

# Magnetic Phases in Heavy Fermion Systems

Robert Peters

July 2014

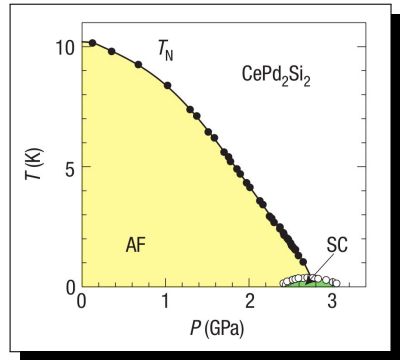
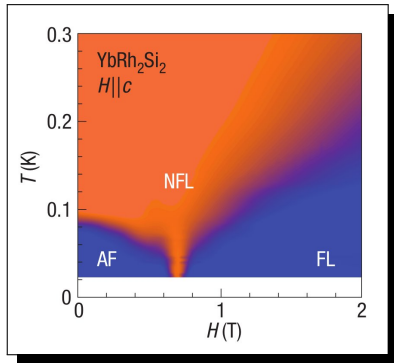


# Outline

- Introduction: model and method
- the phase diagram of the Kondo lattice model
  - weak coupling: RKKY dominated phases
  - strong coupling: Kondo dominated phases

## Heavy fermion systems

Due to the existence of strongly localized  $f$ -electrons, one can observe a variety of long-range ordered phases in  $f$ -electron systems.

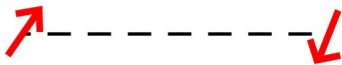


P. Gegenwart, Q. Si, F. Steglich: Nature Physics 2008

# Heavy fermion systems

competing effects in  $f$ -electron materials

RKKY interaction

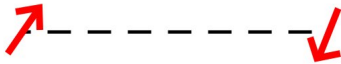


magnetic interaction between different  
magnetic moments

# Heavy fermion systems

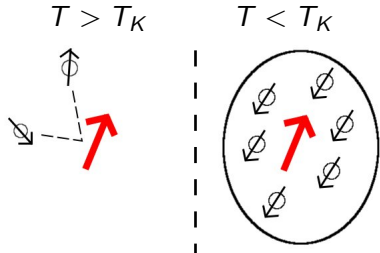
competing effects in  $f$ -electron materials

