Spin-charge order in Kondo-Lattice Model on triangular lattice

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Frustrated Magnetism @ JNU *Feb. 10, 2015*

In collaboration with ...

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Motivation

Question: what happens when charge carriers are introduced in a frustrated magnet?

- Do the charge carriers induce new magnetic groundstates?
- How is the charge transport affected by the magnetic order?

Interplay between:

electron itineracy, local moment magnetism & frustrated geometry

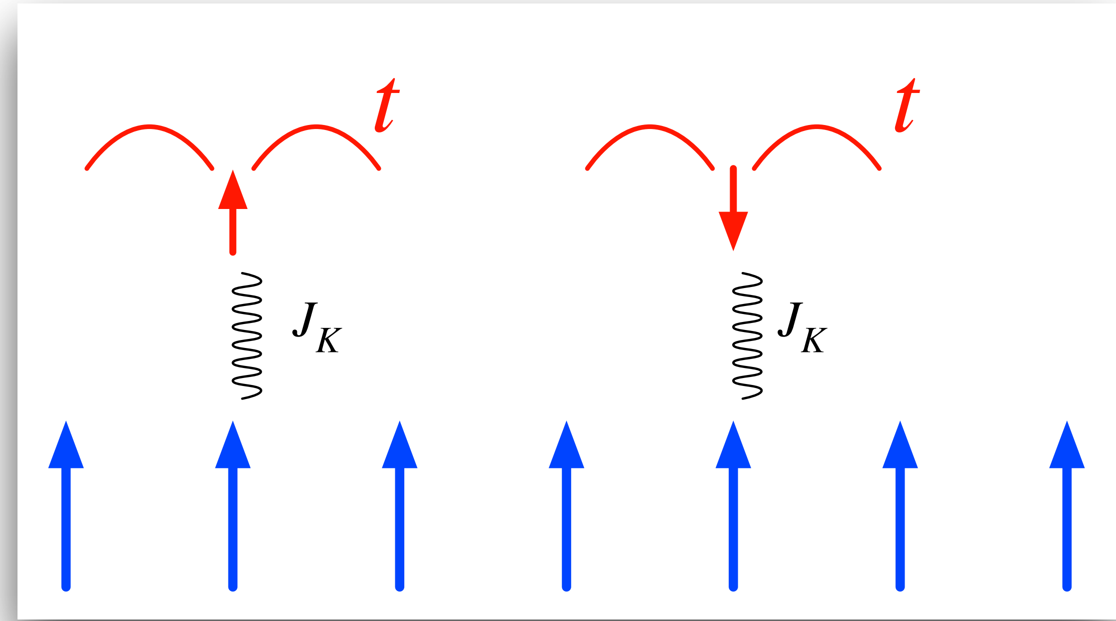
Outline of the talk

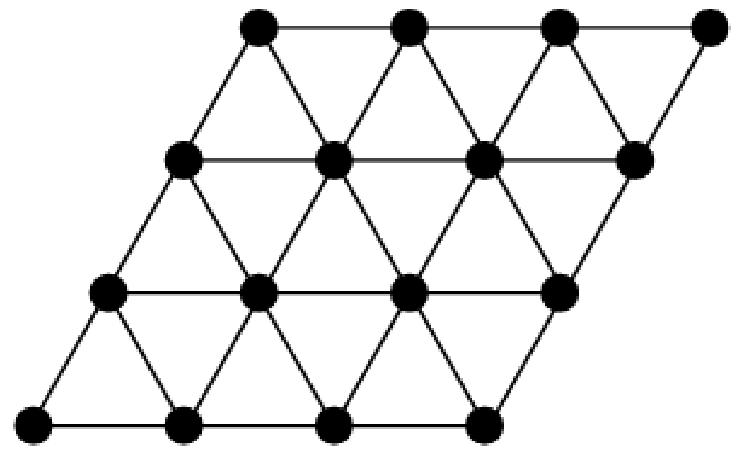
- Kondo-lattice model on a triangular lattice
- Weak coupling: Fermi surface nesting, perturbation theory
- Strong coupling: effective spinless Hamiltonian; Monte Carlo combined with diagonalization
- spin-charge ordered phases at $n=1/3$ and $n=2/3$
- Summary

Kondo lattice model on triangular lattice

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + H.c.) + J_K \sum_i \mathbf{S}_i \cdot \sigma_i$$

Parameters: $t, \; J_K, \; n$





Degrees of Freedom: (i) Localized Spins, (ii) Itinerant Fermions

Two possible ways to realize such models in real materials:

(i) Introduce magnetic impurities in metals/semiconductors (*e.g.* DMS)
(ii) Introduce charge carriers in a magnetic insulator (*e.g.* Manganites, heavy-fermion systems, etc.)

Classical approximation for spins

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + J_K \sum_i \mathbf{S}_i \cdot \sigma_i$$

Full quantum problem: size of the Hilbert space grows exponentially; as hard as a multi-orbital Hubbard problem

For large localized spins (S = 3/2, 2, …): assume the spins to be classical

Born-Oppenheimmer: fast variables (electrons) and slow variables (spins)

- What is the ground state of the localized classical spin sub-system?
- How are the itinerant electrons affected by the spins?

$$\mathcal{Z} = \int \mathcal{D}\{\mathbf{S}\}\; Tr\; e^{-\beta H} \equiv \int \mathcal{D}\{\mathbf{S}\}\; e^{-\beta H_{eff}(\{\mathbf{S}\})}$$

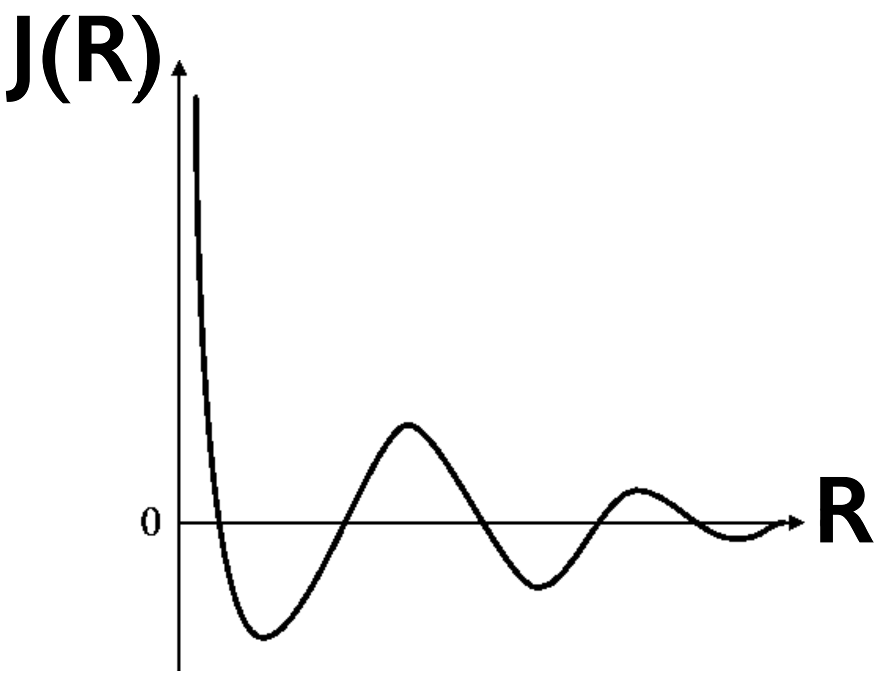
$$H_{eff}(\{\mathbf{S}\}) = -k_B T\; ln(Tr\; e^{-\beta H})$$

