Magnetic phases of the one-dimensional frustrated Kondo lattice

XX Training Course in the Physics of Strongly Correlated Systems

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DER FORSCHUNG | DER LEHRE | DER BILDUNG

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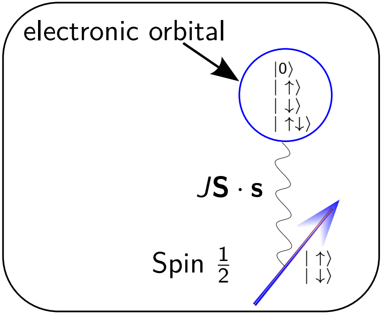
Model and method

Model and method

Kondo lattice model

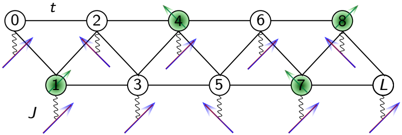
One atom:



8 local basis states in total

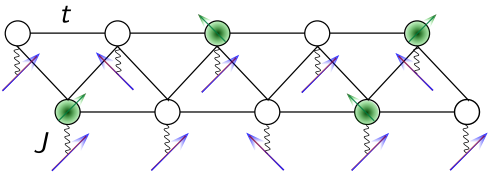
lattice:

$$H = -t \sum_{\langle i,j\rangle\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + J \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i$$



Kondo lattice model – included physics

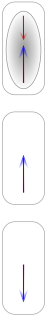
- indirect magnetic coupling (RKKY)
  - Ferromagnetism
  - Antiferromagnetism
- Kondo effect
- Heavy fermions
- Spin liquid
- ...



Strong coupling limit

Lacroix [1985]

Kondo model ($J = \infty$) ⟺ Hubbard model ($U = \infty$)



$|e\rangle$

$|\uparrow\rangle$

$|\downarrow\rangle$

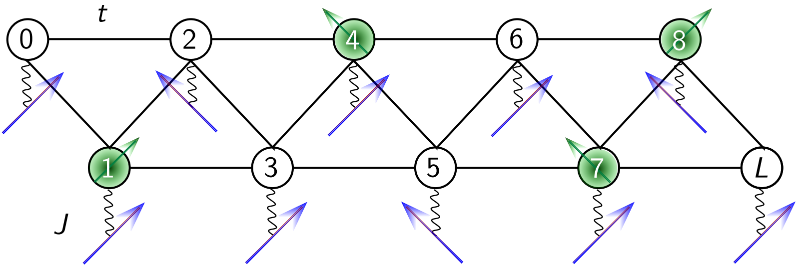
❗ Effectively the localized spins hop through the lattice

Frustrated geometry

- One-dimensional zig-zag ladder
- $J > 0$: antiferromagnetic Kondo model
- open boundary conditions

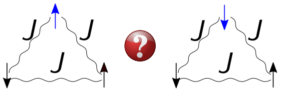
$L = 40$

$t = 1$



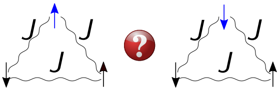
Geometrical frustration

General picture of frustration

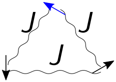


Geometrical frustration

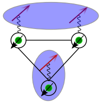
General picture of frustration



trade-offs:

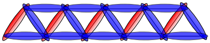


120°
(classical)



Partial Kondo
screening

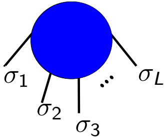
Motome et al. [2010]
Aulbach et al. [2015]



dimerized

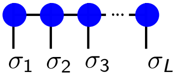
Computational method – DMRG

$|\Psi\rangle = \sum_{\{\sigma\}} T_{\sigma_1 \cdots \sigma_L} |\sigma_1 \cdots \sigma_L\rangle$



General Tensor state d^L

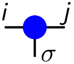
$|\Psi\rangle = \sum_{\{\sigma\}} \mathbf{A}_{\sigma_1} \cdots \mathbf{A}_{\sigma_L} |\sigma_1 \cdots \sigma_L\rangle$



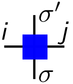
Matrix Product state LdM^2

MPS network allows local optimization of the site tensors with Matrix Product Operators. Schollwöck [2011]

