The Fate of the Mott-Hubbard Transition in 2D

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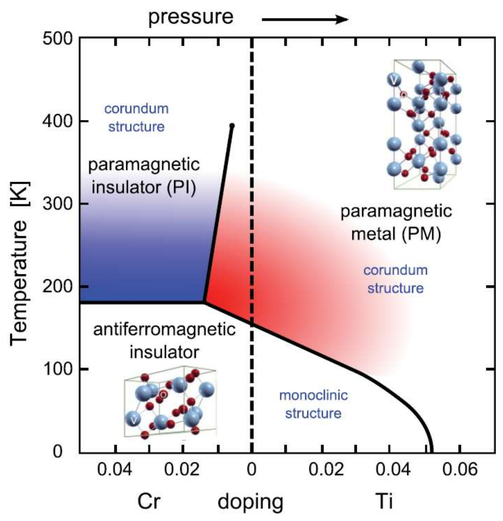
Introduction: The Mott-Hubbard transition



Strongly correlated electron systems can exhibit a vast variety of interesting physical phenomena such as the Mott-Hubbard metal to insulator transition **(MIT [1])**. Due to the strong Coulomb repulsion in the partially filled 3d or 4f orbitals, single particle descriptions (e.g. bandtheory) as well as perturbative descriptions are **not applicable**.

Simple description of electronic correlations

Basic model for correlations:
Hubbard Hamiltonian

$$\mathbf{H} = -\mathbf{t} \sum_{(i,j),\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \mathbf{U} \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

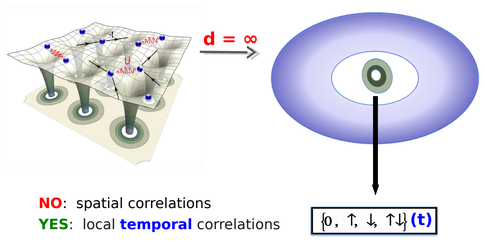
- **t**: electron hopping term *
- **U**: Coulomb repulsion in case of double occupancy

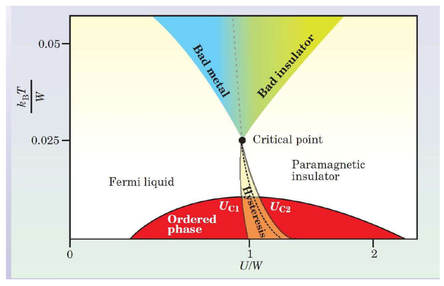
Not solvable analytically in arbitrary dimensions, its properties can be analysed by means of the dynamical mean field theory **(DMFT)**.

* All calculations on this poster have been carried out for the half-filled, two-dimensional Hubbard model and all energies are measured in units of $\mathbf{4t = 1}$.

The dynamical mean field theory (DMFT)

In the **DMFT** [2] the full many-body Hamiltonian is mapped onto a (self-consistent) single-site Anderson impurity model, creating a **spatial mean field** while keeping all **temporal (quantum) fluctuations**.





[3]

Famous **DMFT** results
Non-perturbative analysis of the MIT [3], predictions of spectroscopic experimental results for e.g. $\mathbf{V_2O_3}$ [4], description of δ-phase of **Pu** [5], ...

DMFT also shows **anomalous** physics
Kinks [6], formation of large instantaneous magnetic moments, abrupt change of the out-of-equilibrium behaviour after a quench of the electronic interaction [7].

Paths to the inclusion of non-local correlations beyond DMFT

Cluster extensions of **DMFT**/**Cluster** methods

- Cellular DMFT (**CDMFT** [8])
- Dynamical Cluster Approximation (**DCA** [8])
- Variational Cluster Approximation (**VCA** [9])

} **short range** spatial correlations limited by cluster size

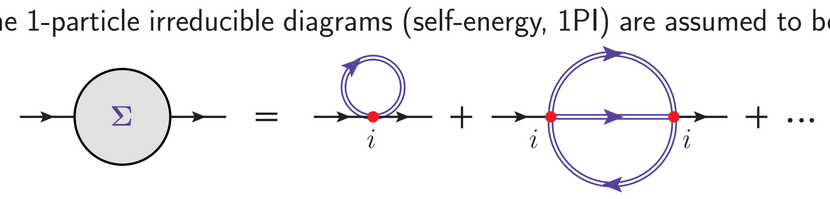
Diagrammatic extensions of **DMFT** based on vertex functions [10, 11]

- Dynamical Vertex Approximation (**DΓA** [12])
- Dual Fermion Approach (DF [13])
- One-particle irreducible approach (1PI [14])
- DMFT and functional RG (DMF^{2}RG [15])

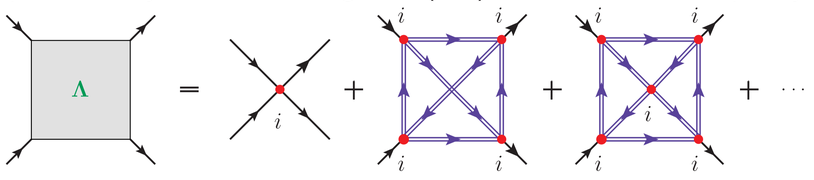
} systematic inclusion of spatial correlations on **every length-scale**

Diagrammatic content and principle of DΓA

In **DMFT** the 1-particle irreducible diagrams (self-energy, 1PI) are assumed to be purely **local**

