The doped Hubbard model

Moritz Reh

Outline

- The Hubbard model
    - Introduction & Motivation
    - Theory
    - Difficulties
    - Phases
- Microscopic approaches
    - Geometric string theory
    - π-flux theory

The Hubbard model - Introduction & Motivation

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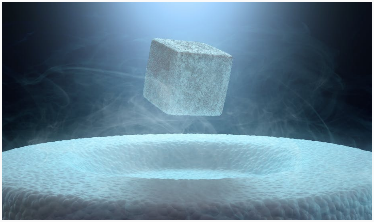
- Goal: Better understanding of the high T_c superconduction in cuprates



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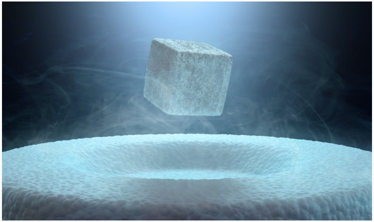

- Physically: Radial wave function in 3d transition metals has small extent

The Hubbard model - Introduction & Motivation

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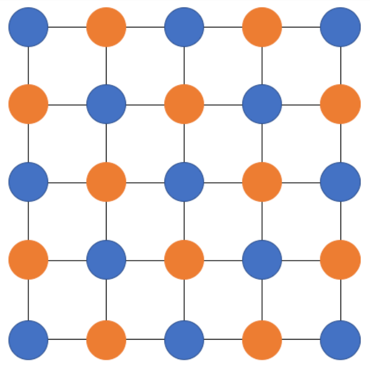

Hubbard model at $T = 0$ and doping $\delta = 0$

The Hubbard model - Introduction & Motivation

- Fermi-Hubbard model: Hopping between neighboring sites and on-site interaction

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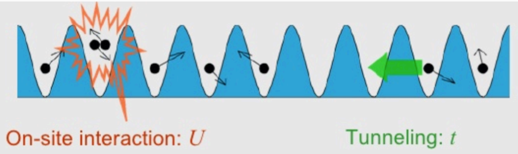
$$H_{Hubb.} = \underbrace{-t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma}}_{Hopping} + \underbrace{U \sum_{i} n_{i,\downarrow} n_{i,\uparrow}}_{Coulomb-repulsion}$$



Fermi-Hubbard scheme, Source: Utrecht University

The Hubbard model - Introduction & Motivation

- Experimental realization: ultracold atoms in an optical lattice ($\rightarrow$ second talk)

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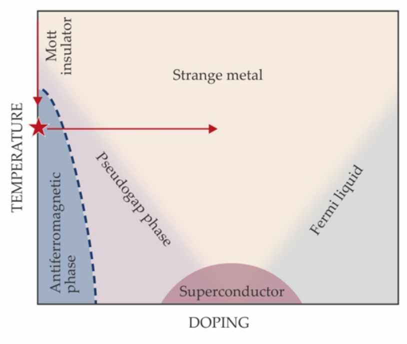
- Recreate phases of cuprate superconductors with the Hubbard Hamiltonian



Phase diagram of the Fermi-Hubbard model, Source: Physics Today

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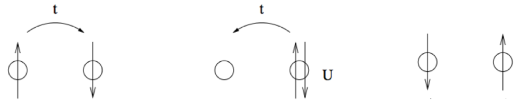
- limit $U \gg t$: no double occupancies



Exchange processes, Source: Augsburg University

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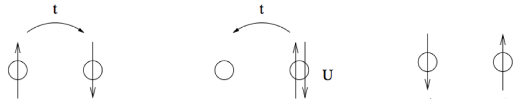

Exchange processes, Source: Augsburg University

- obtain the t-J Hamiltonian for $U \gg t$ ($J = \frac{4t^2}{U}$):

$$H_{t-J} = -t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

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- Additionally: low temperatures, large β ⇒ high value for m (Error control with $\Delta\tau$, see Daniel Kirchhoff slides)

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- Numerical sign problem

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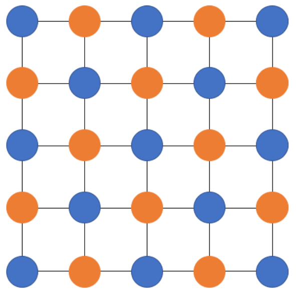

