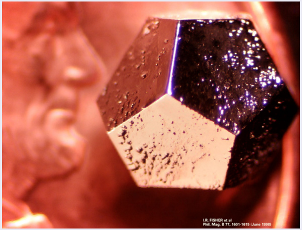
RKKY Interactions in Rare Earth Quasicrystals

Stefanie Thiem
(joint work with John Chalker)

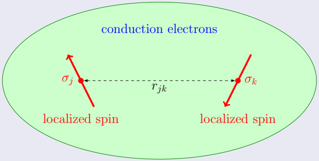
Department of Physics, University of Oxford

Open Statistical Physics
26th March 2014

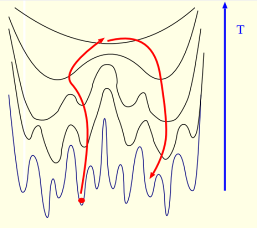
1. Introduction



2. RKKY Interactions



3. Parallel Tempering



4. Conclusion

Introduction

Quasicrystals

Quasicrystals*

Quasicrystals are materials with long-range order lacking a three-dimensional translational periodicity.

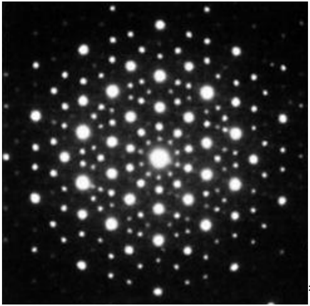
*Senechal, 2006, Notices of the American Mathematical Society, 53

*Shechtman et al., 1984, Phys. Rev. Lett. 53

Quasicrystals

Quasicrystals*

Quasicrystals are materials with long-range order lacking a three-dimensional translational periodicity.


*

Diffraction pattern

---

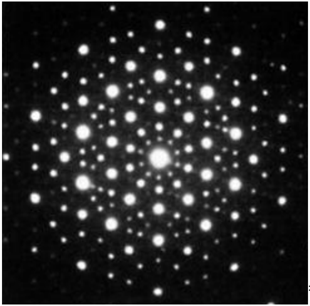
*Senechal, 2006, Notices of the American Mathematical Society, 53

*Shechtman et al., 1984, Phys. Rev. Lett. 53

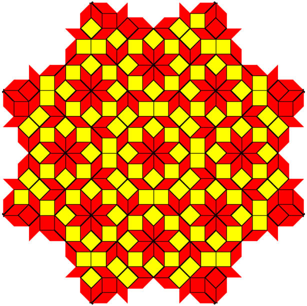
Quasicrystals

Quasicrystals*

Quasicrystals are materials with long-range order lacking a three-dimensional translational periodicity.


*

Diffraction pattern



Ammann Beenker Tiling

*Senechal, 2006, Notices of the American Mathematical Society, 53

*Shechtman et al., 1984, Phys. Rev. Lett. 53

Magnetic Properties of Rare Earth Quasicrystals

- rare earth quasicrystals contain localized magnetic moments (5-10%) which interact via the RKKY mechanism

Magnetic Properties of Rare Earth Quasicrystals

- rare earth quasicrystals contain localized magnetic moments (5-10%) which interact via the RKKY mechanism
- Experiments:
  - Curie-Weiss temperature shows the existence of predominant (anti)ferromagnetic interactions
  - for low temperatures many quasicrystals show a spin-glass-like freezing

Magnetic Properties of Rare Earth Quasicrystals

- rare earth quasicrystals contain localized magnetic moments (5-10%) which interact via the RKKY mechanism
- Experiments:
  - Curie-Weiss temperature shows the existence of predominant (anti)ferromagnetic interactions
  - for low temperatures many quasicrystals show a spin-glass-like freezing
- Open Problems:
  - Is spin glass behaviour associated to quasiperiodic order or to disorder?
  - Are there differences to conventional spin glasses in frustrated periodic systems?
  - ...