Weak Kondo coupling

- Perturbation expansion in J_K/t

RKKY interactions between localized spins

$$H_{RKKY} = \sum_{r,R} J(R)\, \mathbf{S}_r \cdot \mathbf{S}_{r+R}$$

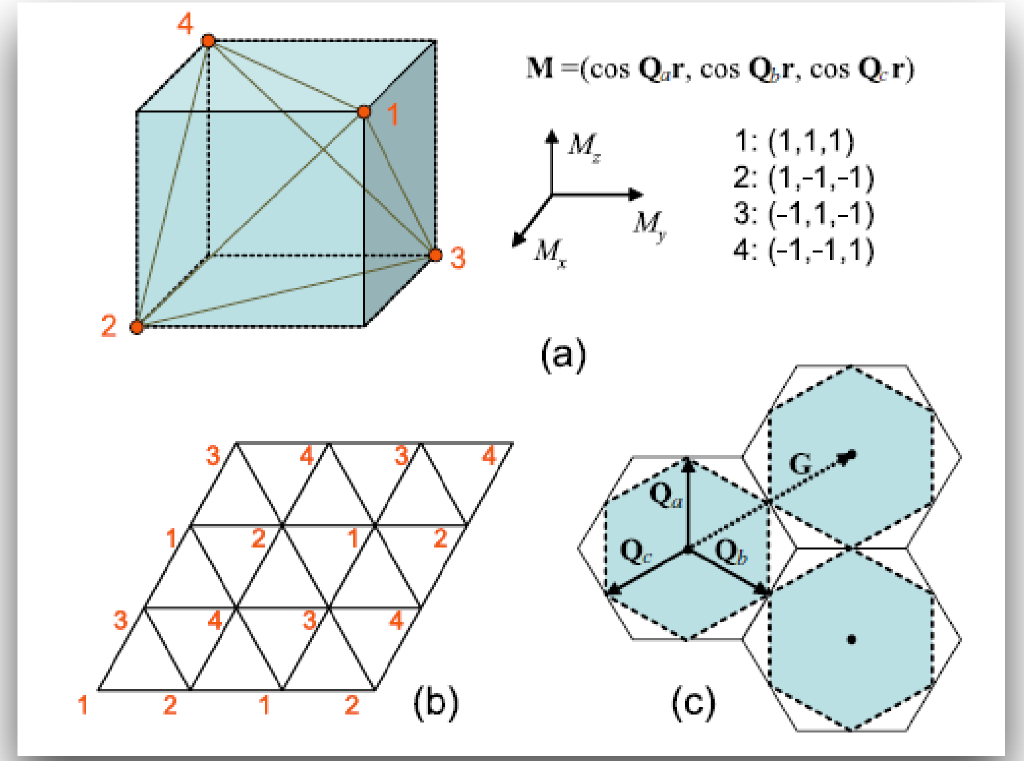


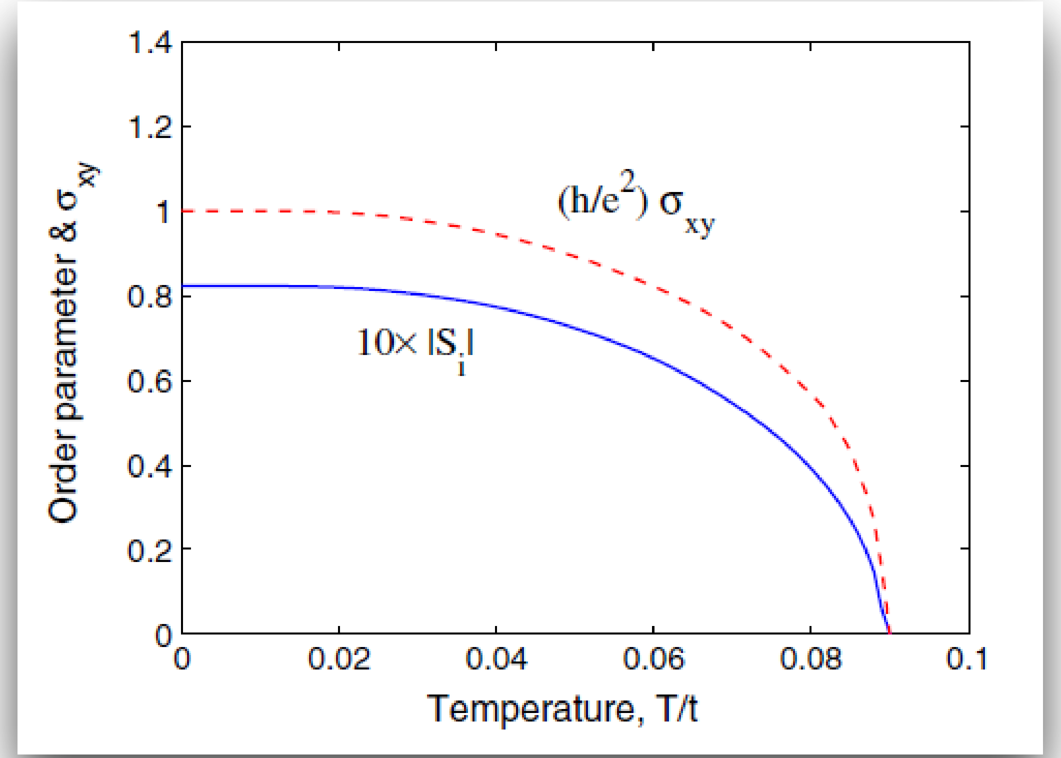
A variety of magnetically ordered states, or glassy states can arise depending on:

- Electronic filling fraction of the conduction band
- Lattice structure for itinerant electrons
- Lattice structure for localized spins

Something even simpler: the shape of the Fermi surface

Non-coplanar state at n=3/4





Ivar Martin & C. D. Batista, PRL '08

- Fermi surface is nested by three Q vectors at n=3/4
- Realization of 4-sublattice non-coplanar magnetic order
- Finite scalar spin chirality, anomalous Hall effect

Multiple-spin interactions in the 4th order perturbation expansion in J_K/t

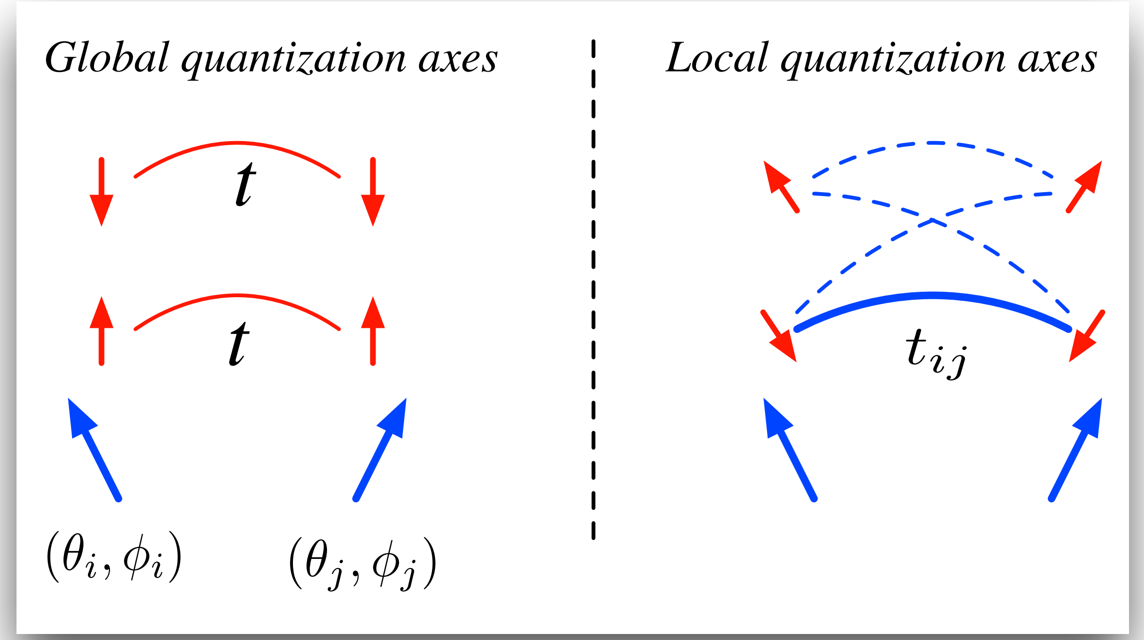
Akagi, Udagawa & Motome, PRL '12

Large Kondo coupling

What happens in the limit $J_K >> t$?

$J_K \to \infty$

Spinless fermions with modified hoppings



$$t_{ij}/t = \cos(\theta_i/2)\cos(\theta_j/2) + \sin(\theta_i/2)\sin(\theta_j/2)\, e^{-\mathrm{i}(\phi_i - \phi_j)}$$

Finite J_K corrections, antiferromagnetic coupling with $J_{AF} \sim t^2/J_K$

$$H = -\sum_{\langle ij \rangle}(t_{ij}\ d_i^\dagger d_j + H.c.) + J_{AF}\sum_{\langle ij \rangle}\mathbf{S}_i \cdot \mathbf{S}_j$$

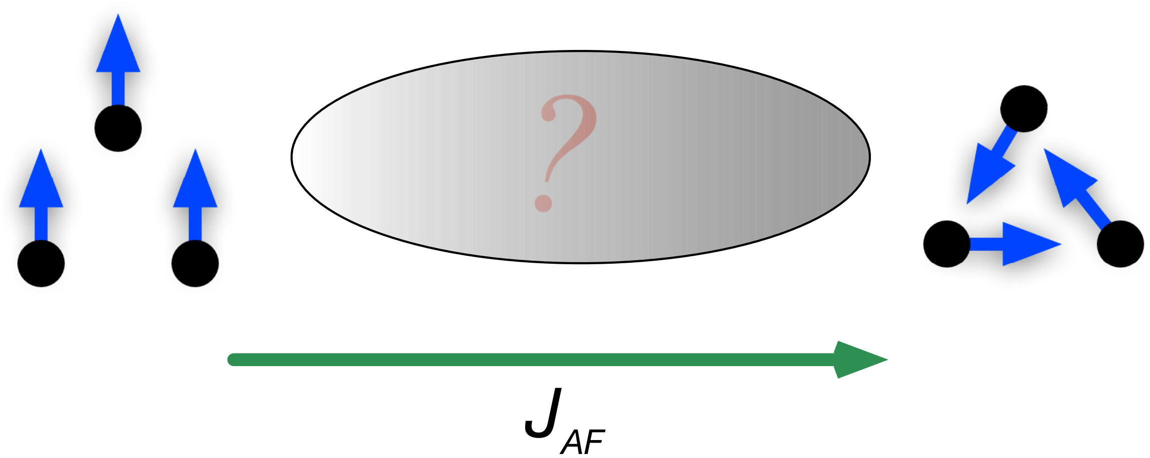
Effective spinless fermion model

$$H = -\sum_{\langle ij \rangle}(t_{ij}\ d_i^\dagger d_j + H.c.) + J_{AF}\sum_{\langle ij \rangle}\mathbf{S}_i \cdot \mathbf{S}_j$$

What are the magnetic ground states of this model?