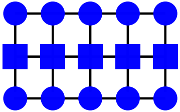
MPS

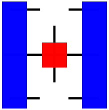
$A_{ij}^{\sigma} =$ 

MPO

$W_{ij}^{\sigma\sigma'} =$ 

expectation value

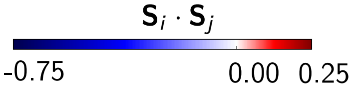
$\langle\Psi|H|\Psi\rangle =$ 

$H_{\text{eff}} =$ 

Results

Results

Nearest neighbour correlations



homogeneous

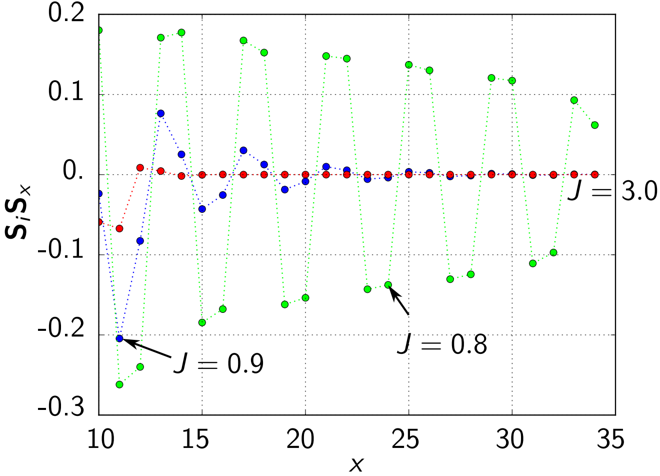
$J = 3.0t$

dimerized

$J = 0.7t$

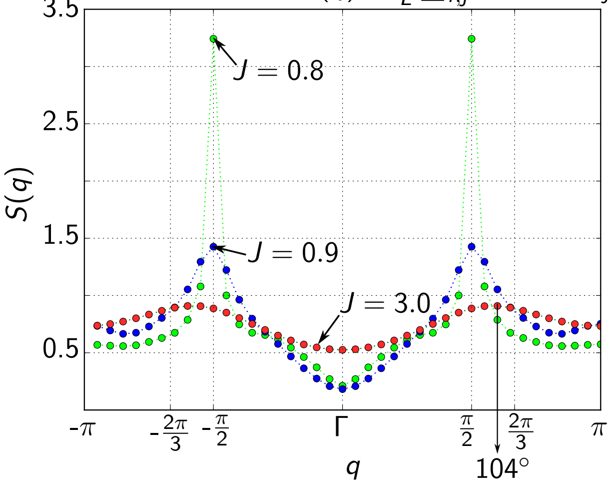
- Two phases at half filling
- Phase boundary: $J \approx 0.9t$
- Homogeneous phase is a spin liquid
- Dimerized phase has long range order

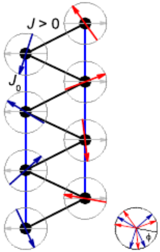
Long range correlations



Spin structure factor

$$S(q) = \frac{1}{L}\sum_{i,j} e^{iq(i-j)}\mathbf{S}_i\mathbf{S}_j$$

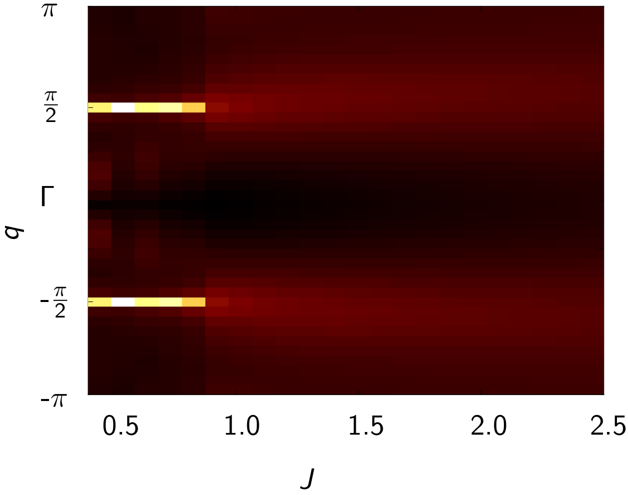




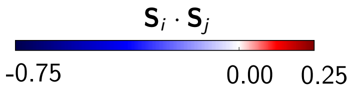
Dublenych [2016]

