Monte Carlo study of a spin-ice type Kondo lattice model on a pyrochlore lattice

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I. Metallic pyrochlore oxides
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III. Phase diagram
IV. Magnetization process
V. Summary

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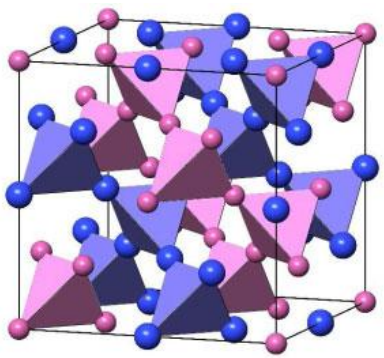
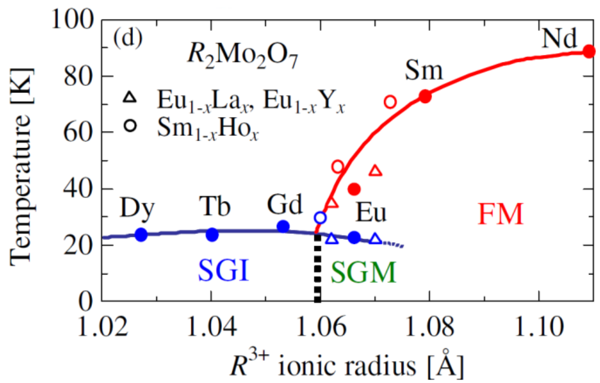
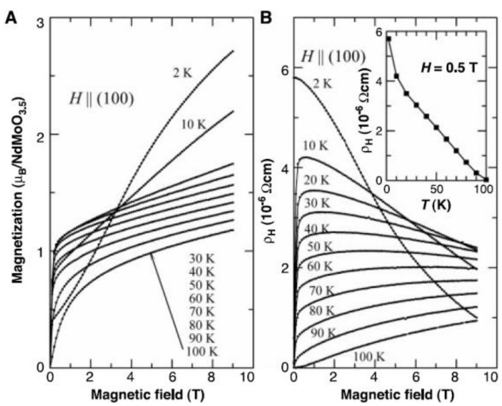
Metallic pyrochlore oxides



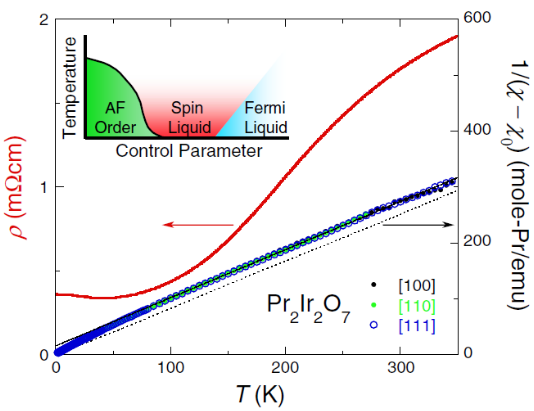


Iguchi *et al.* (`09)

- Geometrical frustration
  - ✓ Embedded pyrochlore networks
  - ✓ 4f localized spins + 3d conduction electrons



Taguchi *et al.* (`01)



Nakatsuji *et al.* (`06)

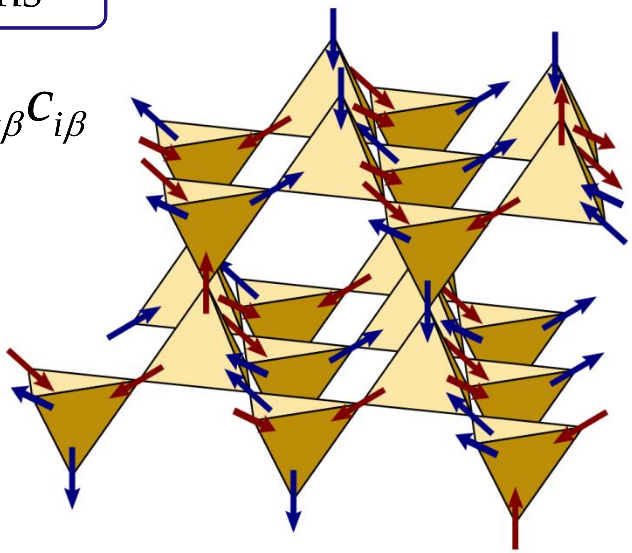
- Peculiar properties
  - ✓ "Diffusive metal" [$R_2Mo_2O_7$]
  - ✓ Resistivity minimum [$Pr_2Ir_2O_7$]
  - ✓ Unconventional Hall effects [$Pr_2Ir_2O_7$, $Nd_2Mo_2O_7$]