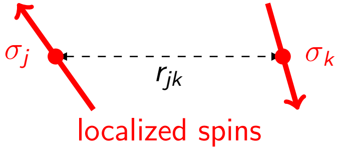
RKKY Interactions for Tight-Binding Models

Ruderman-Kittel-Kasuya-Yosida interactions

RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

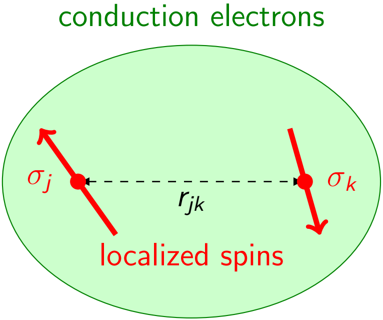
Ruderman-Kittel-Kasuya-Yosida interactions

RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.



Ruderman-Kittel-Kasuya-Yosida interactions

RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

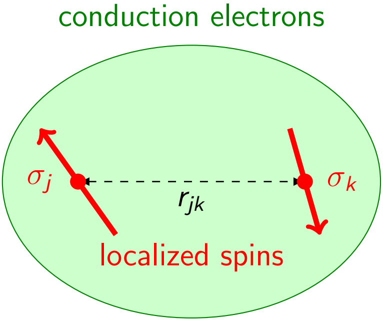


Ruderman-Kittel-Kasuya-Yosida interactions

RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

- exchange interactions between two magnetic moments

$$\mathcal{H}_{\mathrm{RKKY}} = \lambda^2 \chi_{j,k}(E_{\mathrm{F}})\, \sigma_j \sigma_k$$



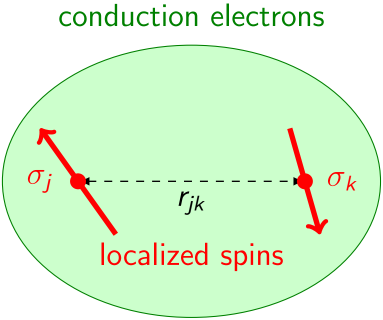
Ruderman-Kittel-Kasuya-Yosida interactions

RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

- exchange interactions between two magnetic moments

$$\mathcal{H}_{\mathrm{RKKY}} = \lambda^2 \chi_{j,k}(E_{\mathrm{F}})\, \sigma_j \sigma_k$$

- coupling λ between conduction electrons and magnetic moments



Ruderman-Kittel-Kasuya-Yosida interactions

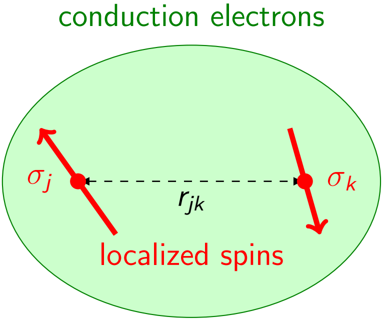
RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

- exchange interactions between two magnetic moments

$$\mathcal{H}_{\mathrm{RKKY}} = \lambda^2 \chi_{j,k}(E_{\mathrm{F}})\, \sigma_j \sigma_k$$

- coupling λ between conduction electrons and magnetic moments
- sea of conduction electrons modelled by tight-binding Hamiltonian

$$\mathcal{H}_{\mathrm{cond}} = \sum_{\langle l,m \rangle} |l\rangle \langle m|$$



Ruderman-Kittel-Kasuya-Yosida interactions

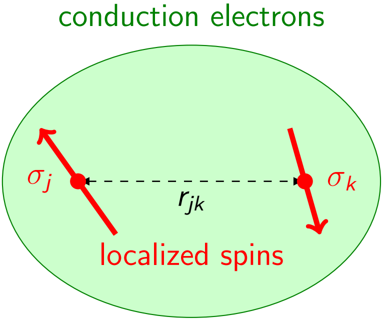
RKKY refers to a coupling mechanism of magnetic moments in a metal by means of an interaction through the conduction electrons.