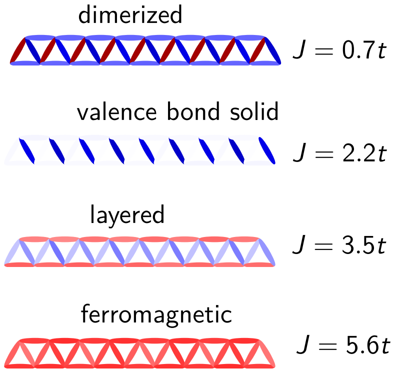
$$\phi = \pi - \arccos\left(\frac{|J|}{4J_0}\right)$$

Spin structure factor



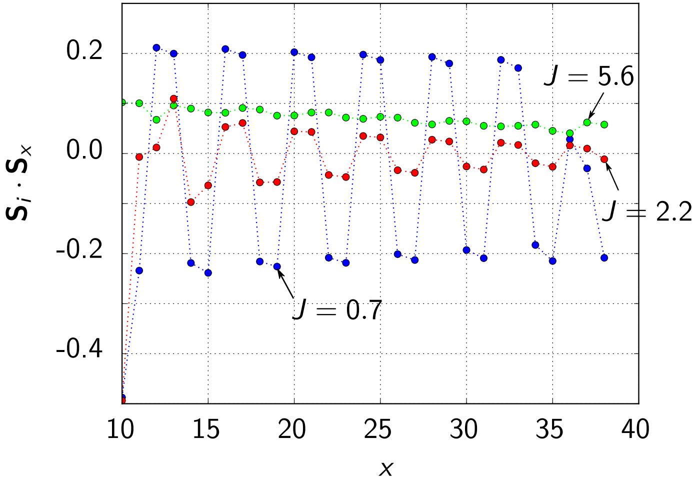
Nearest neighbour correlations



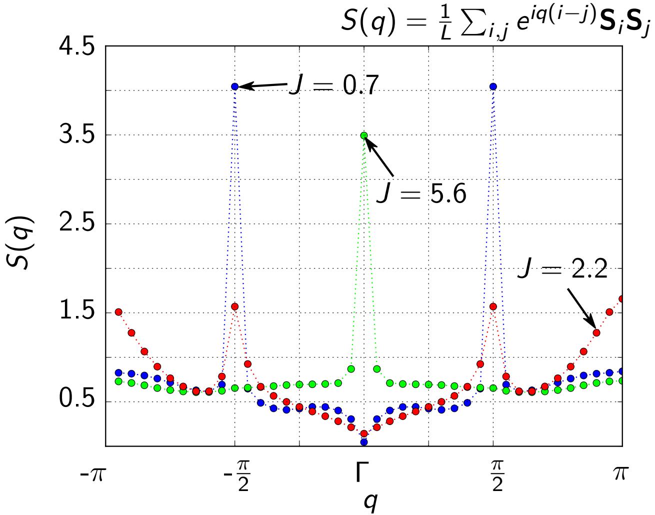


- Four regions at quarter filling
- Phase boundary: $J \approx 5.4t$
- Ferromagnetism at strong J follows from Hubbard model
- Exotic valence bond phase at $J \approx 2.2t$