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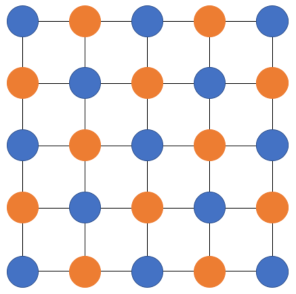

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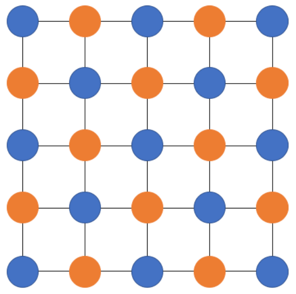
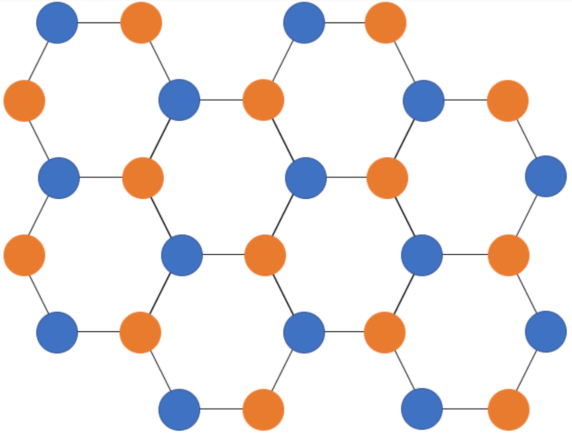


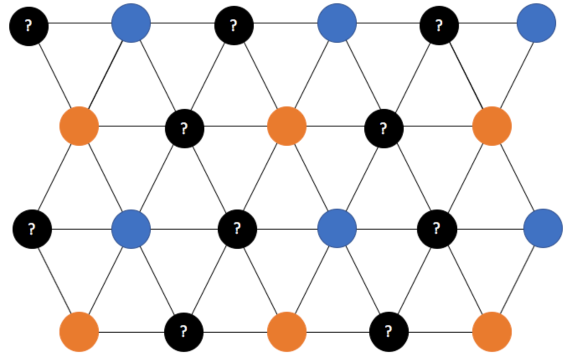
- Bipartite lattices naturally make ideal antiferromagnets
- Antiferromagnetism in non-bipartite lattices is called frustrated antiferromagnetism.

The Hubbard model - Phases



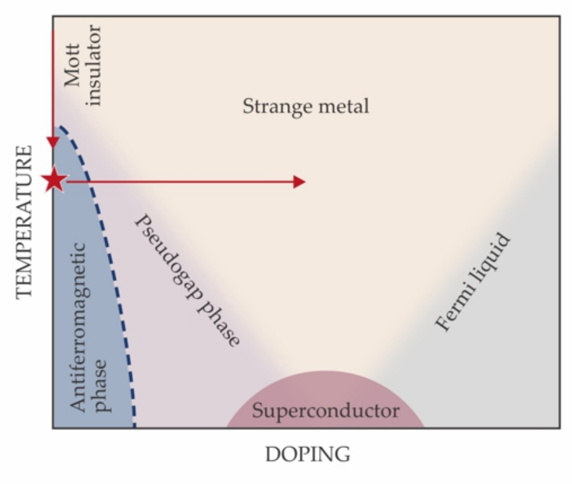
The honeycomb lattice is a bipartite lattice

The Hubbard model - Phases



The triangular lattice is NOT a bipartite lattice

The Hubbard model - Phases



Phase diagram of the Fermi-Hubbard model, Source: Physics Today

Microscopic approaches - Geometric string theory

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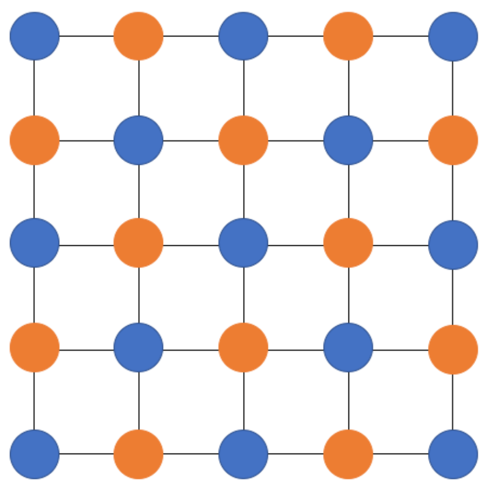
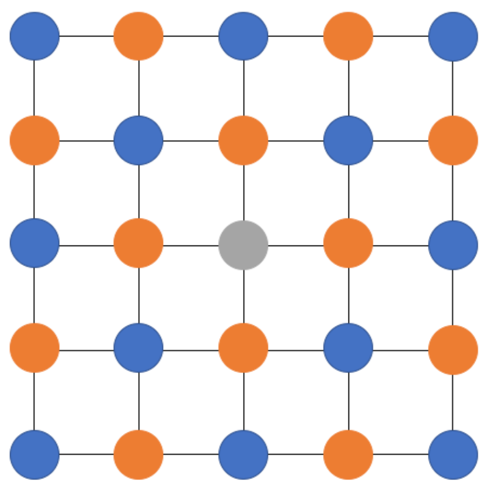
$|\psi\rangle = |\psi_{1/2}\rangle$ AFM ground state



$\Delta E = 0J$

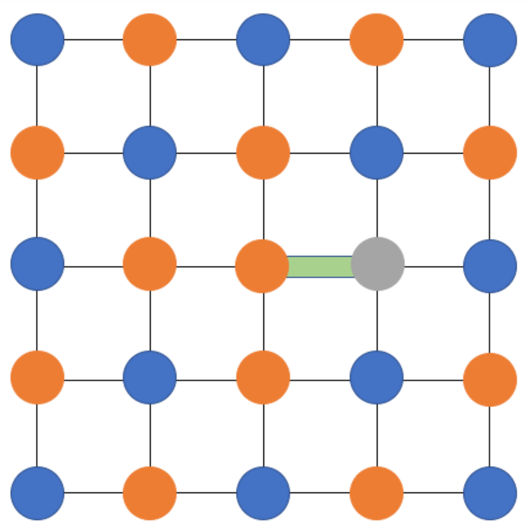
Microscopic approaches - Geometric string theory

$$|\psi\rangle = c_{\vec{j},\sigma}\,|\psi_{1/2}\rangle = |\vec{j} = \begin{pmatrix} 2 & 2 \end{pmatrix}^T, \sigma = \text{blue}, l = 0\rangle$$