Spin-Ice type Kondo lattice model

Itinerant electrons | s-d interactions

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c_{i\sigma}^{+} c_{j\sigma} + H.c.) + J \sum_{i,\alpha,\beta} c_{i\alpha}^{+} S_i \cdot \sigma_{\alpha\beta} c_{i\beta}$$

- Pyrochlore lattice
- S_i : Ising spins along the <111> axis.
- $J = 2.0$, t=1.0



- No direct interactions between the localized spins.
  ⇒ Only effective interactions mediated by itinerant electrons.
  (cf. Ikeda & Kawamura `07)
- Possible geometrical frustration by the electron-mediated interactions.
  ⇒ Importance of long-range interactions

Real space Monte Carlo simulation

Calculating distribution function:

Ising spins

$$\mathrm{Tr}\,\exp(-\beta H) = \mathrm{Tr}_{\{S_i\}}\mathrm{Tr}_{C}\,\exp(-\beta H[\{S_i\}])$$

Itinerant electrons

Ising spins ⇨ Monte Carlo Method

Electrons ⇨
- Diagonalization
- Polynomial expansion
- …

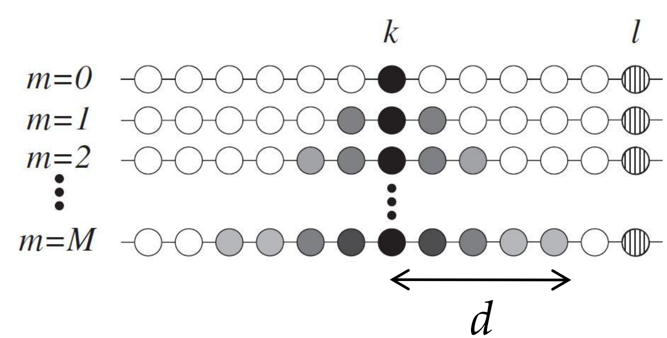
Exact diagonalization: $O[N^4]$

⇒ *Only small systems.*

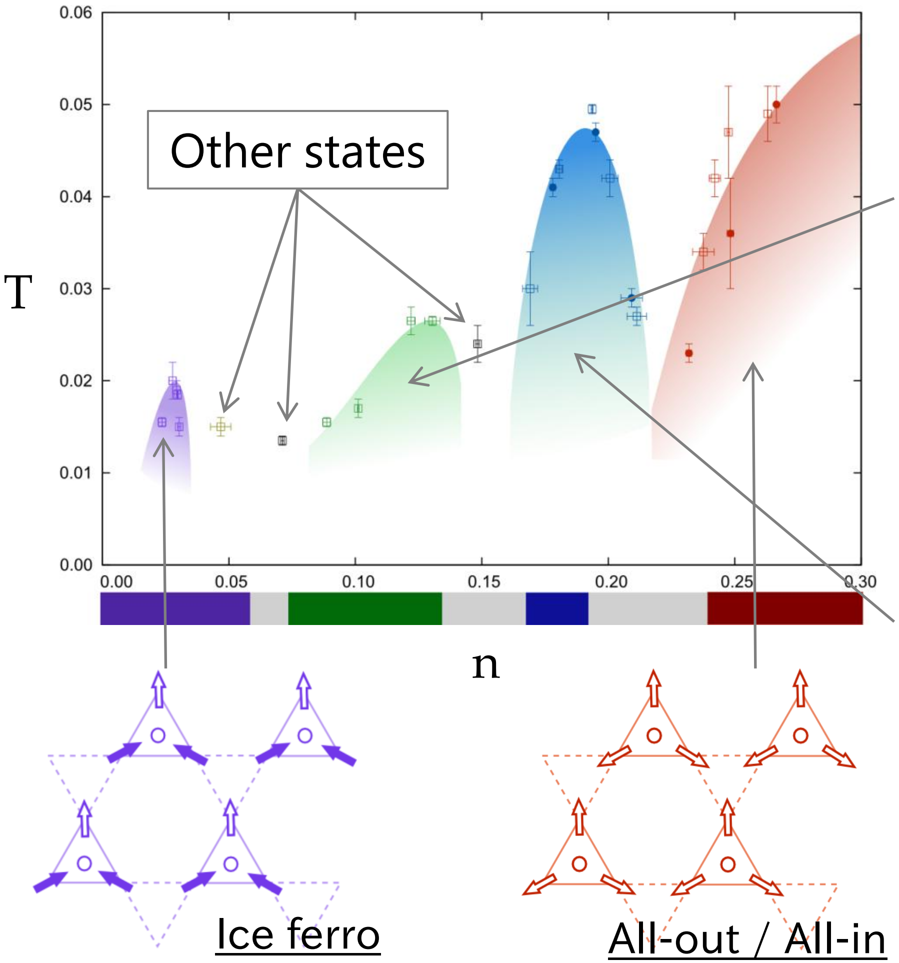
Polynomial expansion: $O[N]$

⇒ ***Much larger systems.***

1. Basis: Site-localized states $|k\rangle$
2. Density matrix ⇒ up to ***M*** th order in Chebyshev polynomials
3. Truncation distance ***d***

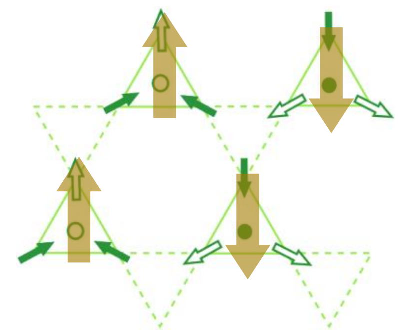


Phase diagram (J=2.0)

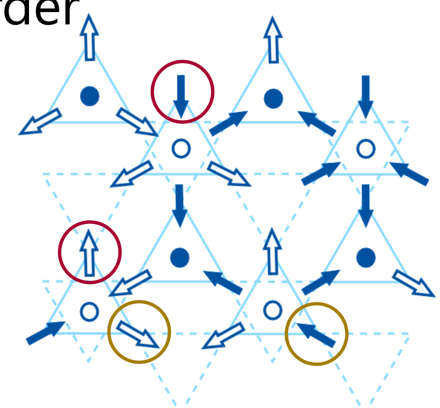


Novel magnetic states:

