Glassy and geometric frustration in a magnetic crystal

Piyush Jeena [1] Ludovic Jaubert [1]

[1]CNRS, LOMA, University of Bordeaux

Introduction

Geometrical Frustation

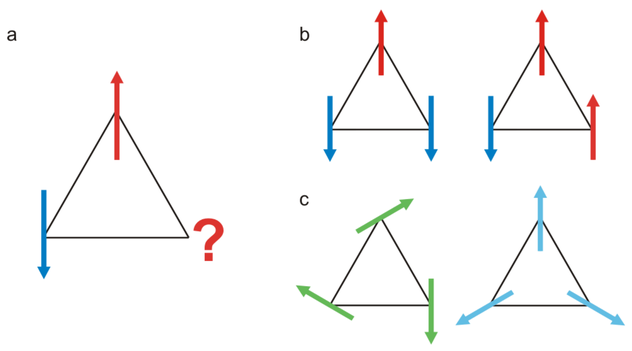


Figure 1. A plaquette of the triangular lattice.

Panel (a) indicates that, for Ising spins, the third spin is frustrated and for any of the two possible orientations, one link will yield a positive contribution to the energy.

Model

Recently studied frustated systems are pyrochlore oxides , with a general formula $A_2B_2Y_7$ (A = rare earth, B = metal(non-magnetic), Y = oxygen).

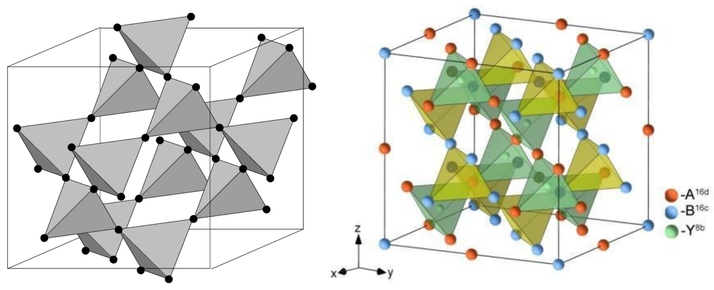


Figure 2. Pyrochlore lattice: The spins are located on the corner of every tetrahedra.

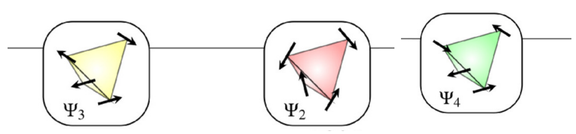
The model hamiltonian is the usual nearest- neighbor interactions compatible with the point group symmetry,T_d , of the pyrochlore lattice :

$$H_{ex} = \sum_{ij} J_{ij}^{\mu\nu} S_i^\mu S_j^\nu = \sum_t H_{tet}^{ex}[t], J_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix} \quad (1)$$

We studied the rare-earth pyrochlore oxide $Er_2Ti_{2-x}Sn_xO_7$ (Shirai et al., 2017) inspired from vastly studied pyrochlore oxides are : $Er_2Ti_2O_7$ (Savary et al., 2012) and $Er_2Sn_2O_7$ (Guitteny et al., 2013) benchmarked with their respective exchange interaction parameters. Here x is the chemical dilution.

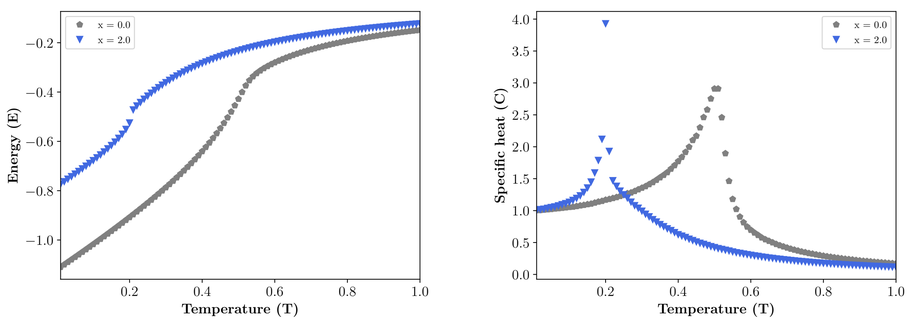
	$Er_2Ti_2O_7$	$Er_2Sn_2O_7$
J_1	0.11 meV	0.07 mev
J_2	-0.06 meV	0.08 meV
J_3	-0.10 meV	-0.11 meV
J_4	-0.003 meV	0.04 meV

Order parameters :: Geometrical frustration (Yan et al., 2017)