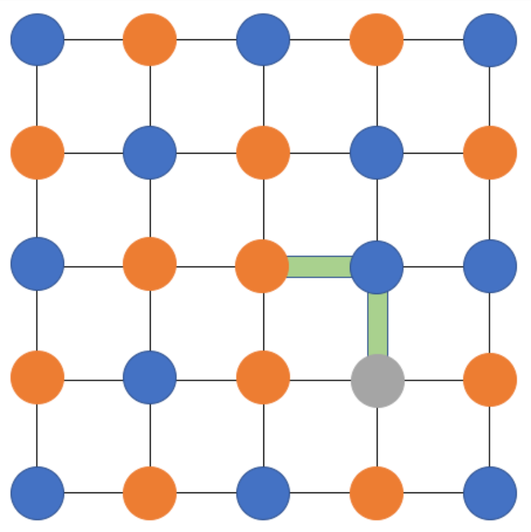


$$\Delta E = 8J$$

Microscopic approaches - Geometric string theory

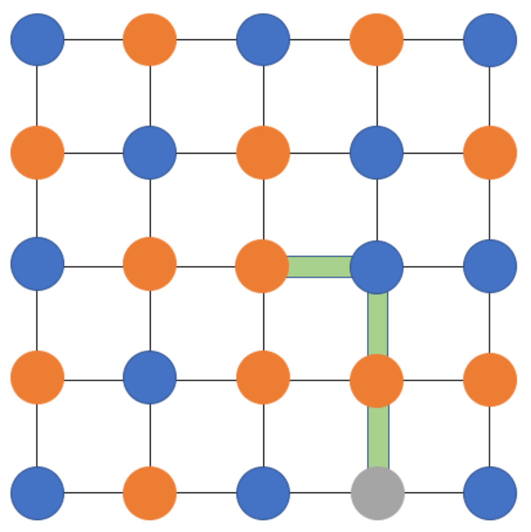


$\Delta E = 20J$



$$\Delta E = 28J$$

Microscopic approaches - Geometric string theory



$$\Delta E = 36J$$

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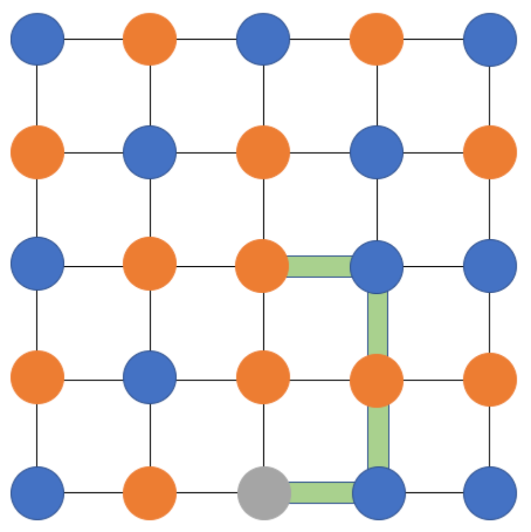
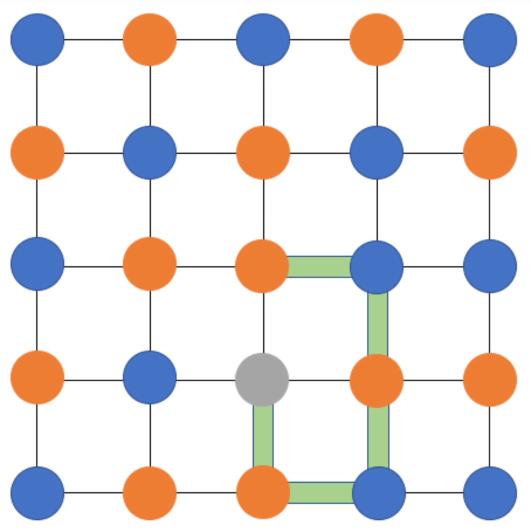


$$\Delta E = 44J$$

Microscopic approaches - Geometric string theory



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Microscopic approaches - Geometric string theory

- Starting point: undoped Heisenberg spin model at half filling

$$H_{Heisenberg} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

with $|\vec{S}| = 1$.

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- Describe the motion of holes with string states:
  trivial string state (hole): $|\vec{j}, \sigma, l = 0\rangle = c_{\vec{j},\sigma} |\psi_{1/2}\rangle$
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- Lets look at the energy change that comes with such strings!

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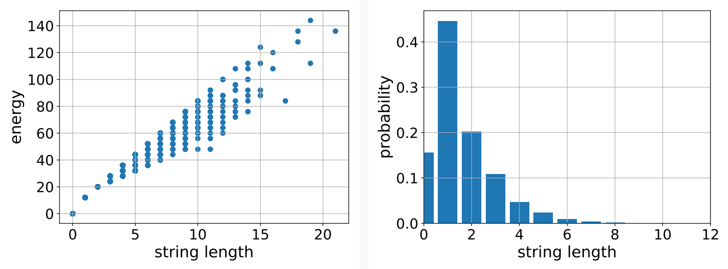
- Simulations on an 8x8 lattice (periodic boundary conditions) show this correlation (simulation with AFM Ising-Spins):



Energies and probabilities of string lengths

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- $H_J = \Sigma_\Sigma V_{Pot}(l_\Sigma)$, $V_{Pot}(l_\Sigma) = \frac{dE}{dl} l_\Sigma + g_0 \delta_{l_\Sigma,0} + \mu_h$

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- linear string tension: $\frac{dE}{dl} = 2J(C_s(\sqrt{2}) - C_s(1))$
  attractive potential: $g_0 = -J(C_s(2) - C_s(1))$
  overall offset: $\mu_h = J(1 + C_s(2) - 5C_s(1))$

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- $C_s(d)$: spin-spin correlator at distance d

$$C_s(d) = (-1)^{|\vec{d}|} \frac{\langle S^z_{\vec{i}} S^z_{\vec{i}+\vec{d}} \rangle - \langle S^z_{\vec{i}} \rangle \langle S^z_{\vec{i}+\vec{d}} \rangle}{S^2}$$