- exchange interactions between two magnetic moments

$$\mathcal{H}_{\mathrm{RKKY}} = \lambda^2 \chi_{j,k}(E_{\mathrm{F}})\, \sigma_j \sigma_k$$

- coupling λ between conduction electrons and magnetic moments
- sea of conduction electrons modelled by tight-binding Hamiltonian

$$\mathcal{H}_{\mathrm{cond}} = \sum_{\langle l,m \rangle} |l\rangle \langle m|$$

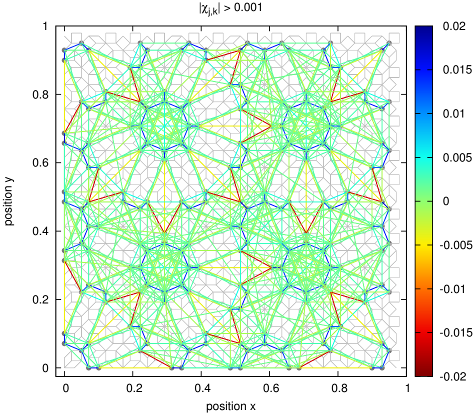


- magnetic susceptibility for $T = 0$

$$\chi_{j,k}(E_{\mathrm{F}}) = \frac{1}{\pi} \int_{-\infty}^{\infty} \Im(G^0_{j,k}(E) G^0_{k,j}(E)) \mathrm{sign}(E_{\mathrm{F}} - E) \mathrm{d}E$$

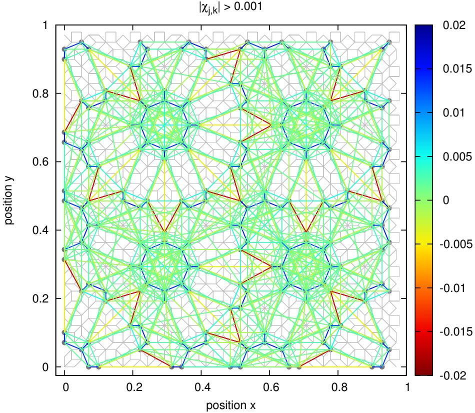
RKKY Interactions for Ammann-Beenker Tiling

spins at vertices with 5 nearest neighbours and
$E_F = 1.95$ (pseudogap).



RKKY Interactions for Ammann-Beenker Tiling

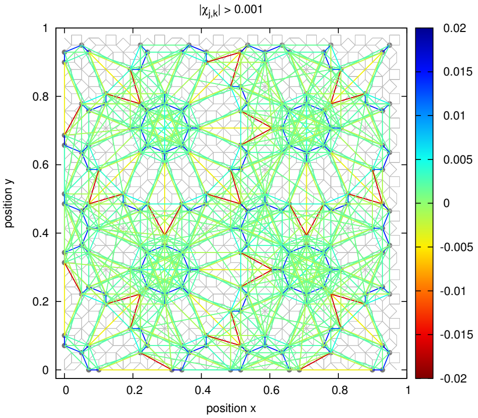
spins at vertices with 5 nearest neighbours and
$E_F = 1.95$ (pseudogap).



- broad range of interaction strengths for same local environment

RKKY Interactions for Ammann-Beenker Tiling

spins at vertices with 5 nearest neighbours and $E_F = 1.95$ (pseudogap).



- broad range of interaction strengths for same local environment
- comparison to RKKY formula for periodic systems $\chi(r) \propto 1/r^d$ reveals significant differences

Parallel Tempering

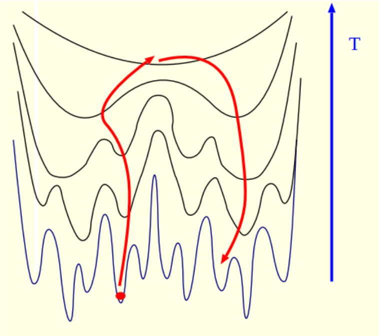
Parallel Tempering*

- Monte Carlo method aimed at significantly reducing of the correlation times between local minima in the energy landscape

*Swendsen and Wang, 1986, Phys. Rev. Lett. 57

Parallel Tempering*

Energy Landscape



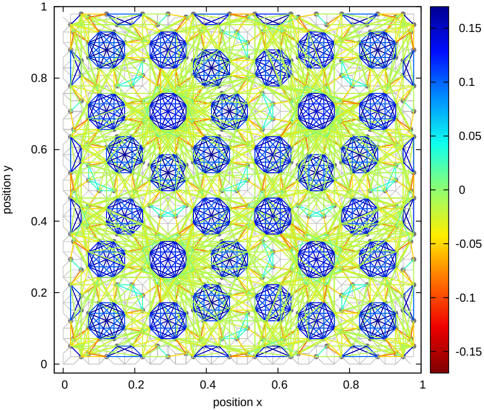
- Monte Carlo method aimed at significantly reducing of the correlation times between local minima in the energy landscape
- M copies (replicas) of the system with different temperatures T_m