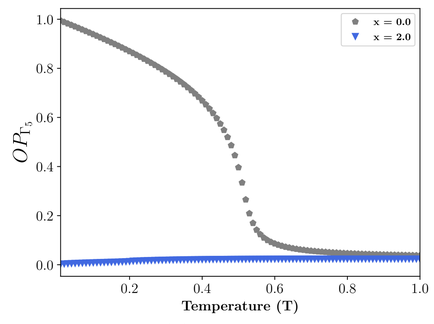
	Definition in terms of spin components	Associated ordered phases
OP_{Γ_5}	$\begin{pmatrix} \frac{1}{2\sqrt{6}}(-2S_0^x + S_0^y + S_0^z - 2S_1^x - S_1^y - S_1^z + 2S_2^x + S_2^y - S_2^z + 2S_3^x - S_3^y + S_3^z) \\ \frac{1}{2\sqrt{2}}(-S_0^y + S_0^z + S_1^y - S_1^z - S_2^y - S_2^z + S_3^y + S_3^z) \end{pmatrix}$	Ψ_2 and Ψ_3
OP_{PC}	$\begin{pmatrix} \frac{1}{2\sqrt{2}}(-S_0^y + S_0^z + S_1^y - S_1^z + S_2^y + S_2^z - S_3^y - S_3^z) \\ \frac{1}{2\sqrt{2}}(-S_0^x + S_0^z + S_1^x - S_1^z + S_2^x + S_2^z - S_3^x - S_3^z) \\ \frac{1}{2\sqrt{2}}(-S_0^x + S_0^y + S_1^x - S_1^y + S_2^x + S_2^y - S_3^x - S_3^y) \end{pmatrix}$	Palmer Chalker

x = 0.0 :: $Er_2Ti_2O_7$, x = 2.0 :: $Er_2Sn_2O_7$

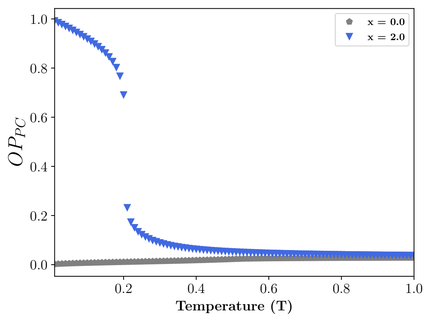


(a) Energy vs T

(b) Specific heat vs T



(c) OP_{Γ_5} vs T



(d) OP_{PC} vs T

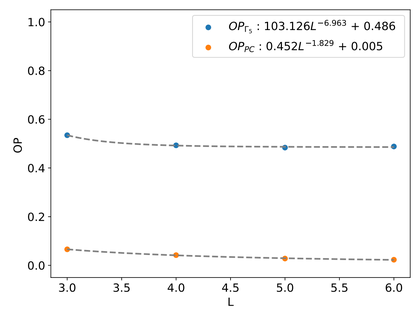
Quenched Disorder

- The idea is to tune the Hamiltonian of our system via non-magnetic dilution $x \in (0 -> 2)$ and explore the existing magnetic orders.
- The model to induce chemical quenched disorder is to choose the interaction bonds based upon the nearest neighbouring non magnetic ions(Ti,Sn) surrounding a particular Er-Er bond of a tetrahedron. There are three possibilities for the interaction bond parameters :

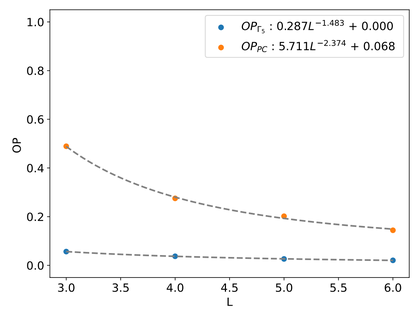
	$Er_2Ti_2O_7$	$Er_2Sn_2O_7$
J_1	0.11 meV	0.07 mev
J_2	-0.06 meV	0.08 meV
J_3	-0.10 meV	-0.11 meV
J_4	-0.003 meV	0.04 meV

Type of bond values	Neighbouring atoms
$Er_2Sn_2O_7$	Sn < – > Sn
$Er_2Ti_2O_7$	Ti < – > Ti
intermediate	Sn < – > Ti or Ti < – > Sn

Finite size scaling at T = 0.01 K



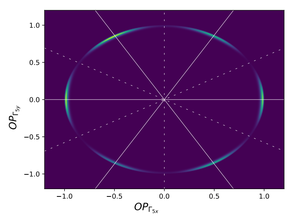
(a) Dilution x = 1.1



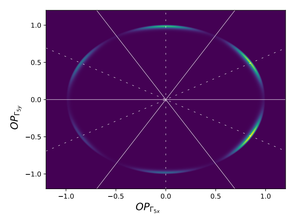
(b) Dilution x = 1.6

PDF (Andrade et al., 2018) of OP_{Γ_5} Order by Disorder

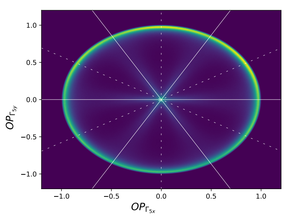
$$\begin{pmatrix} OP_{\Gamma_{5x}} \\ OP_{\Gamma_{5y}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2\sqrt{6}}(-2S_0^x + S_0^y + S_0^z - 2S_1^x - S_1^y - S_1^z + 2S_2^x + S_2^y - S_2^z + 2S_3^x - S_3^y + S_3^z) \\ \frac{1}{2\sqrt{2}}(-S_0^y + S_0^z + S_1^y - S_1^z - S_2^y - S_2^z + S_3^y + S_3^z) \end{pmatrix}.$$



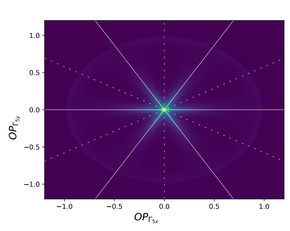
(a) Dilution x =0.0



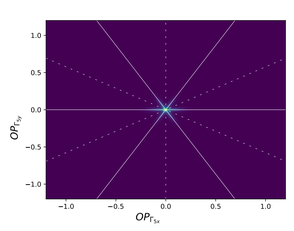
(b) Dilution x = 0.5



(c) Dilution x = 1.0



(d) Dilution x = 1.5



(e) Dilution x = 2.0

Champion et al., PRB (RC) 68, 020401 (2003)

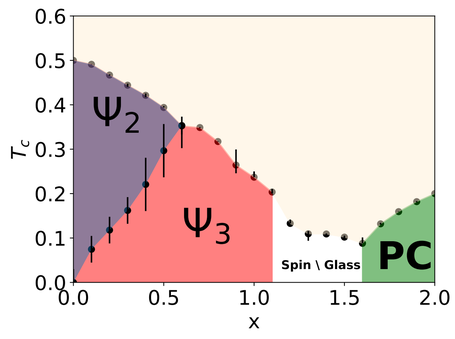
Poole et al., JPCM 19, 452201 (2007)

Maryasin and Zhitomirsky, PRB 2014

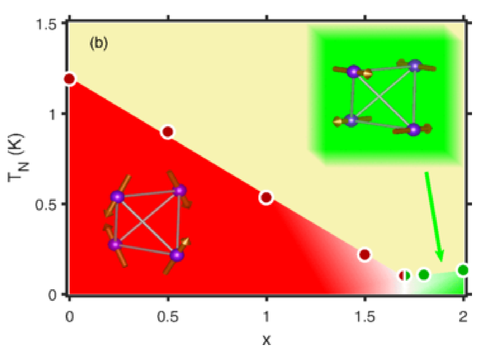
Andreanov and McClarty, PRB 2015

Andrade et al., 2018

Phase Diagram



(a) Numerical results



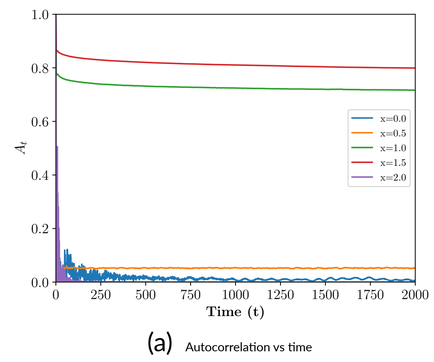
(b) Experimental, Shirai et al., 2017

Figure 3. Phase diagram of $Er_2Ti_{2-x}Sn_xO_7$: critical temperature T_c vs dilution x.

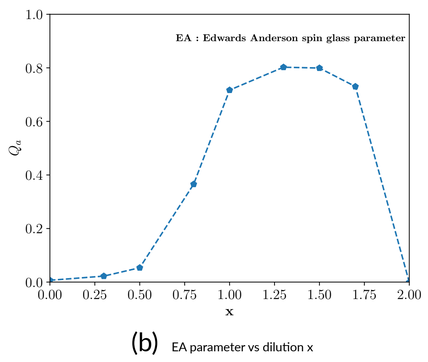
Semi-classical Spin dynamics

$$H_{ex} = \sum_{ij} J_{ij}^{\mu\nu} S_i^\mu S_j^\nu, \frac{dS_i}{dt} = S_i \times (\sum_{ij} J_{ij} S_j) \quad (2)$$

$$S_i(t+\Delta t) = S_i(t) + \frac{k_{1,i}}{6} + \frac{k_{2,i}}{3} + \frac{k_{3,i}}{3} + \frac{k_{4,i}}{6}, A(t) = \sum_{a,b,c,d} \frac{\frac{4}{N}\sum_i S_i(0).S_i(t) - \frac{4}{N}\sum_i S_i(t).\frac{4}{N}\sum_i S_i(0)}{1 - (\frac{4}{N}\sum_i S_i(0))^2} \quad (3)$$



(a) Autocorrelation vs time



(b) EA parameter vs dilution x