Report for the short visit ref: 1872 (Marion MOLINER)

Classical Shastry-Sutherland lattice.

Purpose of the visit

This visit allowed to continue the collaboration started between Andreas Honecker (Goettingen), Pierre Pujol (Toulouse), Daniel Cabra (La Plata/Strasbourg) and Marion Moliner (Strasbourg).
We are studying, both analytically and numerically, the ground state properties of classical Shastry-Sutherland systems. The objective is to determine what conditions can lead to plateaux in the magnetization curves of those frustrated classical antiferromagnets.
At this stage of the project numerical simulations were required. This visit allowed Marion Moliner to profit from the numerical expertise of the Goettingen group.

Rare-earth tetraborides compounds RB_4 crystallize in the tetragonal system and are characterized by a plane of orthogonal dimers. This dimer system is equivalent to the Shastry-Sutherland lattice, which is a square lattice with additional diagonal coupling (see Fig. 1). Recent experiments on terbium tetraboride TbB_4 [1] showed that it presents plateaux in its magnetization curve that were suggested to be due to anisotropy [2]. We are considering another scenario including lattice distortions. The large total angular momentum of TbB_4 justifies a classical approach.

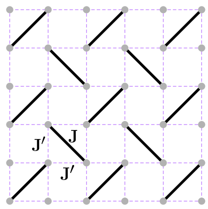

Figure 1: The Shastry-Sutherland Lattice

In previous Monte Carlo Simulations we observed magnetization plateaux at one-third of the saturation magnetization in classical Shastry-Sutherland systems at finite temperature. This suggests that it may be due to an *Order by Disorder* effect [3]. Analytical calculations showed that this should be affected by the system size as it has already been studied in the pyrochlore lattice [4].

Description of the work carried out during the visit

Classical Monte Carlo simulations were performed in order to study the *Order by Disorder* scenario that was suggested analytically. For this the Shastry-Sutherland lattice was implemented in the ALPS codes [5]. Magnetization and specific heat were computed for various systems.
Moreover a numerical study of the ground state of the system in the one-third magnetization plateau was performed. This study was based on the analytical calculations done before.

Description of the main results obtained

- