imriška[1]

[1]Computational physics group of Prof. Matthias Troyer,
Institut für theoretische Physik,
Eidgenössische Technische Hochschule, Zürich

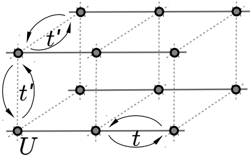
Passugg, Graubünden, CH, June 10 - 13, 2014

Model

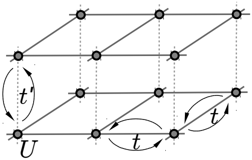
Hubbard model:

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

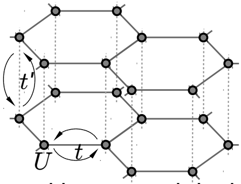
$$\hat{\mathscr{H}} = -\sum_{\langle i,j \rangle, \sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$



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:

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

Neglect spatial & temporal fluctuations:

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

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

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 $Z \to \infty$ ($dim \to \infty$).

Quantum models: variational approach.

DMFA/DMFT concept

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:

$$\frac{1}{\Omega_{BZ}} \int_{BZ} \mathrm{d}\mathbf{k}\, G_{lat}(\mathbf{k}) = G_{lat,local} = G_{imp}$$

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

DMFT solution scheme

Iterative solution scheme:

Monte Carlo solver: G_{imp}

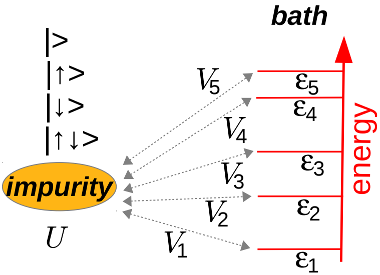
$$G^0_{imp} = [\overline{G}^{-1} + \Sigma]^{-1} \qquad \Sigma = {G^0_{imp}}^{-1} - {G_{imp}}^{-1}$$

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

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

impurity + bath

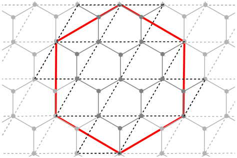
Anderson impurity model



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

Dynamical Cluster Approximation (DCA)

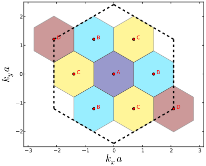
DCA: cluster extension of the DMFA (exact for infinite cluster)



9-cell cluster
on hexagonal lattice

$\leftarrow$ realspace

reciprocal space $\rightarrow$



- Mapping in reciprocal space:

$$\frac{1}{\Omega_{patch}} \int_{patch} \mathrm{d}\tilde{\mathbf{k}}\, G_{lat}(\mathbf{K} + \tilde{\mathbf{k}}) = G_{imp}(\mathbf{K}) \qquad (1)$$

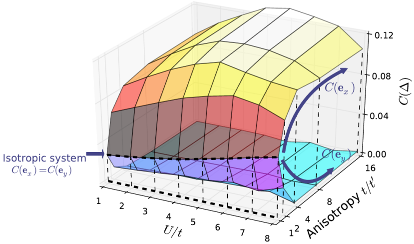
- Selfconsistency: $\Sigma^{\mathrm{lat}}(\mathbf{K} + \tilde{\mathbf{k}}, i\omega_n) \approx \Sigma^{\mathrm{imp}}(\mathbf{K}, i\omega_n)$
- Solution scheme: iterative as for DMFT, for each **K**-point

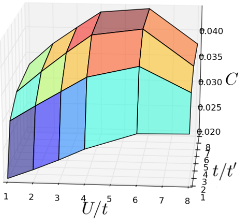
Nearest-neighbor spincorrelations

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

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

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

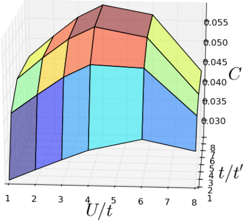




Layered lattices
at $S/N = 0.8$
at half filling

$\leftarrow$ layered square

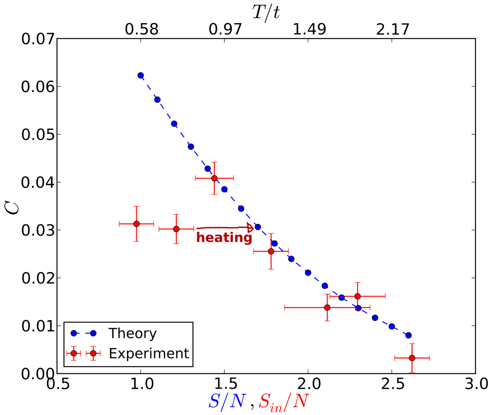
layered honeycomb $\rightarrow$



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

Coupled 1D chains: comparison with experiment

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



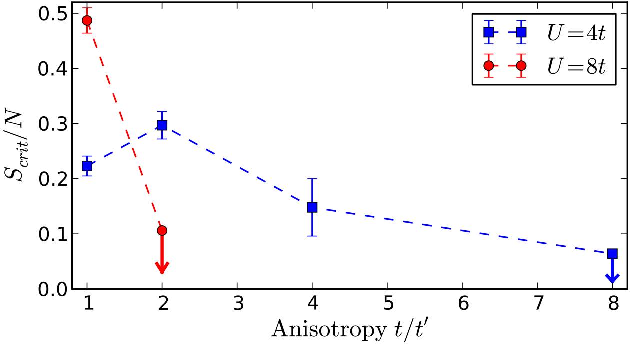
Main plot: coupled 1D chains, $U/t = 1.4375$, $t/t' = 7.36$

Ref.: PRL **112**, 115301 (2014)

Long-range order

- 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_{crit}/N for isotropic cubic lattice.

Critical entropy per particle for half filled coupled 1D chains



Acknowledgement

Prof. **Matthias Troyer**'s Computational Physics Group
(ITP, ETH Zürich)
Dr. **Lei Wang** Dr. **Mauro Iazii**

Assistant Prof. **Emanuel Gull**
Computational condensed matter physics group
(Physics department, University of Michigan)

Prof. **Tilman Esslinger**'s Quantum Optics Group
(Institute for Quantum Electronics, ETH Zürich)
Dr. **Daniel Greif** Dr. **Thomas Uehlinger**
Gregor Jotzu

Assistant Prof. **Leticia Tarruell**
Ultracold quantum gases
ICFO, Castelldefels (Barcelona), Spain