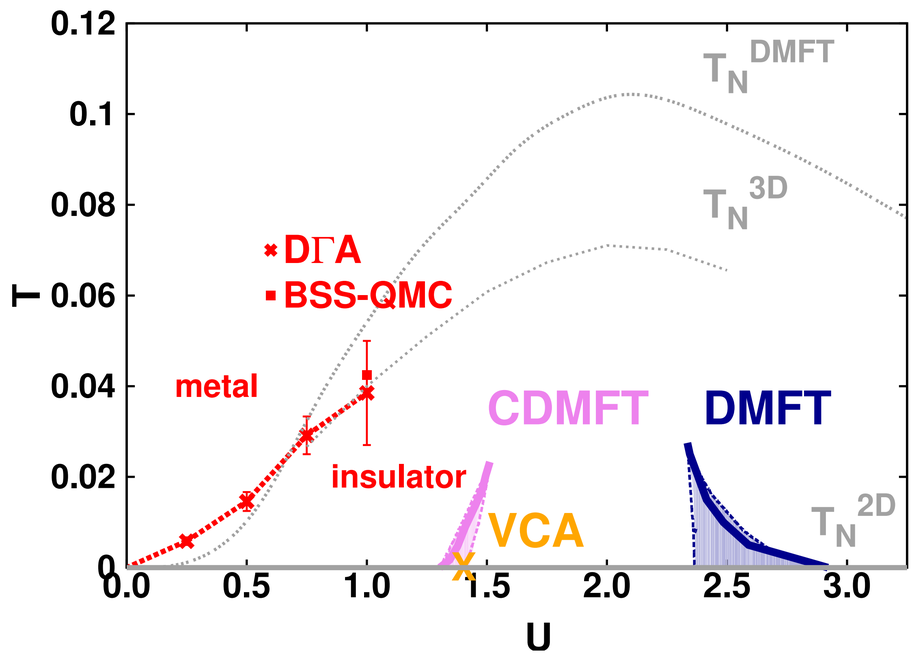


In **DΓA** the 2-particle fully irreducible diagrams (2PI) are assumed to be purely **local**



what results in a (systematically) **non-local** self-energy.

Phase diagram in two and infinite dimensions [16]



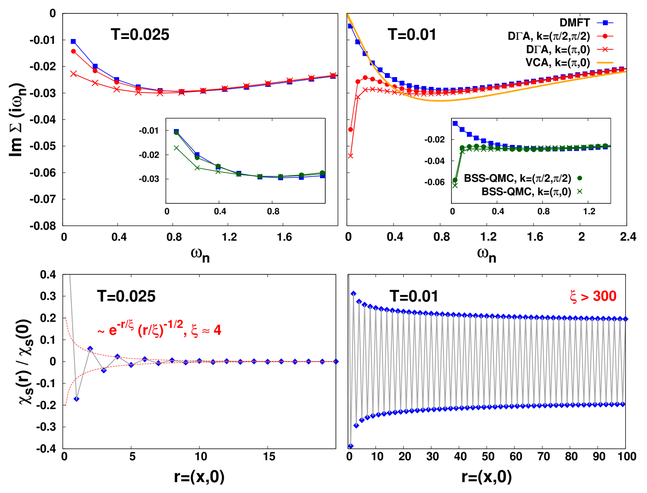
Inclusion of **short-range spatial correlations** (**CDMFT** [8], **VCA**) leads to:

- reduction of $\mathbf{U_C}$ (but $\mathbf{U_C}$ still finite)
- shrinking of the coexistence region
- inversion of slope of transition line

Inclusion of **spatial correlations on all length scales** (**DΓA**) results in:

- only a crossover region remaining from the MIT (confirmed by **BSS-QMC** [17])
- for $\mathbf{U > 0}$, at low enough **T**, an insulator is always found $\Rightarrow$ no MIT in **2D**

One- and two-particle level analysis at U=0.5 [16]

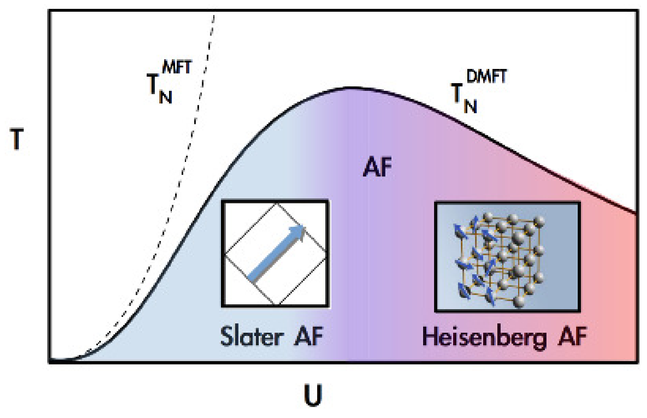


For **T** slightly above the **DΓA** crossover line the self-energy shows (w.r.t. **DMFT** renormalized) metallic behaviour, which changes drastically below the crossover line.

The spin correlation function in real space exhibits antiferromagnetic **fluctuations**, which become (quasi-) **long-ranged**, going to smaller **T**.

$\Rightarrow$ **Long-ranged spin fluctuations** open the gap.

Stabilizing the magnetism: Slater vs. Heisenberg [16]



Which part of the energy stabilizes antiferromagnetic behaviour in the weak-coupling regime? If **T** is lowered **DΓA** shows a **decrease in double occupancy** of $\approx \mathbf{1\%}$, which corresponds to an equal decrease in potential energy, indicating **Slater-paramagnons** as the driving force of the fluctuations.

Conclusions and outlook

- The MIT is **absent** in the (half-filled) Hubbard model in two dimensions: For every finite value of the local Coulomb interaction an insulating gap is opened at low enough temperature (crossover).
- The gap is opened by **long-ranged antiferromagnetic spin fluctuations**.
- The nature of those fluctuations is **Slater-like** in the weak-coupling regime.
- **Outlook:** Frustration of the lattice by adding next-to-nearest-neighbour hopping or doping.

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