Microscopic approaches - π-flux theory

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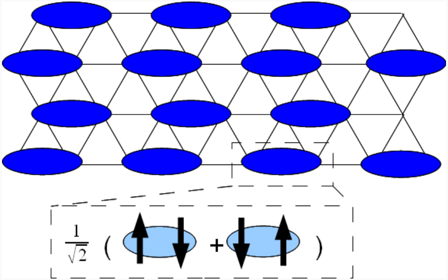
- Resonating valence bond (RVB) theory: Theory to describe superconduction in cuprates by valence bonds



Nearest neighbor valence bonds, Source: Wikipedia

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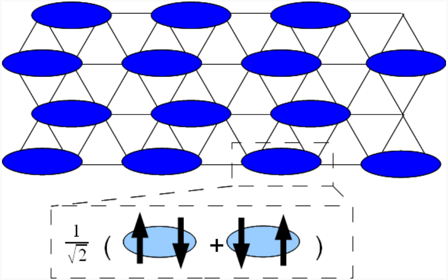

Nearest neighbor valence bonds, Source: Wikipedia

- Doping allows electrons to act as mobile cooper pairs

Microscopic approaches - π-flux theory

- π-flux states: particular class of RVB-wavefunctions, $\theta = \frac{\pi}{4}$

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- Mean-field Hamiltonian (A and B are sublattices):

$$
\begin{aligned}
H_{MF} = &-\frac{1}{2}J^* \sum_{\vec{i} \in A, \sigma} e^{-i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{x},\sigma} + e^{i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{y},\sigma} + h.c. \\
&-\frac{1}{2}J^* \sum_{\vec{i} \in B, \sigma} e^{i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{x},\sigma} + e^{-i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{y},\sigma} + h.c.
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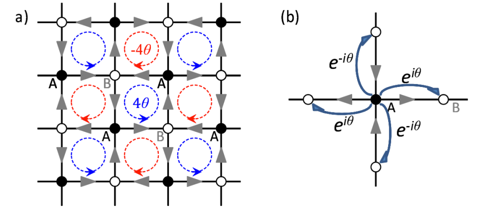
$$-\frac{1}{2}J^* \sum_{\vec{i} \in B, \sigma} e^{i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{x},\sigma} + e^{-i\theta} c^\dagger_{\vec{i},\sigma} c_{\vec{i}+\vec{y},\sigma} + h.c.$$



(a) staggered magnetic field, (b) hopping amplitudes, Source: arXiv 1610.04818

Microscopic approaches - π-flux theory

- MC sampling of Fock states:

$$\rho = \mathcal{P}_{GW} e^{-H_{MF}\beta} \mathcal{P}_{GW}$$

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- probability distribution of Fock-states $|\alpha_{\vec{k}}\rangle$ (momentum space):

$$p_\beta(\alpha_{\vec{r}}, \alpha_{\vec{k}}) = e^{-\beta E(\alpha_{\vec{k}})} \left| \langle \alpha_{\vec{r}} | \alpha_{\vec{k}} \rangle \right|^2$$

with

$$E(\alpha_{\vec{k}}) = \sum_{\vec{k} \; occ. \; in \; \alpha_{\vec{k}}} \epsilon_{\vec{k}}$$

Microscopic approaches - π-flux theory

- artificially add doublon-holon pairs on neighboring sites with opposite spins (Probability $p = 4\frac{t^2}{U^2}$) and measure the anti-moment correlator:

$$C_h(|\vec{d}|) = \langle (1 - n_{\vec{i},\sigma})(1 - n_{\vec{i}+\vec{d},\sigma}) \rangle - \langle 1 - n_{\vec{i},\sigma} \rangle \langle 1 - n_{\vec{i}+\vec{d},\sigma} \rangle$$

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- Fitting parameter: $J^* = 3J$

Thanks for your attention!

- Questions?
- Sources & further reading:
  - Hubbard model:
    - Magnetic Properties of the One-Band Hubbard Model
    - The Two-Dimensional Hubbard Model
    - Antiferromagnetism in the Hubbard model (Talk)
  - Geometric string theory:
    - String patterns in the doped Hubbard model
    - Fabian Grusdt - Geometric string theory (Talk)
    - Meson formation in mixed-dimensional t-J models
  - π-flux theory:
    - The Resonating Valence Bond State in La_2CuO_4 and Superconductivity
    - Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model
    - Large-n limit of the Hubbard-Heisenberg model