*Swendsen and Wang, 1986, Phys. Rev. Lett. 57

Results for Ammann-Beenker Tiling

Ising spins $\sigma = \pm 1$ with RKKY interactions

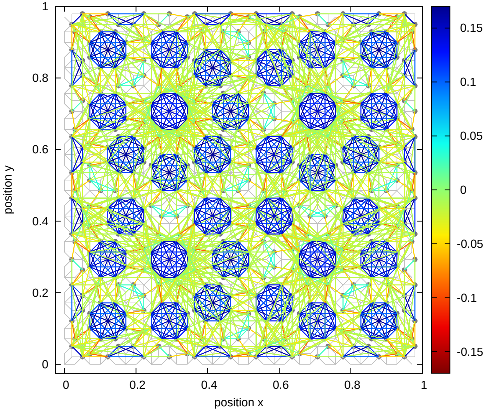
here: $E_{\mathrm{F}} = 0$, spins at positions with 4 nearest neighbours

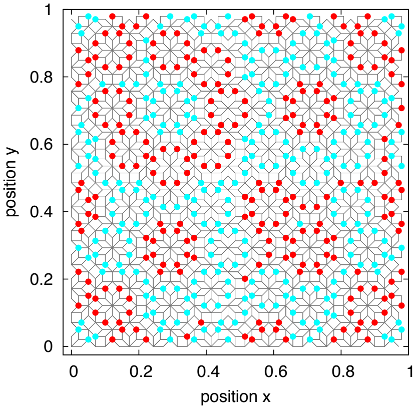


Results for Ammann-Beenker Tiling

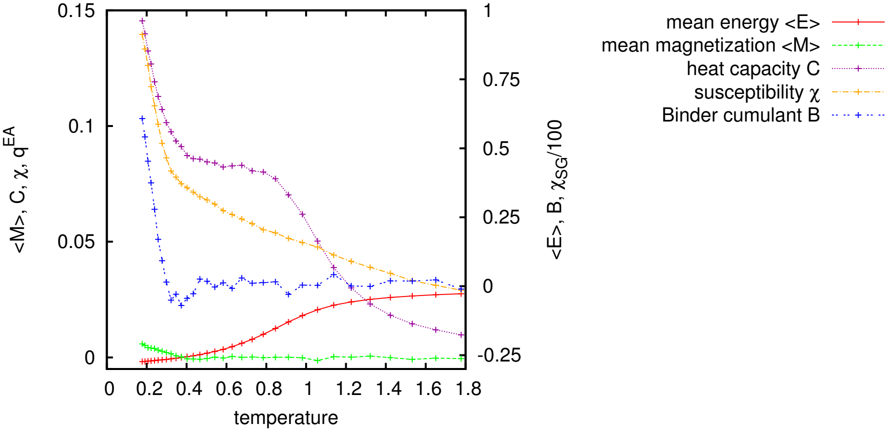
Ising spins $\sigma = \pm 1$ with RKKY interactions