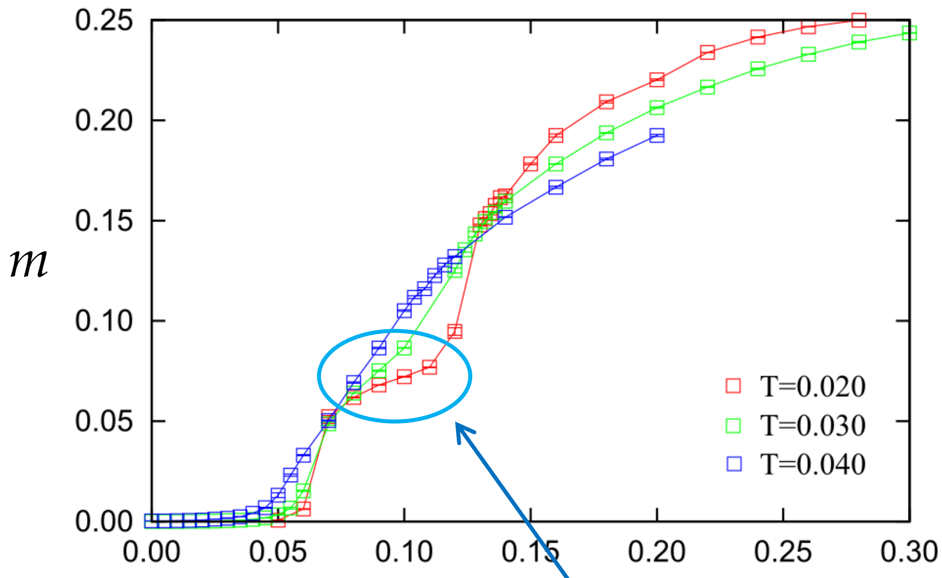
- Stripe order
  - ✓ Ice rule
  - ✓ Stripe ordering of tetrahedra
    ⇒ AF order

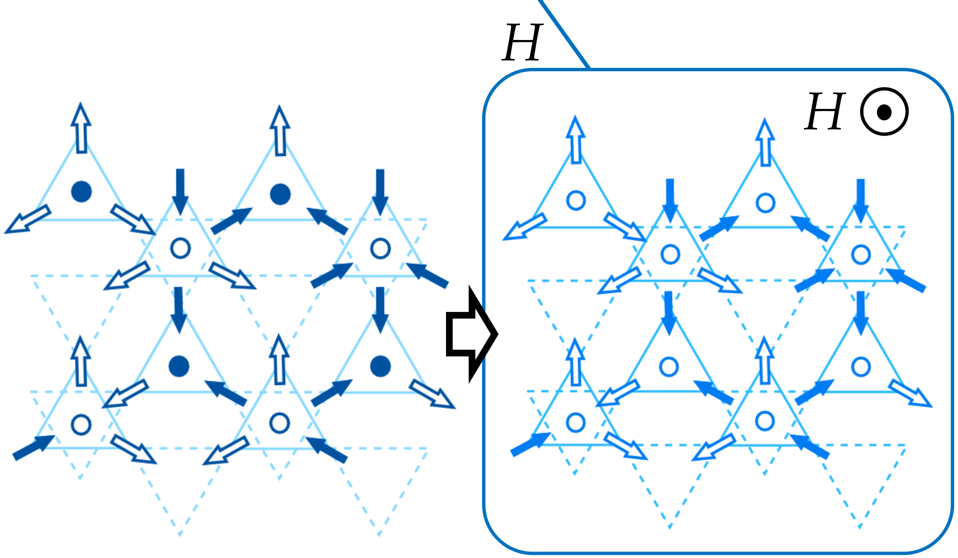


- 32 sublattice order
  - ✓ No ice-rule
  - ✓ AF 3rd n.n.
    ⇒ AF order



Magnetization process (32 sublattice phase)





μ : -3.4
Steps: 900 mcs × 3 bins
Size: N = $4x6^3$

- Magnetic field along <111> axis (Orthogonal to a kagome plane)
- Magnetization plateau around H~0.10 at T=0.02
  - ✓ The magnetic structure in the kagome plane is retained.
  - ✓ The spins in intermediate triangular layer aligns ferromagnetically.

Summary

Employing real-space Monte-Carlo simulation by exact diagonalization method and polynomial expansion technique, we investigated

thermodynamic properties of Spin-Ice type Kondo lattice model.

- ✓ Emergence of novel magnetic phases.
- ✓ Existence of magnetization plateau in one of the novel phase.

Related works (Not shown in poster)

1. Double exchange limit ($J \to \infty$) with anti-ferromagnetic super-exchange interaction on a pyrochlore lattice.
   $\to$ Successive phase transition & novel intermediate phase.
2. Triangular lattice with finite J interactions
   $\to$ Partially disordered phase