RKKY interaction



magnetic interaction between different magnetic moments

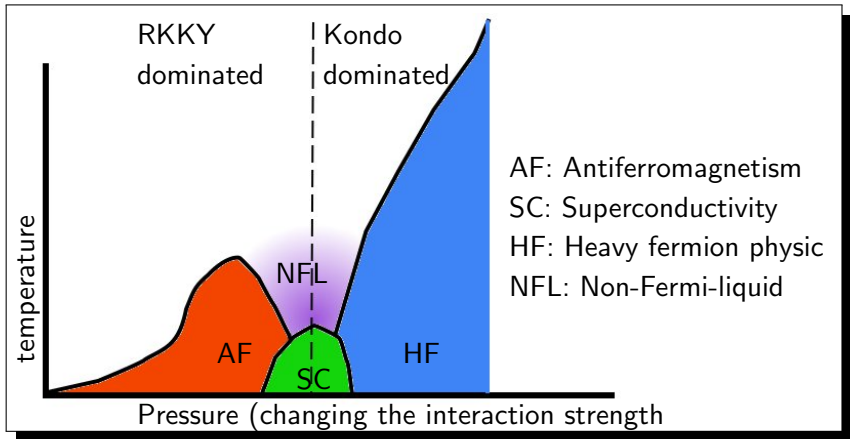
Kondo effect



Screening between magnetic moments and conduction electrons

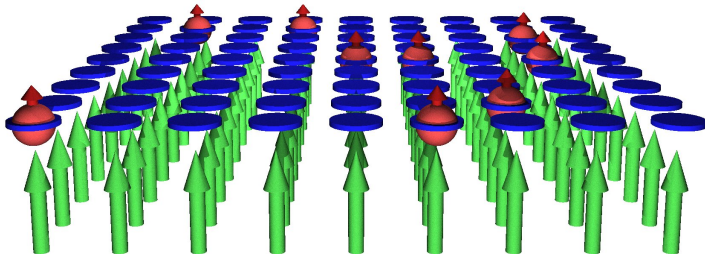
# Heavy fermion systems

## Doniach phase diagram



# Magnetic phase diagram of heavy fermion systems

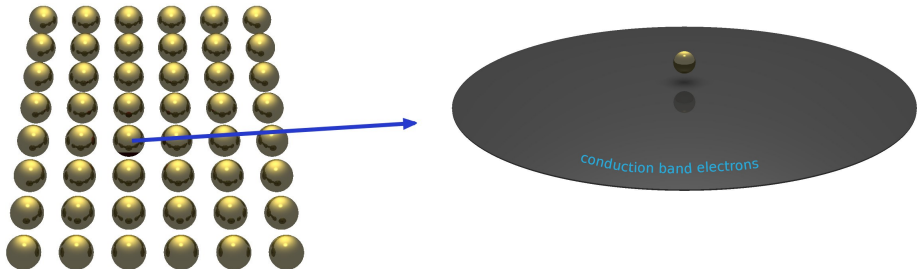
- lattice with conduction electrons
- lattice of magnetic moments
- local antiferromagnetically coupling between both



$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_i \vec{s}_i \vec{S}_i$$

# Dynamical mean field theory

dynamical mean field theory (DMFT)

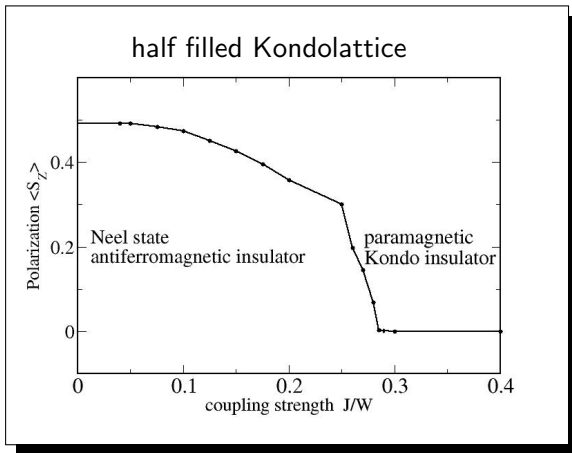


DMFT maps the lattice model onto a self-consistent impurity calculation

DMFT: PRL, W. Metzner and D. Vollhardt (1989); RMP, A. Georges et al. (1996)

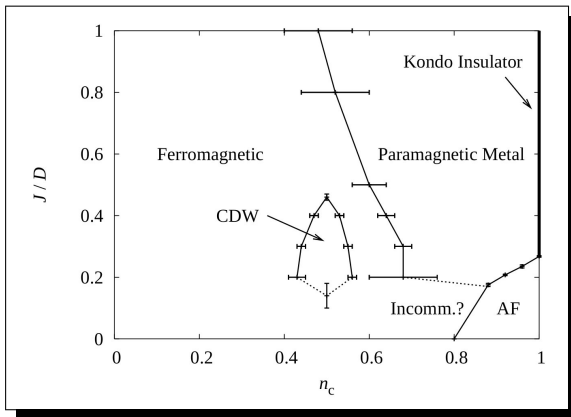


# Dynamical mean field theory



# Dynamical mean field theory

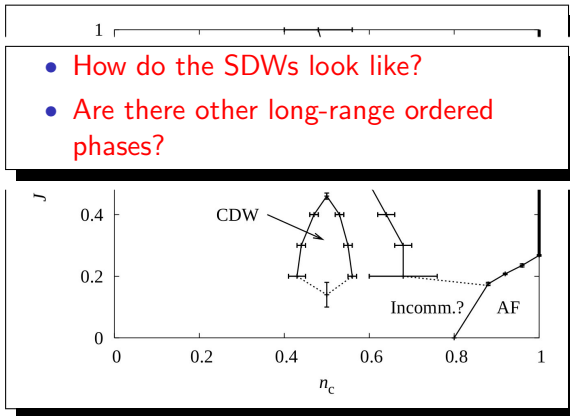
phase diagram calculated by susceptibilities