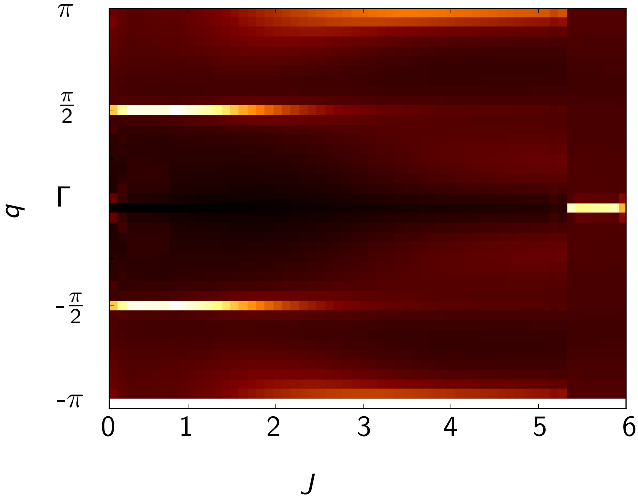
Long range correlations



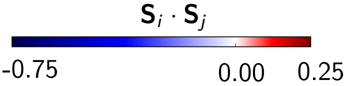
Spin structure factor

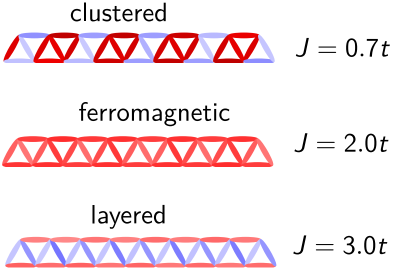


Spin structure factor



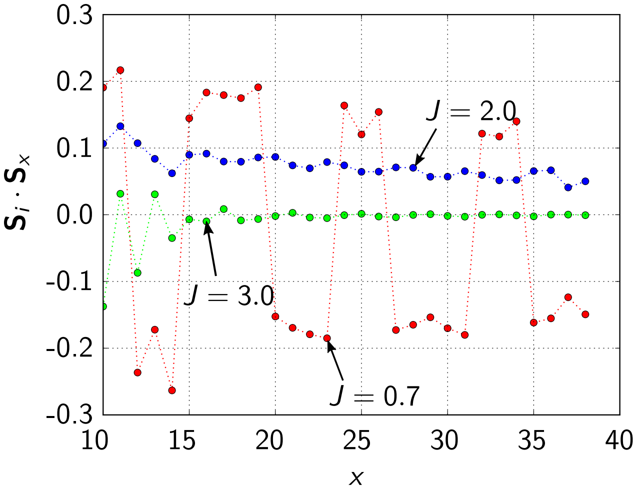
Nearest neighbour correlations



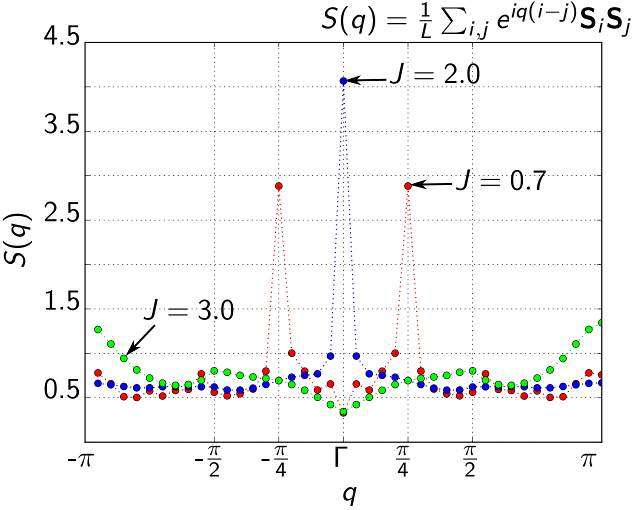


- Three regions at three-quarter filling
- Phase boundaries: $J \approx 1.0t$ and $J \approx 2.2t$
- $J \to \infty$: Luttinger Liquid (same as Hubbard model)
- The clustered phase has wavevector $\frac{\pi}{4}$

