Report

This is the scientific report about my 4 months visit to Rudolph Peierls Centre for Theoretical Physics, Oxford University, partially funded by the ESF (HFM activity, reference number 1261). As a 1^{st} year PhD student from the ENS Lyon (France) under the supervision of Peter Holdsworth, this stay in England was a unique opportunity for me to create or strenghten collaborations with local researchers such as J.T. Chalker (Oxford), R. Moessner (Oxford) and S.T. Bramwell (UC London). The general aim of our research is the theoretical understanding of the behaviour of the spin-ice model on the pyrochlore lattice, with NN ferromagnetic interactions and subjected to an external magnetic field along the [001] direction. The Ising like magnetic moments sit on the vertices of the pyrochlore lattice, as shown in figure 1.*a)* and are forced to lie along the body centered crystal field directions. Ground state configurations require two spins "in" and two spins "out" on each tetrahedron; a condition equivalent to the Bernal and Fowler rules for proton ordering in ice, which allows a macroscopic degeneracy and then a finite entropy at zero temperature. The influence of the field will be to lift this degeneracy in favour of a unique state. In previous numerical work [1], the transition was interpreted as first order, terminating in a critical end point. Here we show that the discontinuity is actually due to loss of ergodicity as the system approaches the topologically constrained manifold of states, and by restoring the equilibrium with a non-local algorithm, this transition appears to be of the *Kasteleyn* type, as we shall explain it below.

At $T = 0$ the system is in a fully magnetized state shown in figure 1.*a)* (black spins). Hence, if a spin on the top layer is flipped, a spin immediately below must follow in order to respect the ice-rule *2in-2out*, followed by spins in consecutive layers, until a line defect has been created, spanning the whole system (red spins in fig.1.*a)*). From a numerical point of view, we consider periodic boundaries and a closed defect line is formed by looping through them. The topological constraint hence ensures that the lowest energy excitation is infinite in extension in the thermodynamic limit and we need an entropic gain at finite temperature to counterbalance it. At each step of the loop development one of the two possible spins is flipped at a cost in Zeeman energy of $2h/\sqrt{3}$, giving a total free energy cost for a loop, in a system of side L:

$$\Delta G = L\left(\frac{2h}{\sqrt{3}} - T\log(2)\right) \propto L(T_K - T) \quad \text{where} \quad T_K = \frac{2h}{\sqrt{3}\log(2)}. \tag{1}$$

When $T < T_K$, no excitations are possible ; the specific heat C_h and the susceptibility χ are exactly zero, but as soon as T goes past T_K the line defects become entropically favourable and the system undergoes a Kasteleyn transition. This explains why a non-local spin dynamic [2, 3] is needed, in opposition to a Metropolis method, which can only flip spins one by one. To guarantee its physical sense, the program has been computed such as to respect the detailed balance condition at each step of the loop construction. As T becomes significant in comparison with J, exceptions to ice-rule shall arise and a Metropolis program must be run in parrallel to the loop algorithm which only propagates on the ground state manifold. In figure 1.*c)* we show Monte Carlo data of M vs T/T_K for an $N = 4\times10^6$ spin system, with each data point being the average over 5.10^5 loop moves and 5.10^5 Metropolis steps. The data for $h = 0.01J$ show overwhelming evidence for a three dimensional Kasteleyn transition. As the temperature decreases, M increases continuously towards its saturation value $M_{sat} = 1/\sqrt{3}$ at $T = T_K$, which suggests a repulsion between line defects. This is understandable since a 1^{st} line defect in the system will lower the number of possible configurations for a 2^{nd} line which is then less entropically favourable. On the other hand, the slope is discontinuous at T_K, as expected for a Kasteleyn transition. For larger fields the discontinuity is rounded because of violation of the ice-rule and the saturation occurs at a lower temperature with respect to $T_K(h)$.

In addition to our numerical studies, we have been able to solve analytically and exactly a related model that shows a Kasteleyn transition : a Cayley tree of tetrahedra, illustrated in figure 1.*b)*. Each tetrahedron, besides the central one, is connected to another one towards the center of the tree and to three others outside which creates the ramifications of the tree. Since there are no connections between the developping branches, it is possible to establish a recursion relation between the magnetization of one layer and the one right after. The asymptotic limit of this sequence represents actually the thermodynamic limit of the Cayley tree, which is shown on figure 1.*c)* (solid lines) and falls very close to the simulation data for the pyrochlore lattice. The slight difference is due to the fact that the dimension 3 is the upper critical dimension of the Kasteleyn transition [4] with logarithmic divergence in the specific heat and susceptibility. This leads to a logarithmic dependance of $\Delta M = M_{sat} - M$ which can not be taken into account by an infinite dimensional calculation such as the Cayley tree. We stress here that the comparison is made without any fitting parameters as J, h and T_K are the same for calculation on the Cayley tree and the simulation in each case.