Otsuki et al., J. Phys. Soc. Jpn. 78 (2009) 034719

# Dynamical mean field theory

phase diagram calculated by susceptibilities



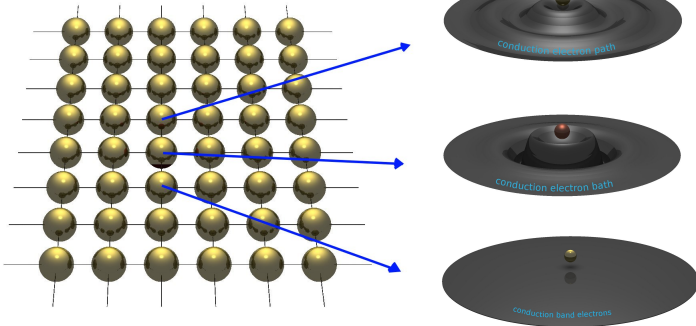
Otsuki et al., J. Phys. Soc. Jpn. 78 (2009) 034719

# inhomogeneous DMFT

Inhomogeneous DMFT is the local approximation of the model, where each lattice site can have a different **local** self-energy.

It has been used to describe cold atoms in a trap, interfaces, superlattices, and surfaces. Furthermore, it can be used in situations where the lattice symmetry is broken spontaneously.

# inhomogeneous DMFT

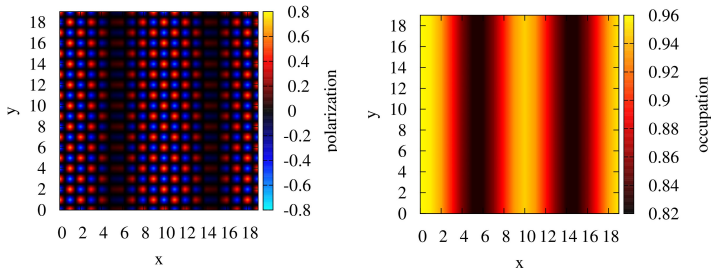


Each lattice site of a finite cluster is mapped onto its own impurity model,  $G_{ij} = (\omega - H_{i'j'} - \Sigma_{i'j'}(\omega))_{ij}^{-1}$

# inhomogeneous DMFT

vertical SDW in the doped Hubbard model

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

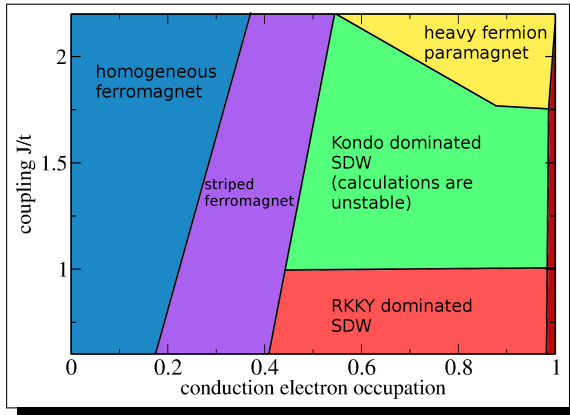


$$U = 8t, \langle n \rangle = 0.9$$

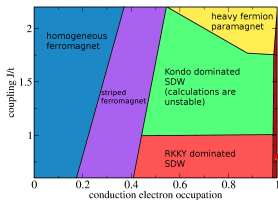
RP and N. Kawakami; PRB 2014

# Magnetic phase diagram of heavy fermion systems

new iDMFT calculations, also stabilizing incommensurate SDW states

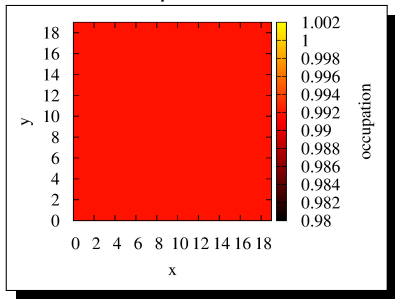


# Magnetic phase diagram of heavy fermion systems

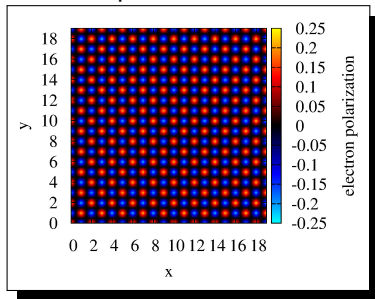


Neel state at half filling

occupation

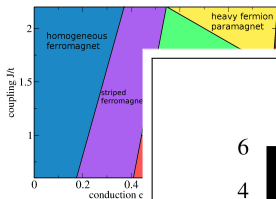


polarization



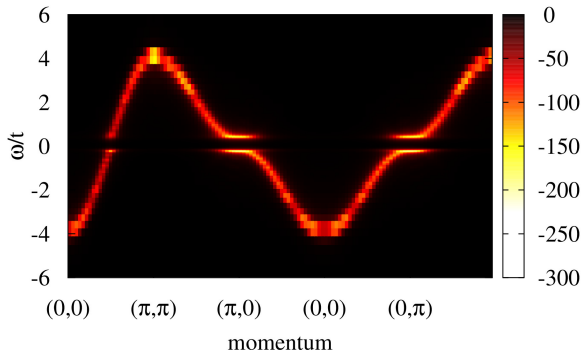


# Magnetic phase diagram of heavy fermion systems



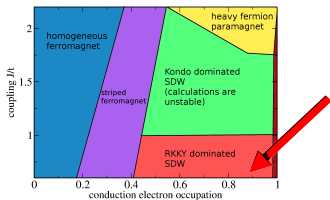
Neel state at half filling

Density of States



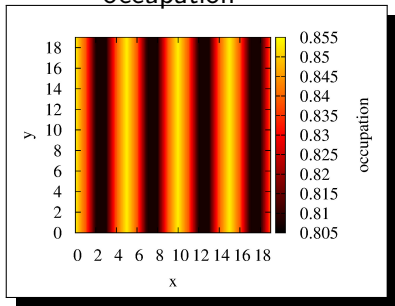
electron polarization

# Magnetic phase diagram of heavy fermion systems

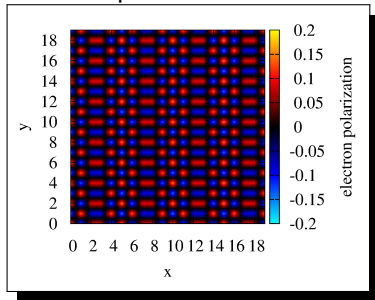


RKKY dominated SDW state

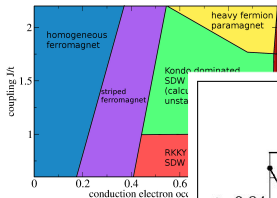
occupation



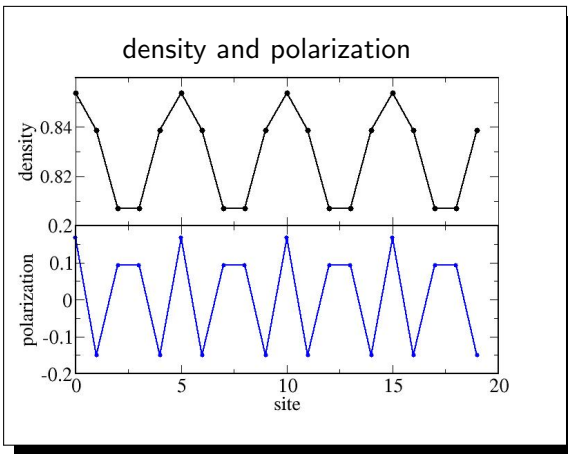
polarization



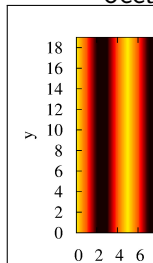
# Magnetic phase diagram of heavy fermion systems



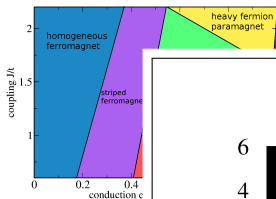
## RKKY dominated SDW state



OCCL

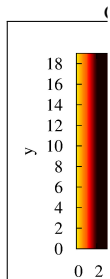
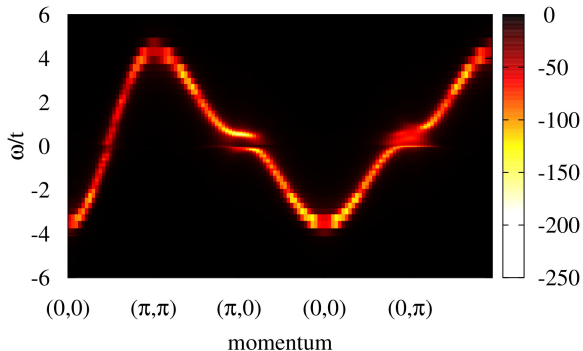


# Magnetic phase diagram of heavy fermion systems



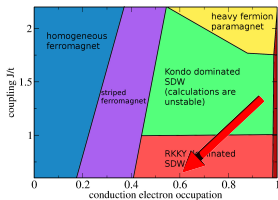
RKKY dominated SDW state

Density of States



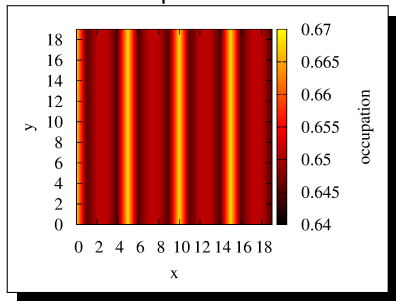
electron polarization

# Magnetic phase diagram of heavy fermion systems

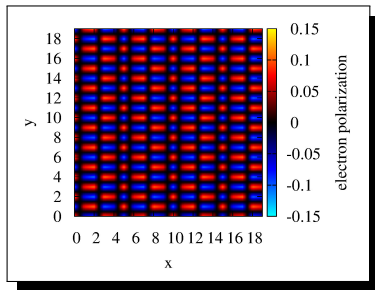


## RKKY dominated SDW state

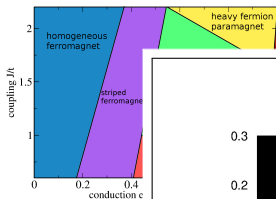
occupation



polarization

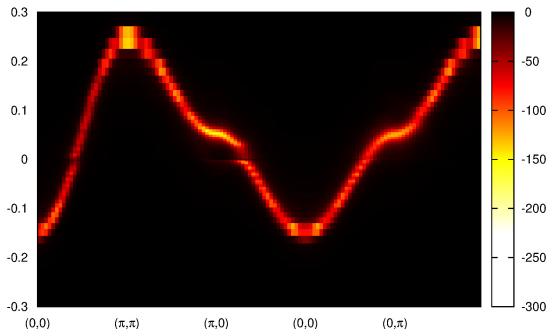


# Magnetic phase diagram of heavy fermion systems



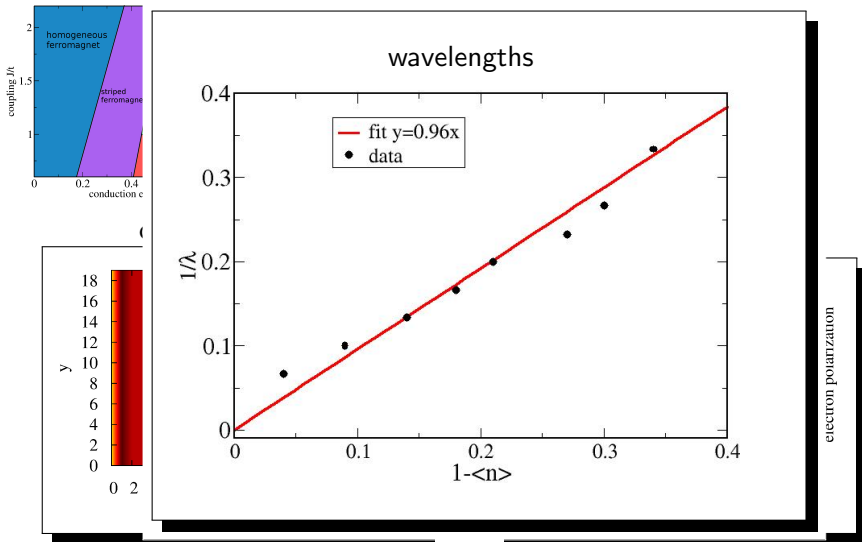
RKKY dominated SDW state

Density of States

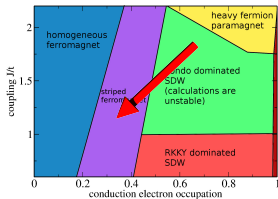


electron polarization

# Magnetic phase diagram of heavy fermion systems

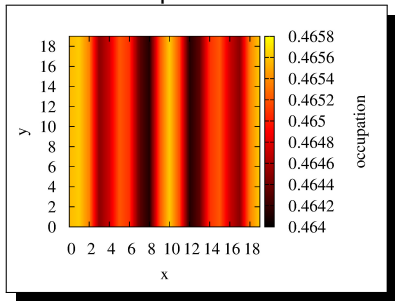


# Magnetic phase diagram of heavy fermion systems

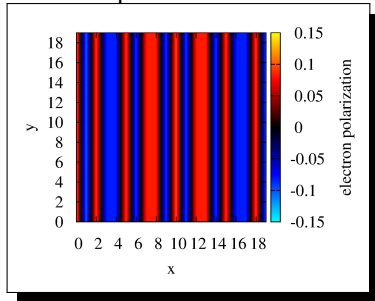


## Striped ferromagnet

occupation

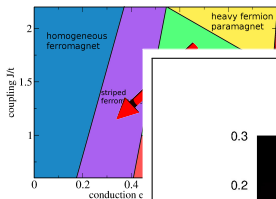


polarization



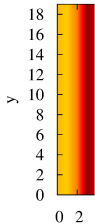
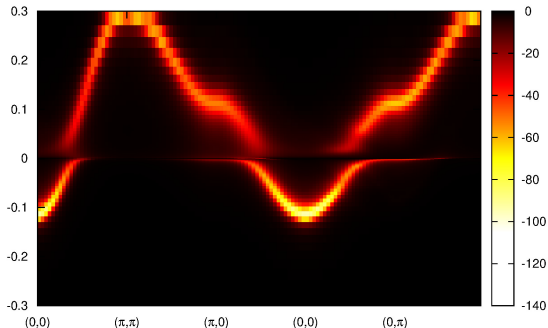


# Magnetic phase diagram of heavy fermion systems



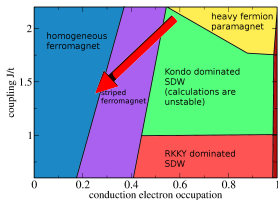
## Striped ferromagnet

### Density of States



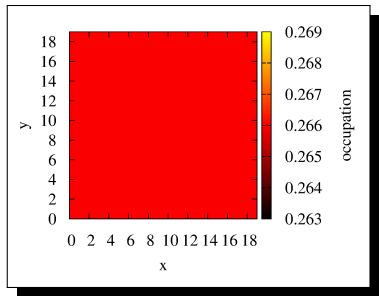
electron polarization

# Magnetic phase diagram of heavy fermion systems

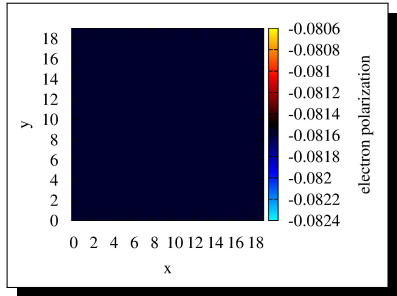


## Ferromagnet

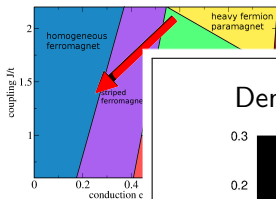
### occupation



### polarization

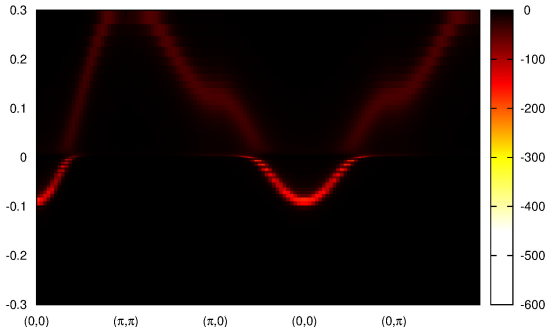


# Magnetic phase diagram of heavy fermion systems



## Ferromagnet

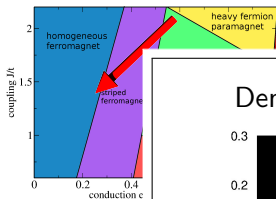
### Density of States - majority electrons



RP, N. Kawakami, T. Pruschke; PRL (2012)

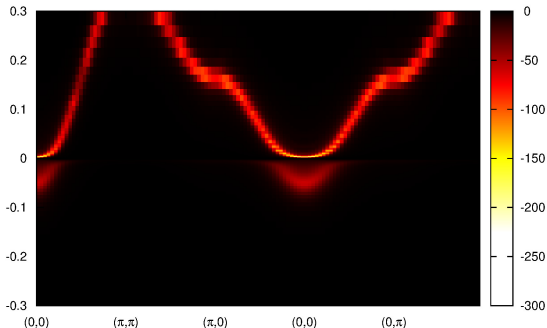
electron polarization

# Magnetic phase diagram of heavy fermion systems



## Ferromagnet

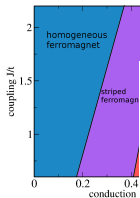
### Density of States - minority electrons



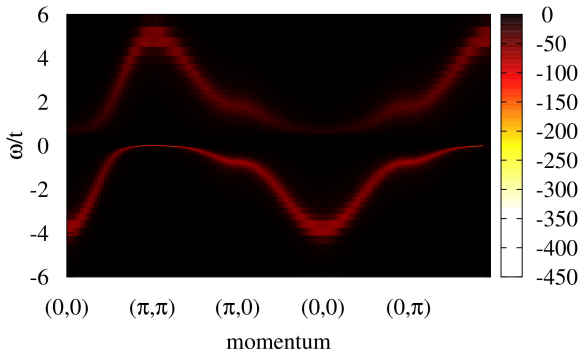
RP, N. Kawakami, T. Pruschke; PRL (2012)

electron polarization

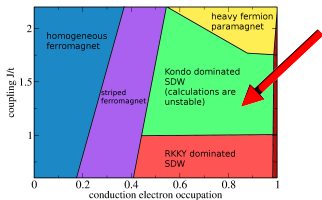
# Magnetic phase diagram of heavy fermion systems



heavy fermion paramagnet

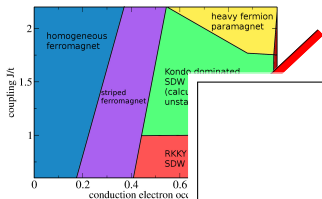


# Magnetic phase diagram of heavy fermion systems

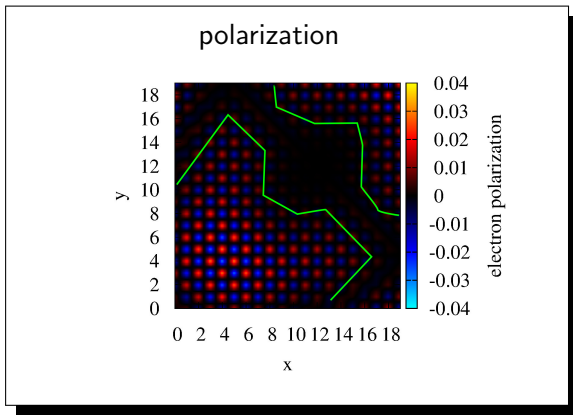


**Kondo dominated SDW, close to QCP**  
NO CONVERGENCE

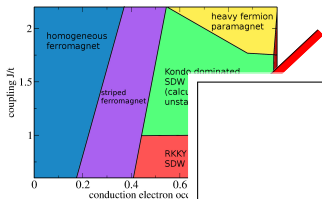
# Magnetic phase diagram of heavy fermion systems



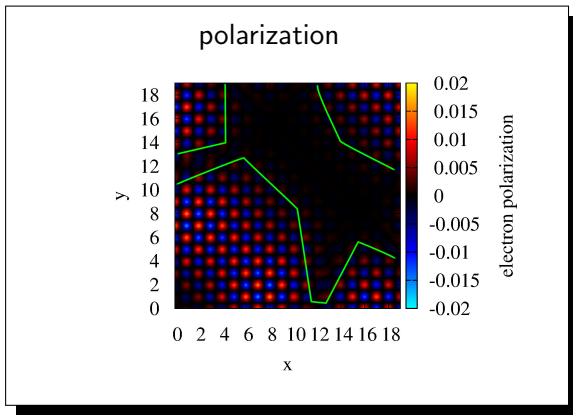
**Kondo dominated SDW, close to QCP**  
**NO CONVERGENCE**



# Magnetic phase diagram of heavy fermion systems

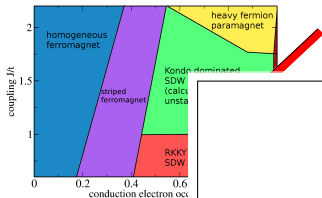


**Kondo dominated SDW, close to QCP**  
**NO CONVERGENCE**

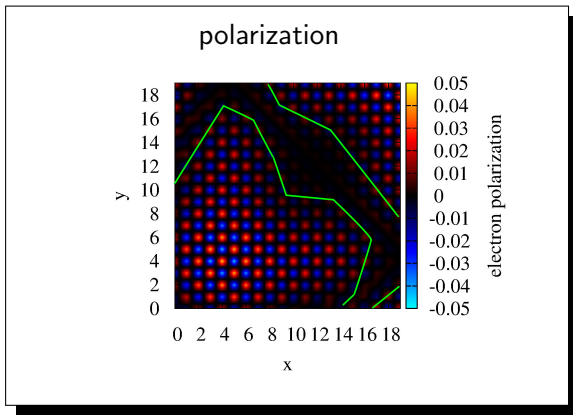




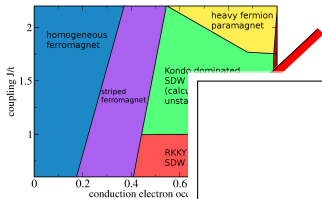
# Magnetic phase diagram of heavy fermion systems



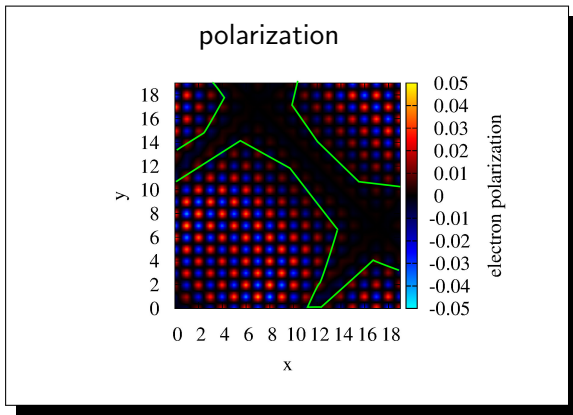
**Kondo dominated SDW, close to QCP**  
**NO CONVERGENCE**



# Magnetic phase diagram of heavy fermion systems



**Kondo dominated SDW, close to QCP**  
**NO CONVERGENCE**



## Summary

- By using the iDMFT, I have studied the magnetic phases of the Kondo lattice model
- There are several different types of SDW phases
- Such SDWs are a mixture of antiferromagnetic bonds and ferromagnetic bonds
- They are accompanied by a charge density wave.
- Close to the quantum critical transition, even iDMFT seems not to converge