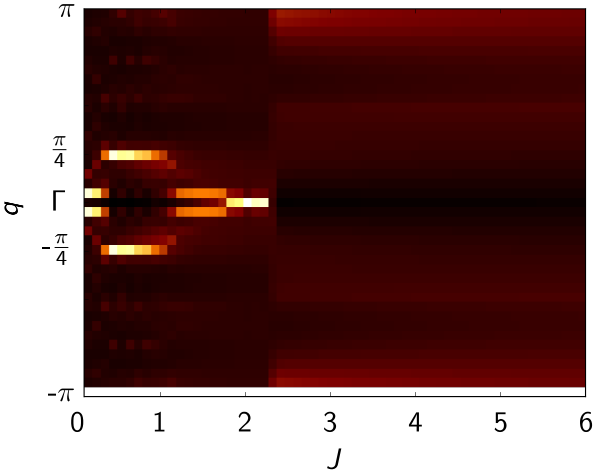
Long range correlations



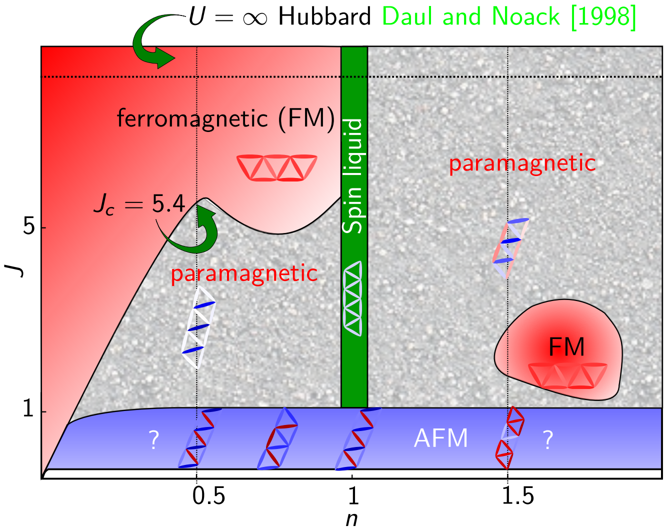
Spin structure factor



Spin structure factor



$J - n$ phase diagram



Conclusion

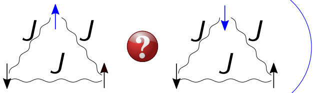
Conclusion

Conclusion

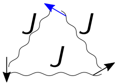
- Frustration is avoided by inhomogeneous correlations
  - Dimerized phase
  - Valence bond phase
  - Clustered phase
- Half filling: phase transition from spin liquid to long range order
- Quarter filling: exotic valence bond groundstate
- Three-quarter filling: clustered groundstate with $q = \frac{\pi}{4}$

Conclusion

General picture of frustration

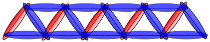


trade-offs:



120°
(classical)

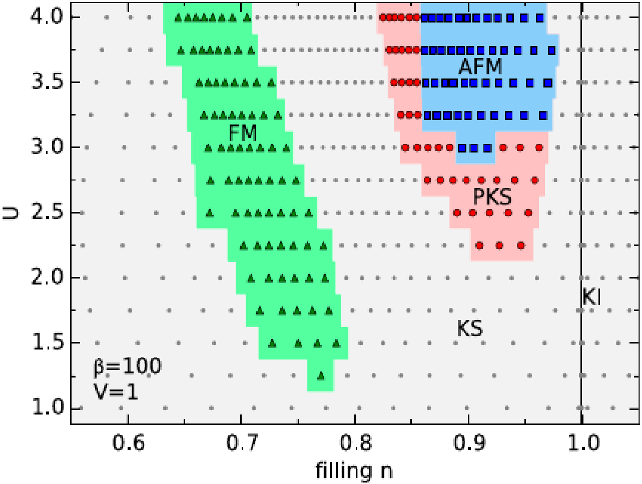
Partial Kondo
screening



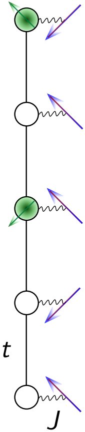
dimerized

Thank you for your attention!

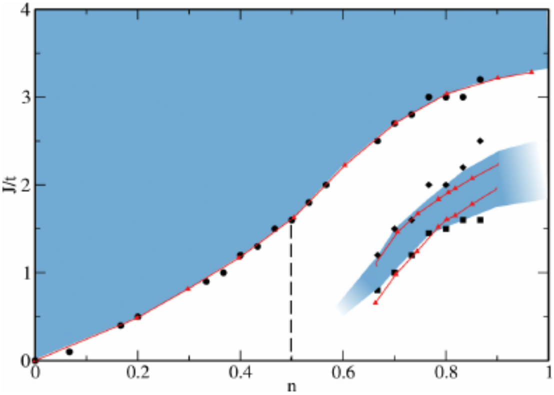
DMFT for periodic Anderson model



Kondo model – one-dimension

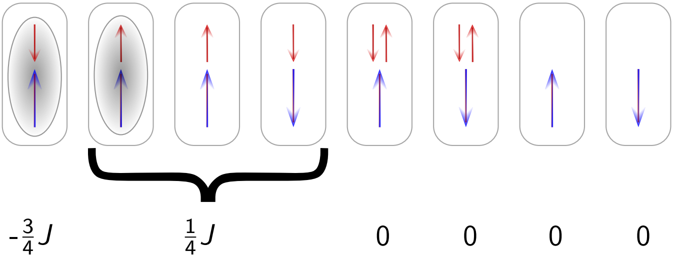


Peters and Kawakami [2012]