$J_{AF} = 0$

Ferromagnetic GS



Large J_{AF}

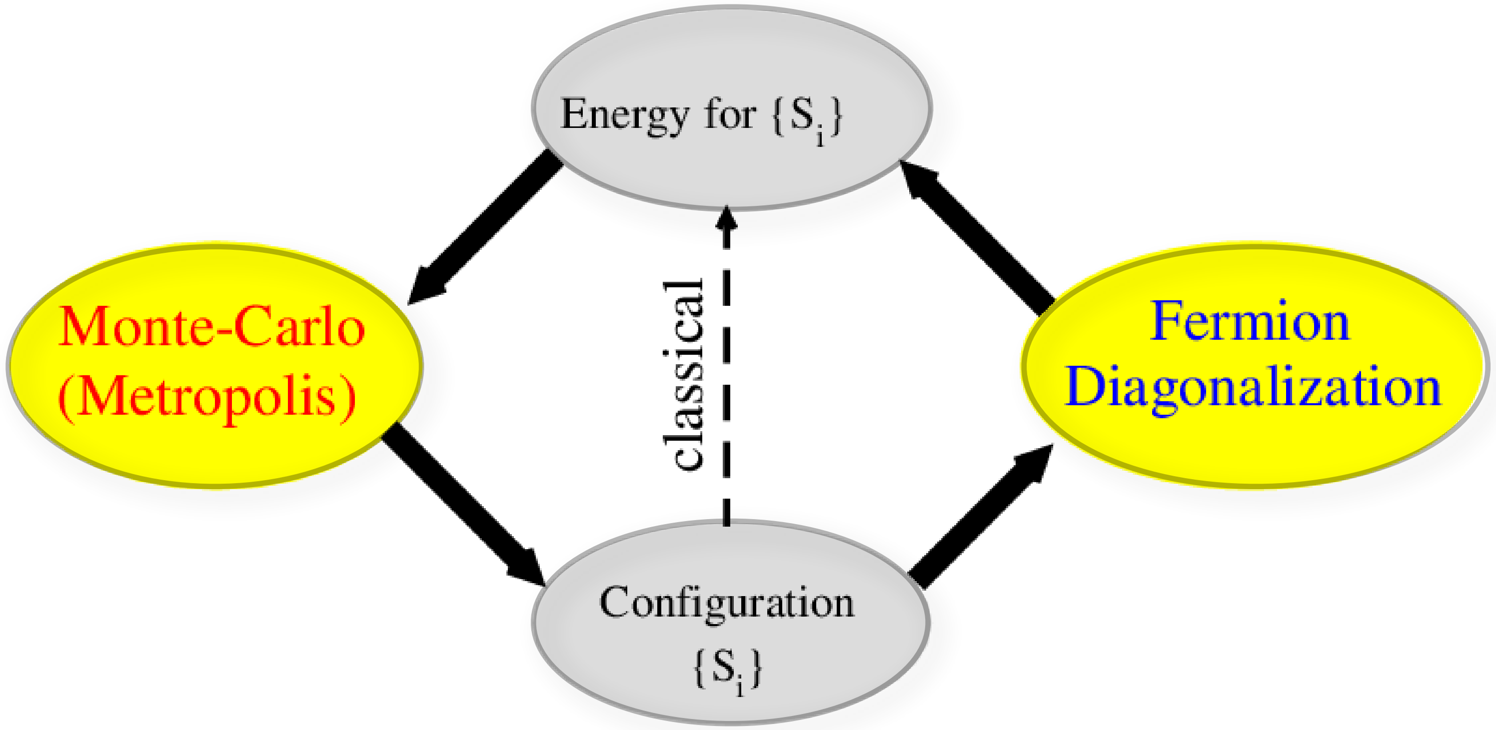
120° state

How to find the ground states for intermediate J_{AF} ?

Need to integrate out the electrons and arrive at effective spin-only model

$$H_{eff}(\{\mathbf{S}\}) = -k_B T\ ln(Tr\ e^{-\beta H})$$

Classical Monte Carlo + Diagonalization

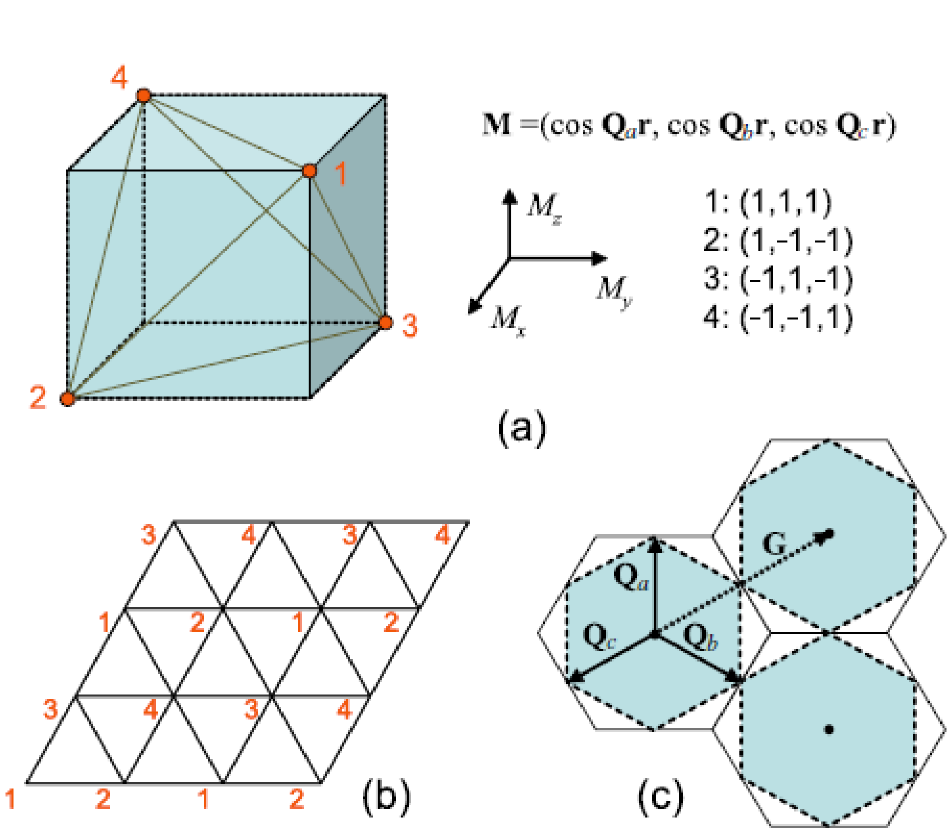


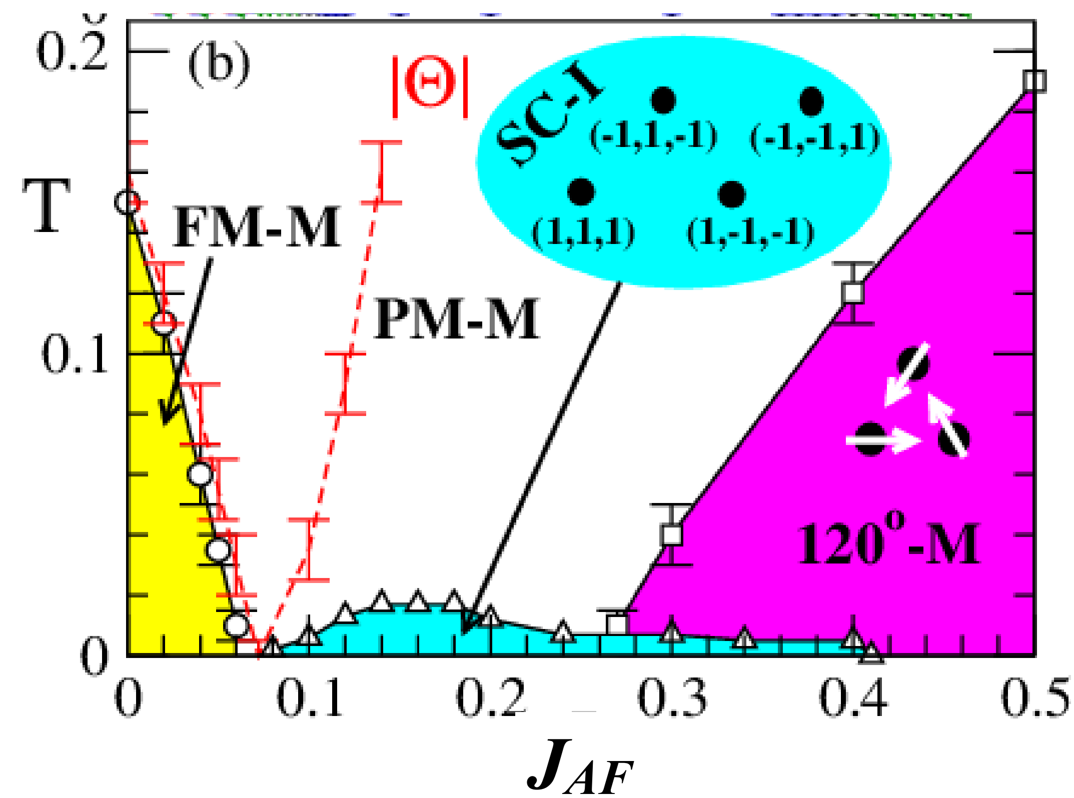
- Classical Monte Carlo for spins (Metropolis algorithm)
- Energy of a classical spin configuration involves fermion contribution
  (Diagonalization of the fermionic Hamiltonian at each Monte Carlo step)
- The algorithm is numerically exact, scales as N^4 with the number of sites N
- We simulate clusters upto N=144 on triangular lattice

The method has been extensively used for studying models of manganites
Dagotto et al., Phys. Rep. 344, 1 (2001)

Noncoplanar state at n=1/2

- The 4-sublattice non-coplanar phase at n=1/4 also exists at strong coupling
- Finite scale spin chirality $\chi = \langle \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \rangle$





S. Kumar & J. v.d. Brink, PRL '10

Present study: The phases at n=1/3 and n=2/3

Low-temperature structure factors

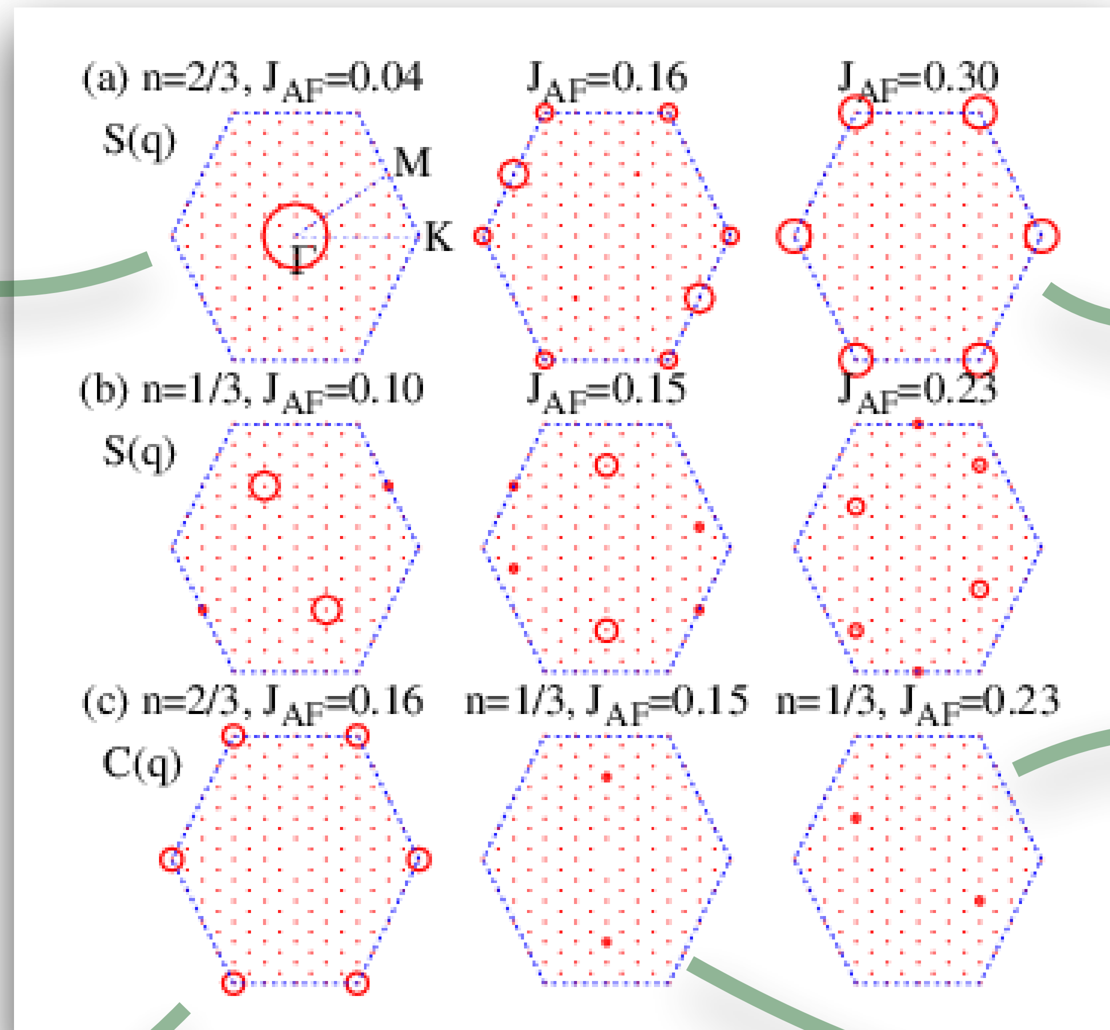
Spin and charge structure factors at *n=1/3* and *n=2/3*

$$S(\mathbf{q}) = \frac{1}{N^2}\sum_{ij}\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle_{av}\; e^{-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$$

$$C(\mathbf{q}) = \frac{1}{N^2}\sum_{ij}\langle \delta n_i \delta n_j\rangle_{av}\; e^{-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$$

FM

120º state

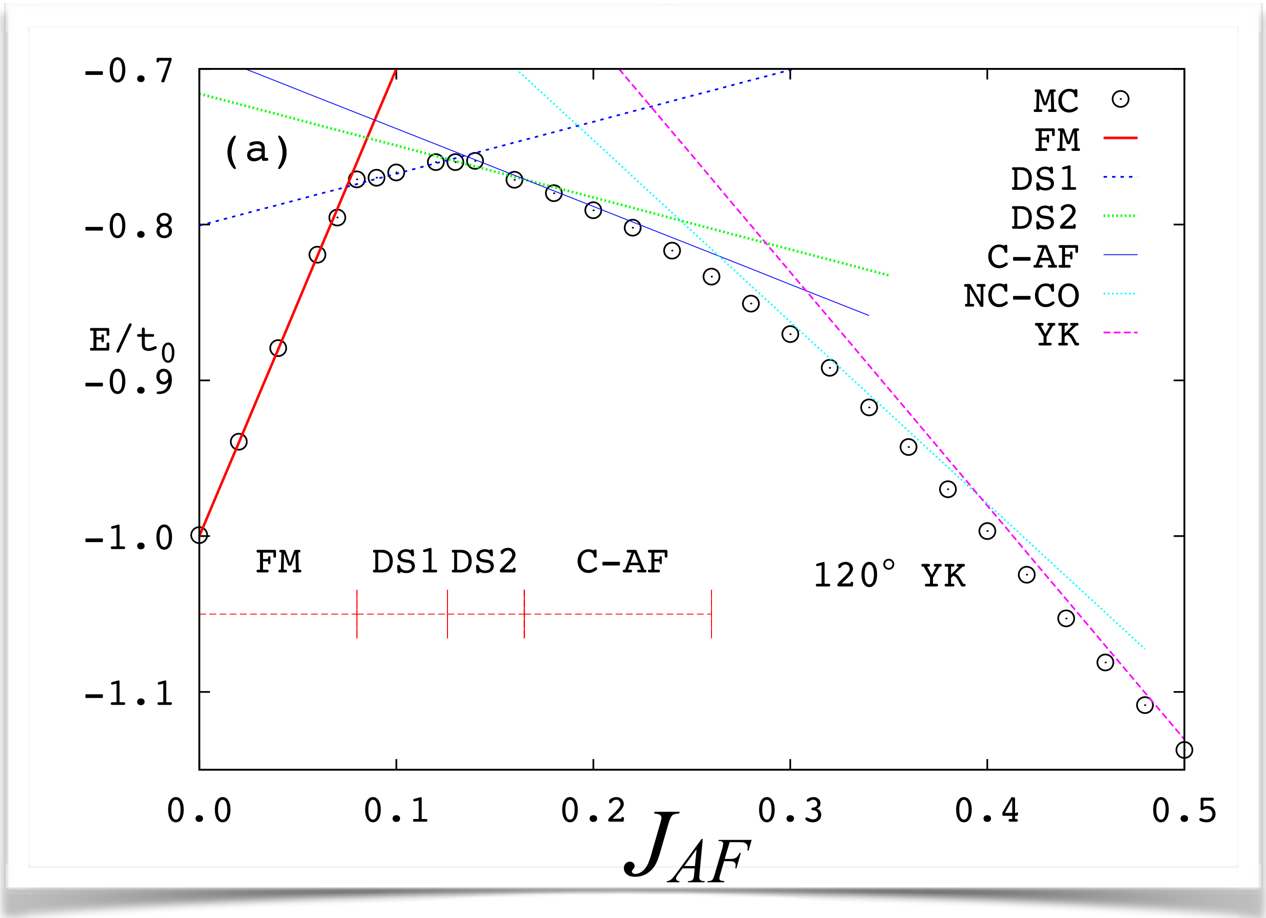


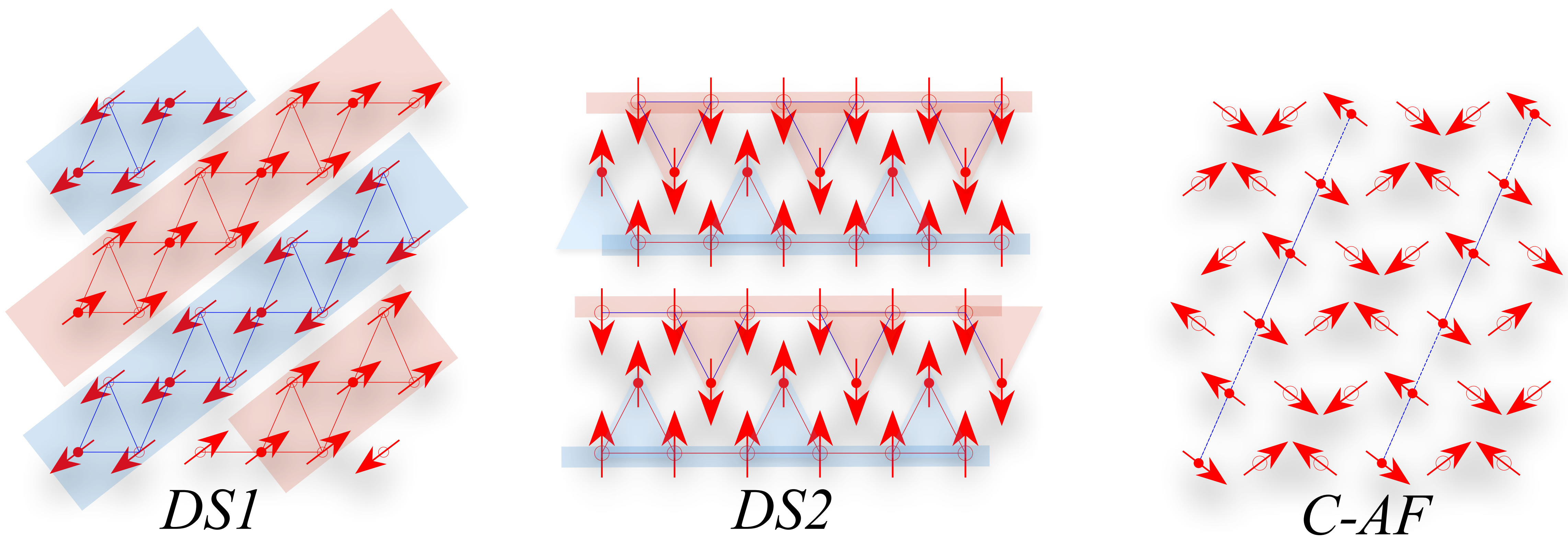
rotationally symmetric Charge Order

Stripe Charge Order

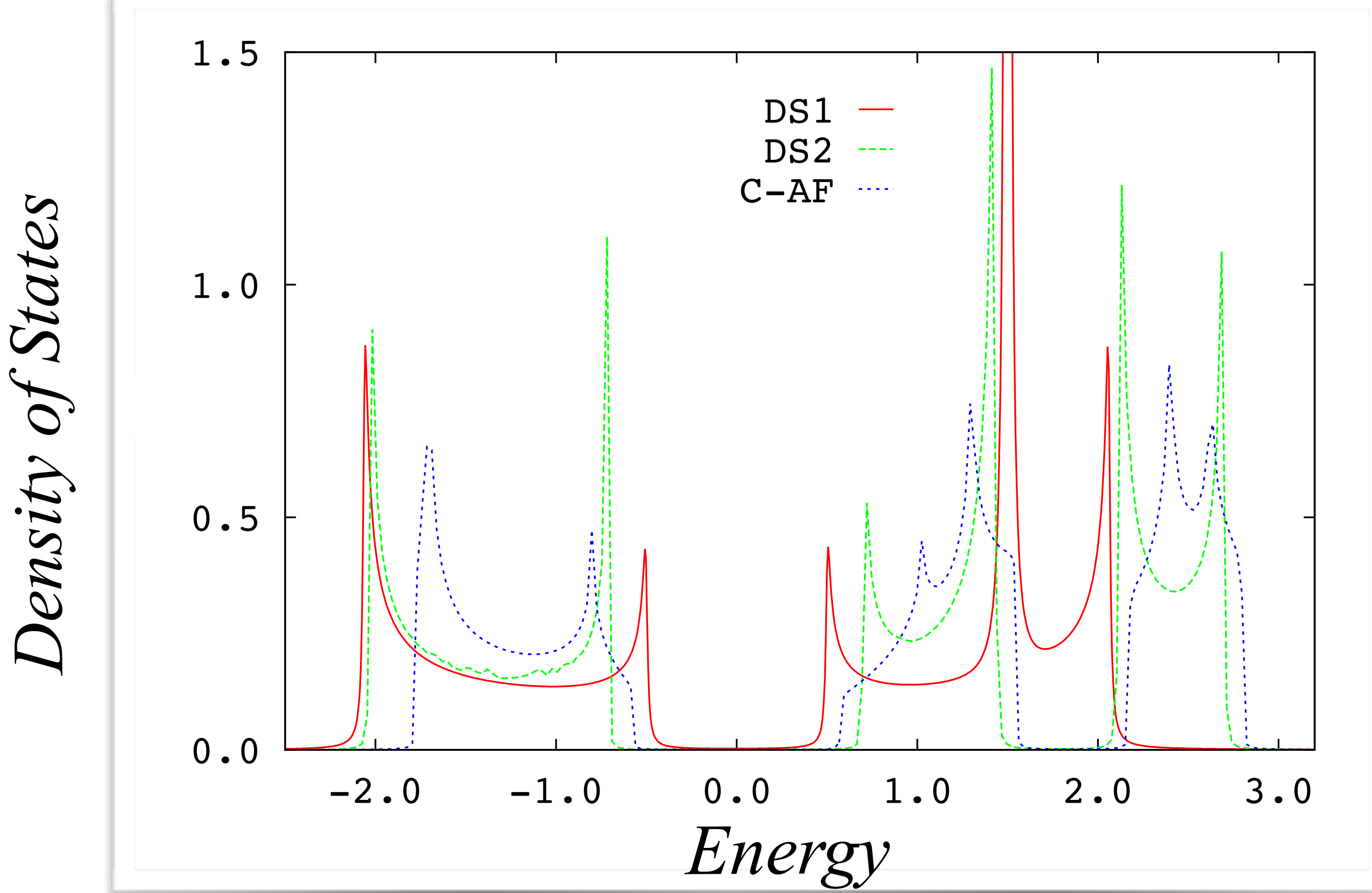
Ground-states at n=1/3

Energy





Low-temperature DOS at n=1/3

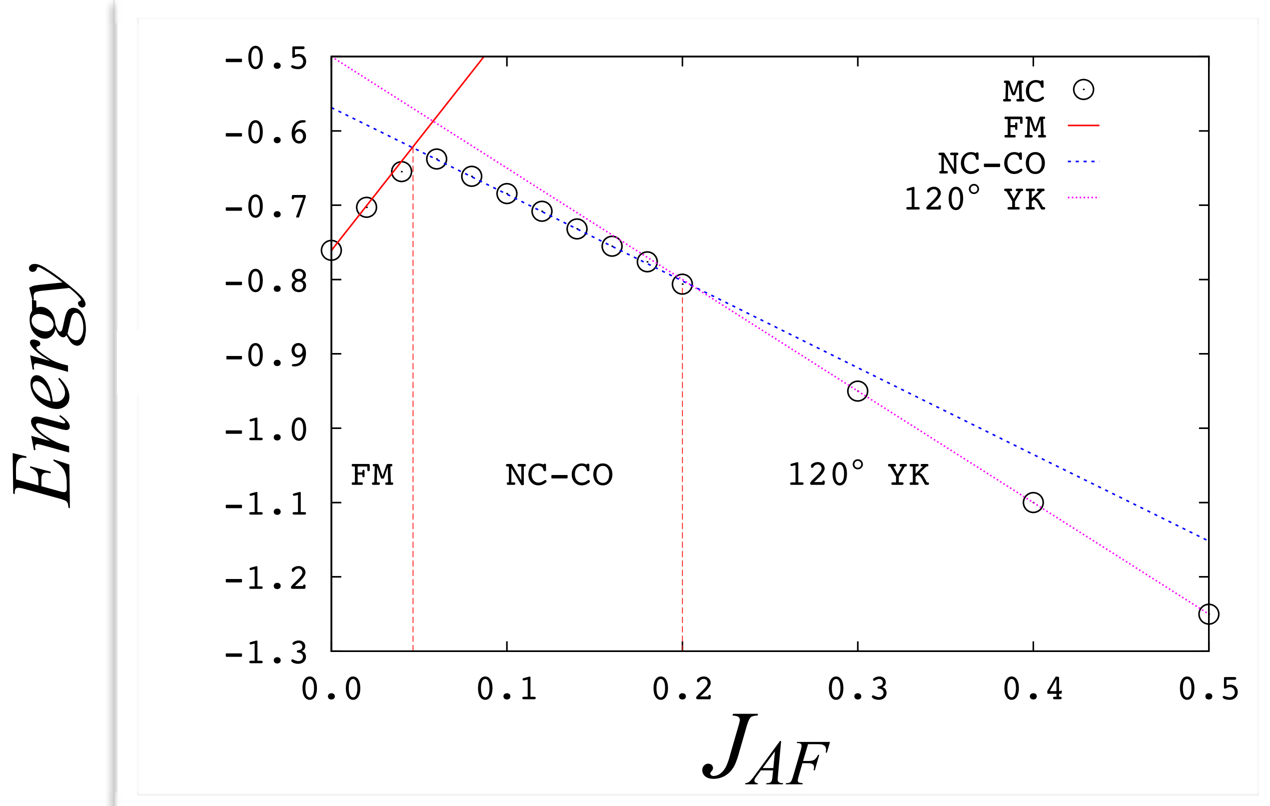


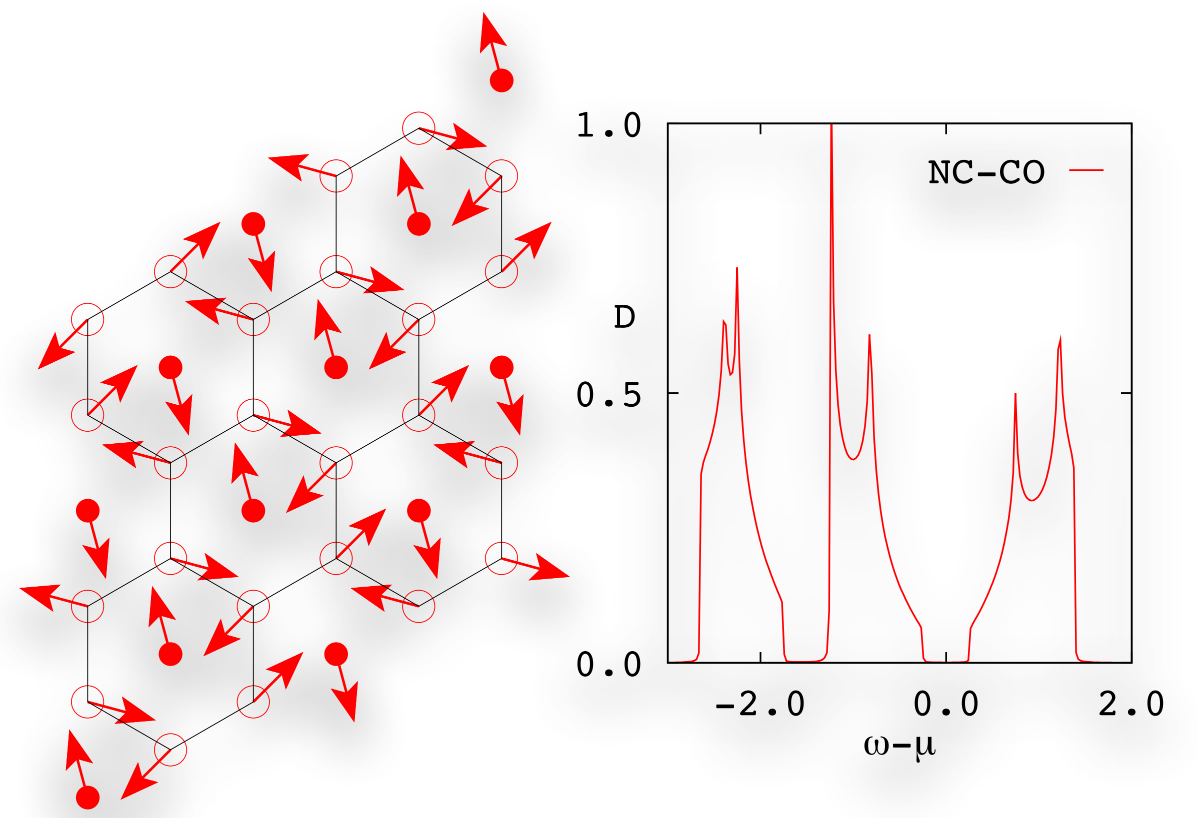
- All the new magnetic phases support gapped electronic spectra
- Opening of gap is responsible for lower energy of these phases
- Band-like effect controlled by magnetic ordering

All these phases were missed in variational calculations:

Akagi and Motome, JPSJ 79, 083711(2010)

Ground-states at n=2/3





- Non-collinear charge-ordered (NC-CO) state at *n=2/3*
- 6 magnetically inequivalent sites; 2 charge-inequivalent sites
- Similar charge ordering in triangular lattice systems: $AgNiO_2$ and $NaCoO_2$

  Bernhard et al., PRL 93, 167003 (2004); Wawrzyska et al., PRL 99, 157204 (2007)
- 6 magnetically inequivalent Co: NMR experiments on $Na_{2/3}CoO_2$

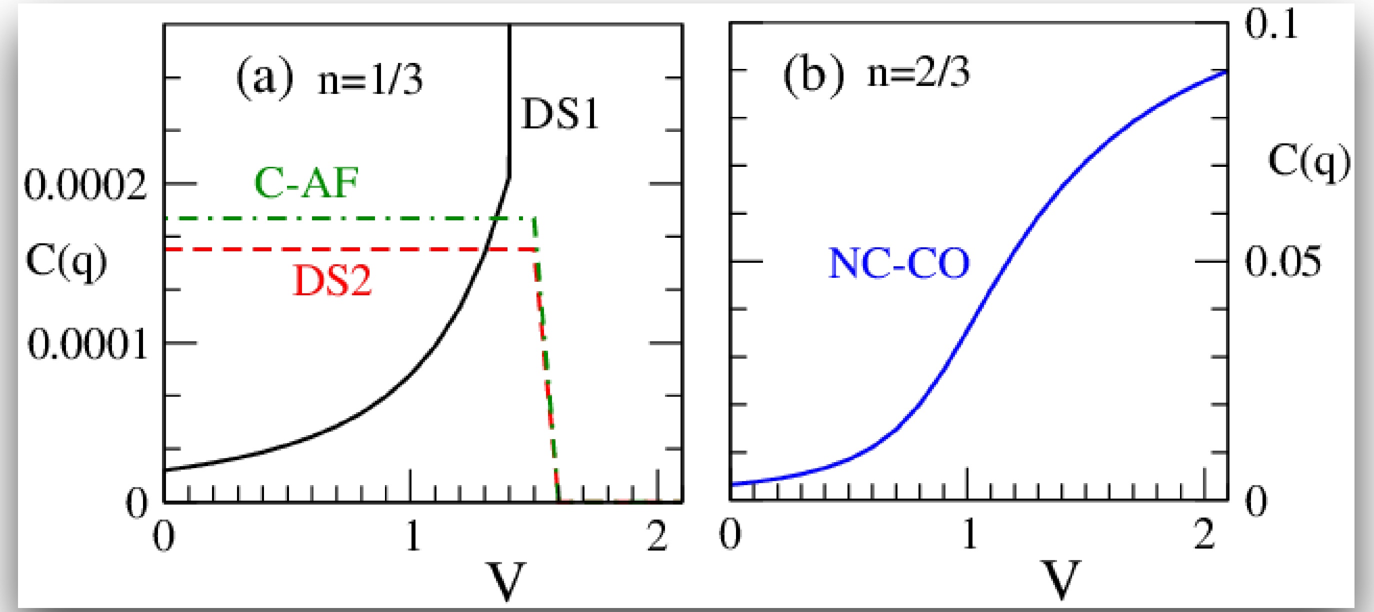
  Mukhamedshin et al., PRL 93, 167601 (2004); arXiv:1403.4567

Effect of Coulomb repulsion

Adding nn Coulomb repulsion between electrons

$$H_1 = V \sum_{\langle ij \rangle} n_i n_j$$

Within Hartree-Fock, the effect of *V* on *C(q)*



- Two of the phases C-AF and DS2 are unstable beyond a critical *V*
- The charge ordering in DS1 and NC-CO is further enhanced

Summary and open questions

- Four new spin-charge ordered ground states in strong-coupling Kondo lattice model on triangular lattice.
- All four phases are insulating. Magnetically induced band-like insulators (?).
- *n=2/3*: six magnetically inequivalent sites. Resemblance with experiments on $Na_{2/3}CoO_2$.

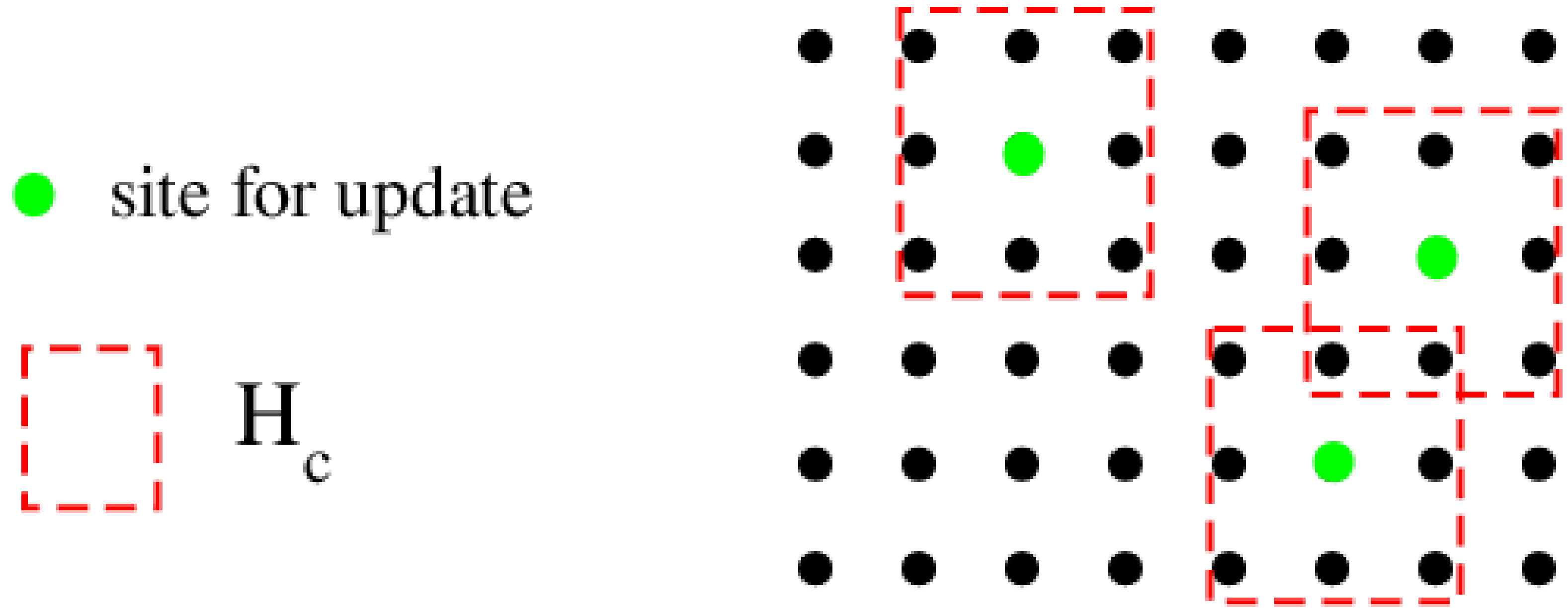
arXiv:1412.2319

- A general description in terms of effective classical spin models
- Role of quantum nature of the localized spins?
- Search for such unusual phases in multi-orbital Hubbard models

Thank you

Traveling Cluster Approximation (TCA)

- Only energy differences are needed for Monte-Carlo updates
- Is it necessary to diagonalize the full Hamiltonian for estimating energy difference?



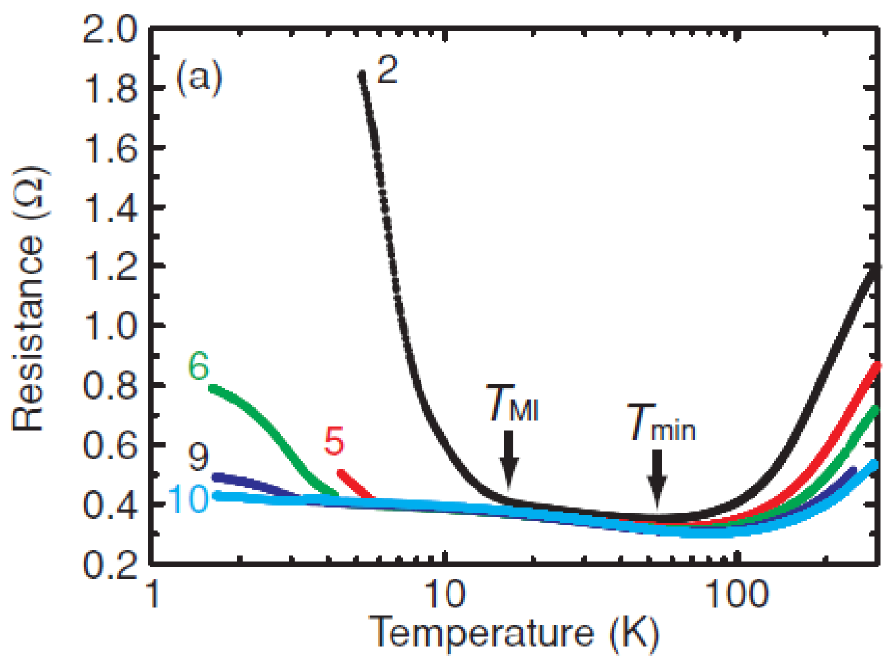
- Fermion spectrum on a smaller cluster centered around the update site
- Computation time scales as NN_c^3, system sizes $N \sim 10^3$ sites can be studied
- Access to electronic properties requires diagonalizing the full Hamiltonian

S. Kumar and P. Majumdar, EPJB '06

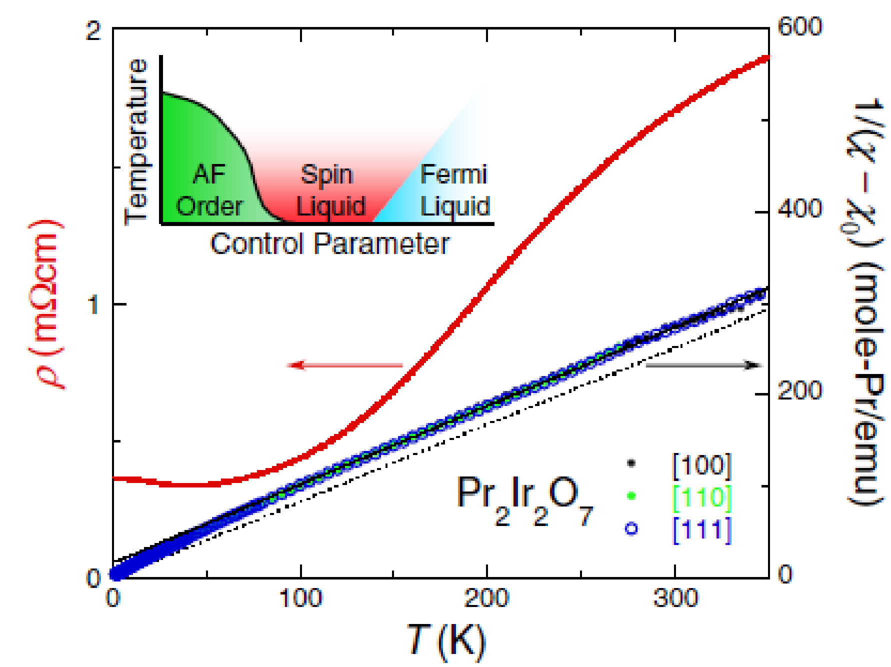
Metallic Spin-Ice Systems

- Unconventional magnetism and transport in $Pr_2Ir_2O_7$:
- 5d conduction electrons from Ir and 4f localized moments from Pr

Nakatsuji et al. PRL '06



Sakata et al. PRB '11



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Non-Kondo Mechanism for Resistivity Minimum in Spin Ice Conduction Systems

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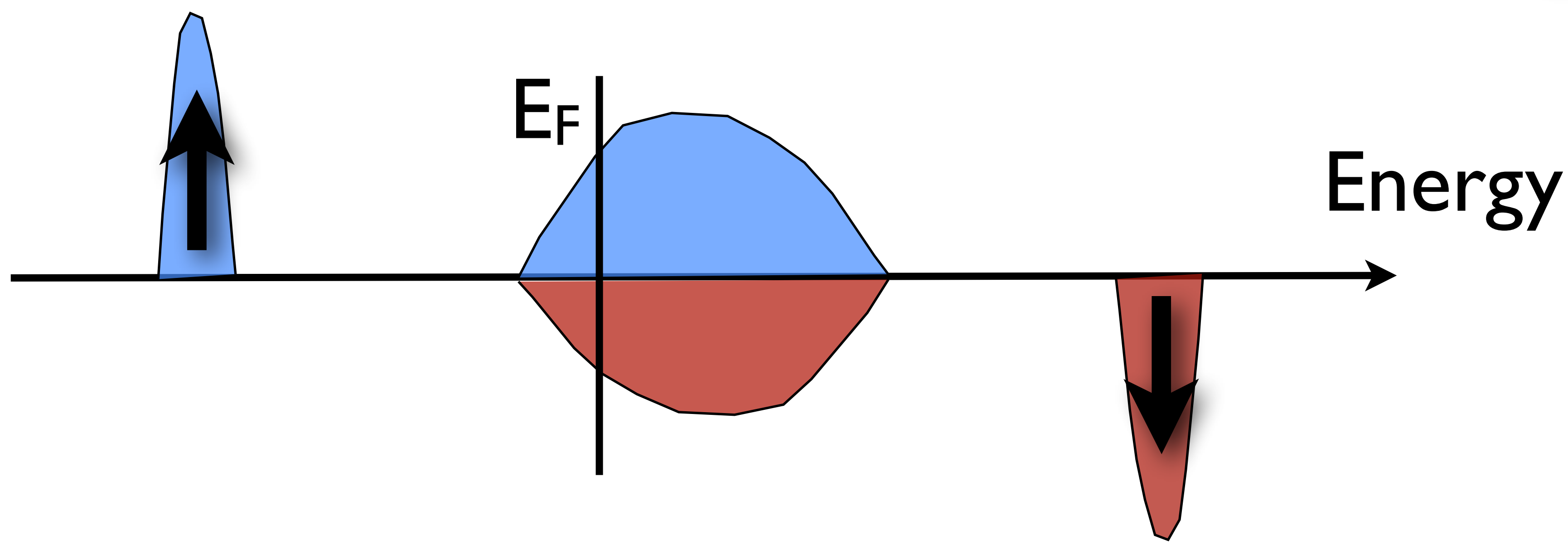
(Received 3 October 2011; published 10 February 2012)

The minimum in resistivity: scattering of electrons from spin-ice like magnetic states

Another class of metallic magnets

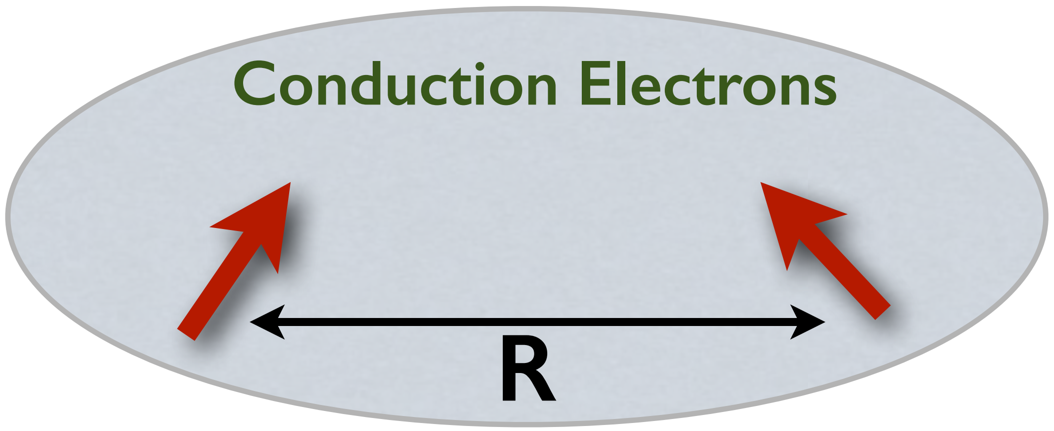


- Many materials have partially filled low-energy levels, which give rise to local magnetic moments ($RMnO_3$, $R_2M_2O_7$, other rare earth magnets)
- In addition, there is also a band of conduction electrons that is partially filled
- Magnetic metals where different bands are responsible for magnetism and electrical conduction

Two possible ways to realize these metallic magnets:

(i) Introduce magnetic impurities in metals
(ii) Introduce charge carriers in a magnetic insulator

Magnetic moments in the presence of itinerant fermions

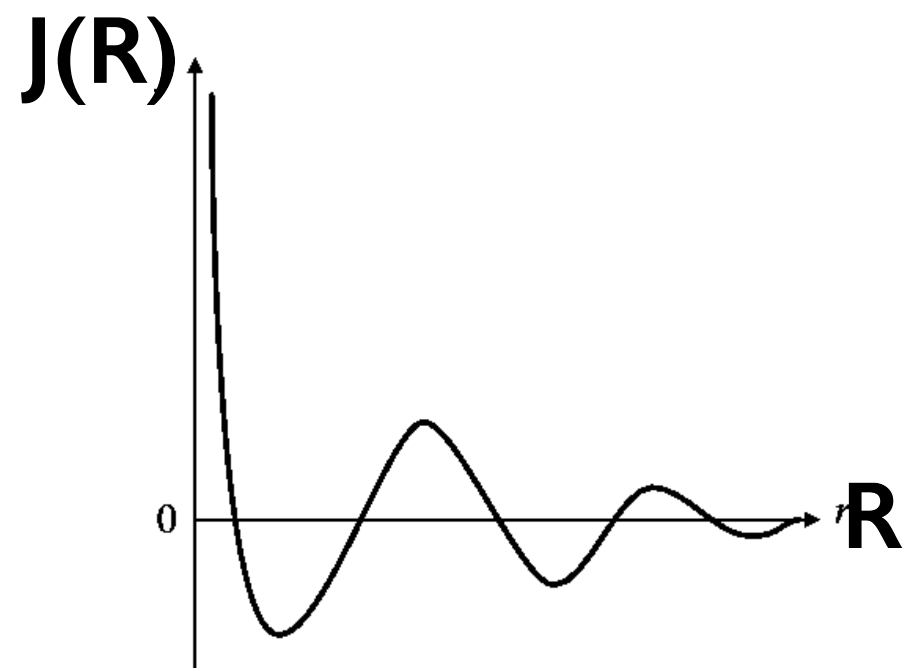


Kondo-lattice model

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) - J_H \sum_i \mathbf{S}_i \cdot \sigma_i$$

For $J_H << t$: Second order perturbation theory leads to the RKKY Hamiltonian

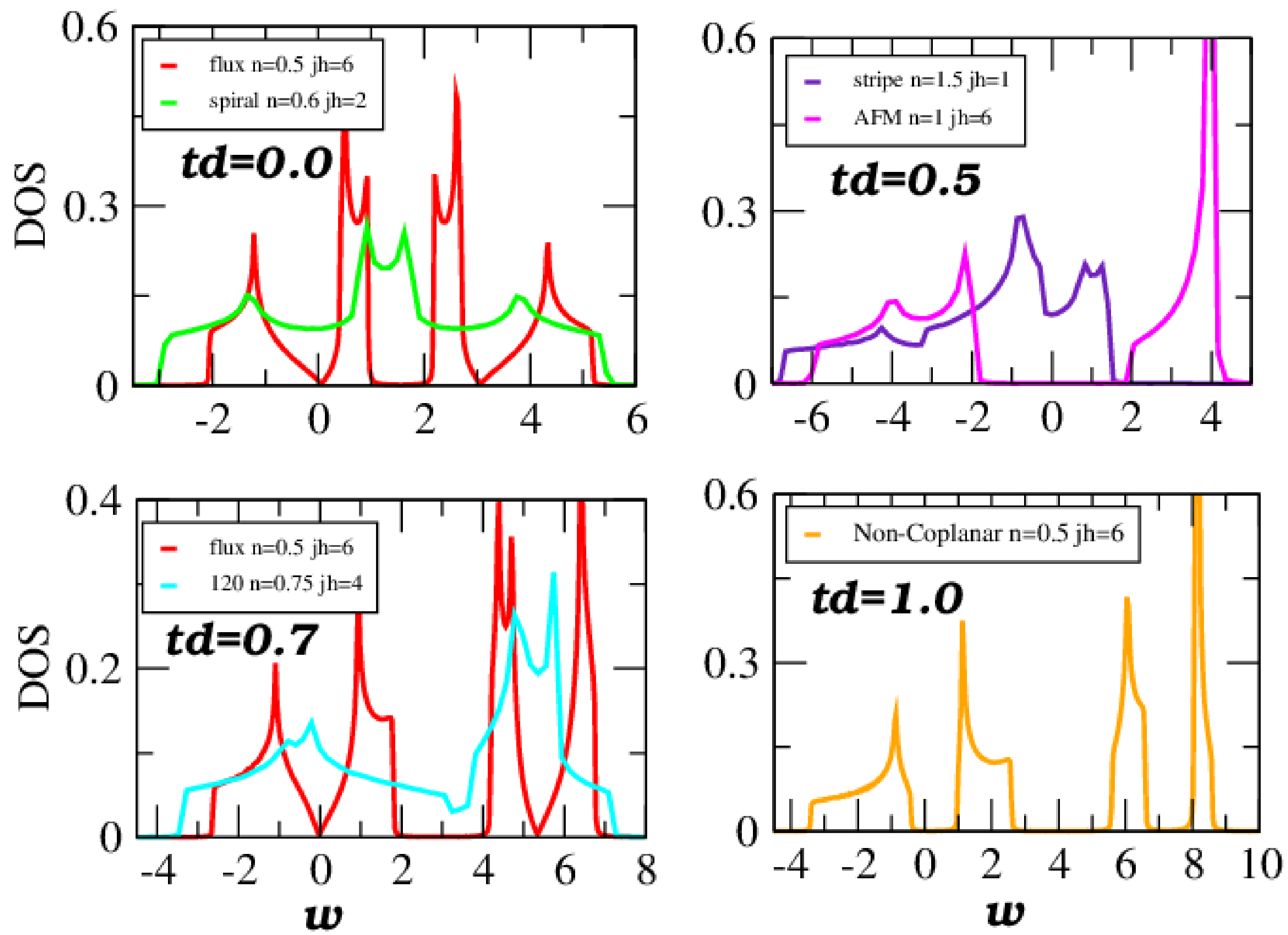
$$H_{RKKY} = \sum_{r,R} J(R)\ \mathbf{S}_r \cdot \mathbf{S}_{r+R}$$



Magnetic interactions are mediated by conduction electrons

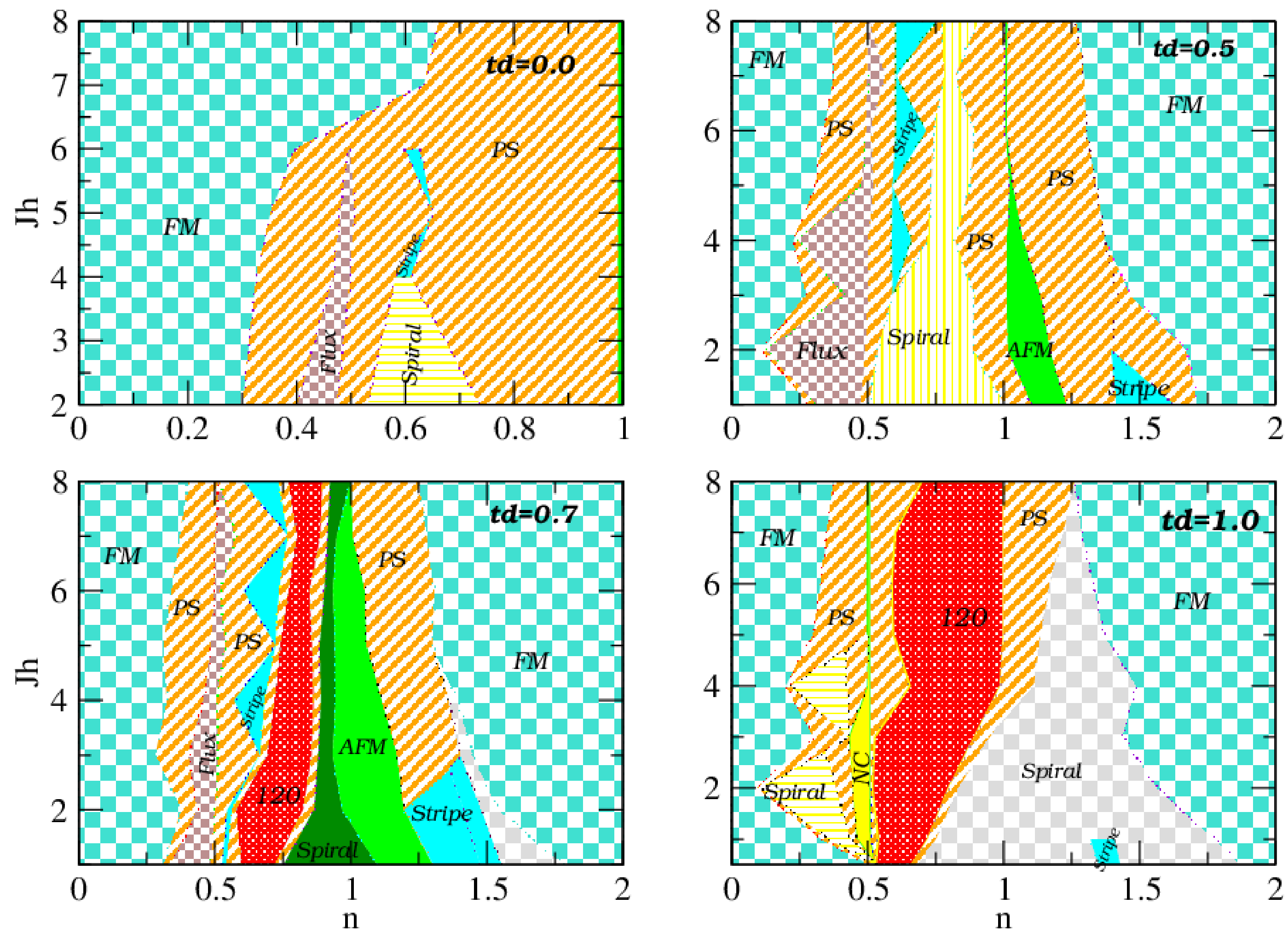
How do the magnetic moments influence conduction?

Kondo-lattice: DOS for various magnetic phases



- DOS in the Kondo-lattice are similar to those in Hubbard model

Phase diagrams for the Kondo-lattice model



All the phases present in the mean-field phase diagram of the Kondo-lattice model are also present in the Hubbard model

Spin-spiral Multiferroics

- A large number of multiferroic materials have been discovered, where a spin-spiral magnetic state is responsible for the ferroelectric state (Type-II multiferroics):

$TbMnO_3$ MnI_2 $NiBr_2$ $AgFeO_2$ CuO and many more

Two Questions:

- Why do spiral states lead to ferroelectric behavior?
- What microscopic interactions stabilize spin-spiral states?

Inverse DM, or spin-current mechanism: (*Katsura et al. PRL 05, Mostovoy PRL 06*)

- Electrical polarization is related to spin current

Collinear Magnetism: No FE distortions *Non-collinear Magnetism: FE distortions*

$$H_{DM} = \sum_{ij} \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

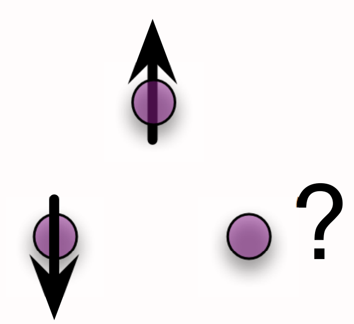
Microscopic models for non-coplanar states

What microscopic interactions stabilize spin-spiral and non-coplanar magnetic states?

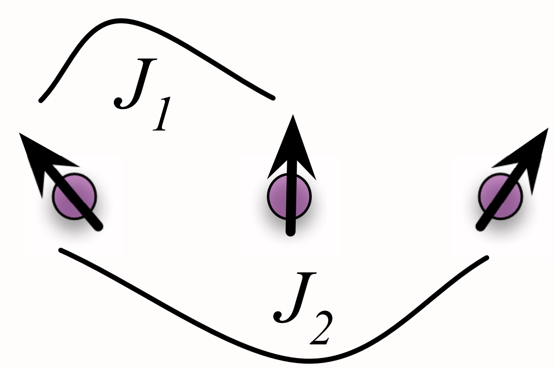
At the level of effective spin models:

- Non-collinear phases: frustrating interactions (geometrical or longer-range exchange)
  Dzyaloshinskii-Moriya (DM) interactions

- Non-coplanar phases: anisotropy terms and longer-range dipolar interactions



Geometrical Frustrations



Long-range interactions

$$H_{DM} = \sum_{ij} \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

Starting with elementary models for electrons in solids:

- Spiral-states are known to exist in the Kondo-lattice model and the Hubbard model?
- Do Kondo-lattice model and Hubbard model also support non-coplanar states?