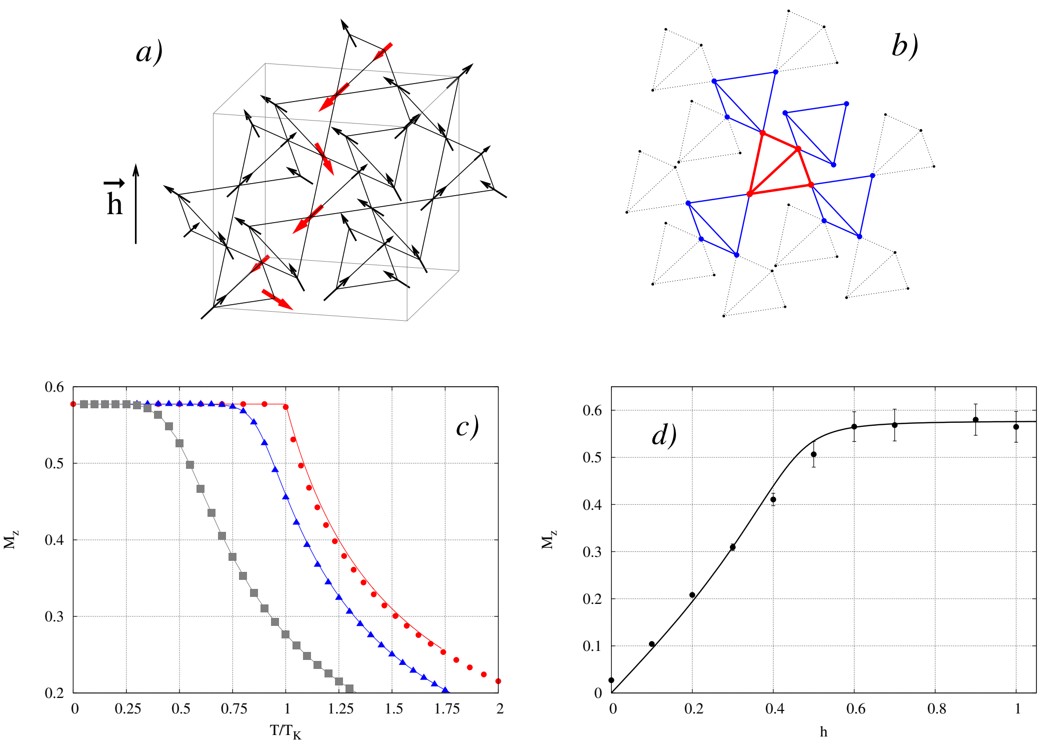

Figure 1: *a)* Pyrochlore lattice where the black spins are in the same direction as $\vec{h}$ whereas the thick red spins correspond to a line defect ; we can notice that the ice-rule is respected. *b)* Cayley tree with a red tetrahedron in the centre, its 4 nearest neighbours (blue) followed by the 12 NNN (only 9 are drawn using dashed lines) ... without any connections between the ramifications once they separate *c)* Component of the magnetization M_z along $\vec{h}$ as a function of T/T_K obtained numerically (dots) and analytically (solid lines) for $h/J = 0.01$, 0.4 et 1 from right to left. *d)* M_z vs h obtained analytically (solid lines) and experimentally (dots) by neutron scattering on the coumpound $Ho_2Ti_2O_7$ at $T = 1.2K$.

What about the experimental situation? Three dimensional Kasteleyn transitions have, in the past, been associated with the trans-gauche disordering transition for polymers imbedded in lipid bilayer systems [5]. Here we propose that spin-ice materials provide a new possibility for their study. Field scans have been performed at fixed low temperature $T = 1.2K$ in Holmium Titanate (where $J = 5.4K$) that we can compare in figure 1.*d)* with our data for M vs h^*. The ratio J/T being of order 1, we can not expect a clear discontinuity of the slope, but the figure does provide strong evidence that a rounded Kasteleyn transition does exist in real spin ice materials and could be more closely approached in future experiments. These results are explained in more details in our paper in preparation [6] and will be presented during the Workshop in Trieste on August 2007 : *Highly Frustrated Magnets and Strongly Correlated Systems.*

References

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