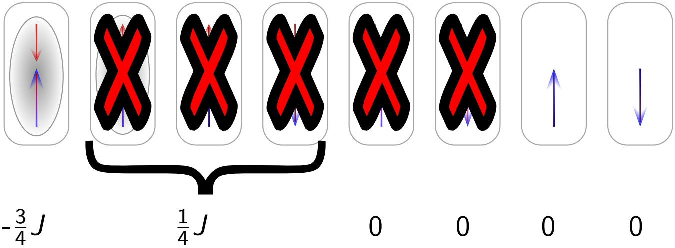
Strong coupling limit

Eight local basis states for the Kondo lattice:



Strong coupling limit

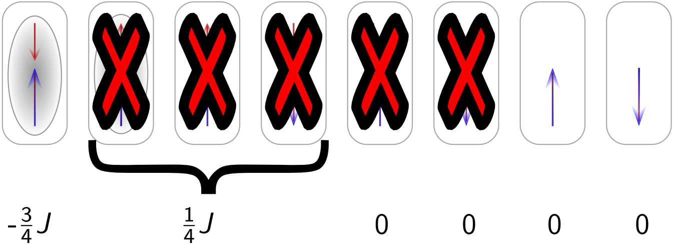
$J = \infty \Rightarrow$ three local basis states for the Kondo lattice:



- $n < 1$: only on-site singlets and empty states
- Construct the hopping parts restricted to these basis states

Strong coupling limit

$J = \infty \Rightarrow$ three local basis states for the Kondo lattice:



- $n < 1$: only on-site singlets and empty states
- $U = \infty$ Hubbard model with opposite sign and half bandwidth Lacroix [1985]

Strong coupling limit

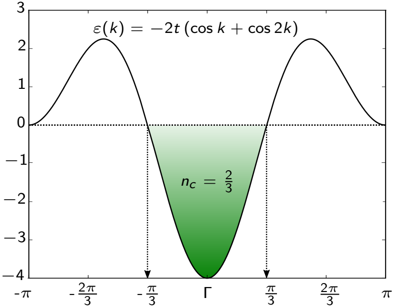
Magnetism in the $U = \infty$ Hubbard model

- one hole $\Rightarrow$ Ferromagnetism (Nagaoka)
- nnn-hopping $\stackrel{n<1}{\Longrightarrow}$ Ferromagnetism
- nnn-hopping $\stackrel{n>1}{\Longrightarrow}$ Luttinger liquid

! Results can be transferred to the Kondo model

! The corrections in $\frac{t^2}{J}$ and $\frac{t^2}{U}$ are not equivalent

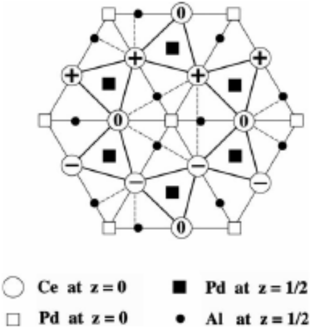
Weak coupling limit



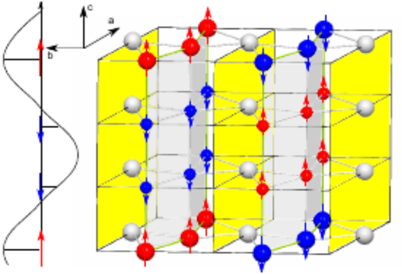
- $n < n_c \Rightarrow$ 2 Fermi points $k_F = \pm\frac{1}{2}n$
- $n > n_c \Rightarrow$ 4 Fermi points
- open boundaries $\Rightarrow$ no exact degenaracy

CePdAl (Cer Palladium Aluminium)

Example for a frustrated Kondo lattice



Oyamada et al. [2008]



Fritsch et al. [2016]

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