here: $E_{\mathrm{F}} = 0$, spins at positions with 4 nearest neighbours

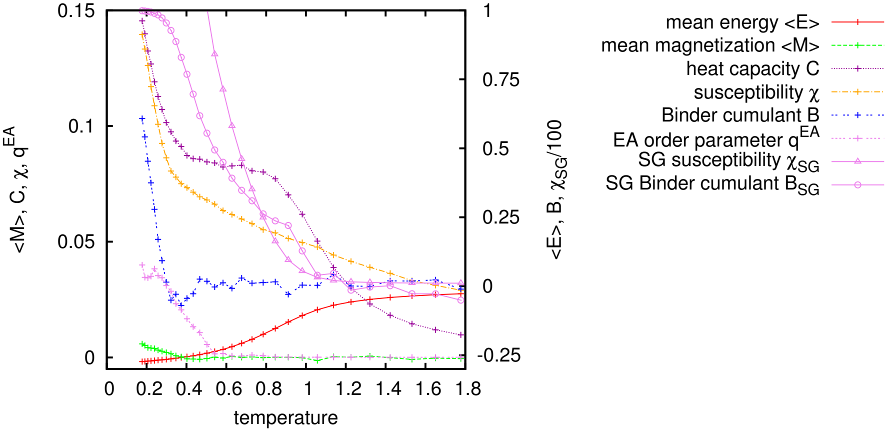




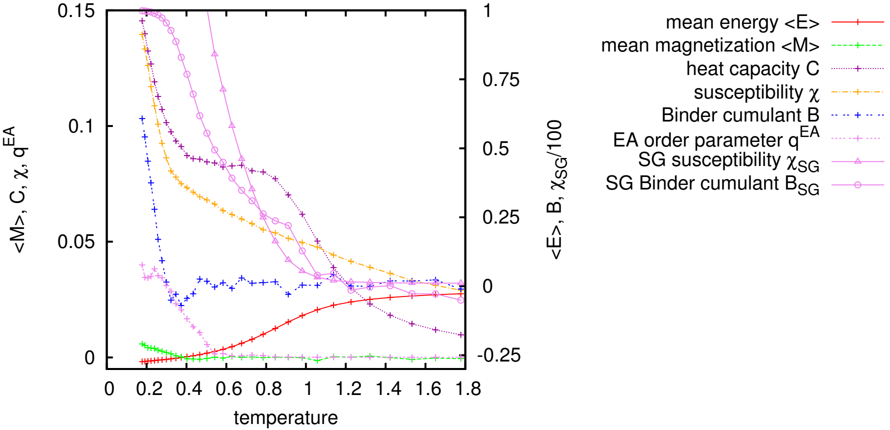
Results for Ammann-Beenker Tiling



Results for Ammann-Beenker Tiling



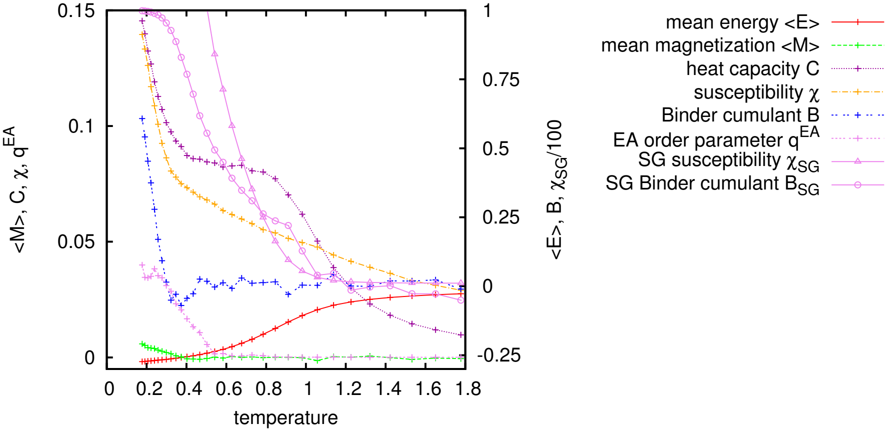
Results for Ammann-Beenker Tiling



- two freezing temperatures for i-ReMgZn and i-ReMgCd*

*Dolinšek et al., 2003, J. Phys.: Cond. Matt. 15

Results for Ammann-Beenker Tiling



- two freezing temperatures for i-ReMgZn and i-ReMgCd*
- neutron scattering data for i-ZnMgTb and i-ZnMgHo indicate the formation of short-range ordered spins†

*Dolinšek et al., 2003, J. Phys.: Cond. Matt. 15

†Sato. Et al., 2006, Phys. Rev. B, 73

Conclusion & Outlook

Conclusion

- RKKY interactions in quasiperiodic tilings are different from periodic systems and strongly depend on the positions of the magnetic moments

Conclusion

- RKKY interactions in quasiperiodic tilings are different from periodic systems and strongly depend on the positions of the magnetic moments
- parallel tempering results shows phase transitions towards a low-temperuture state with similarities to a cluster spin glass

Thank you.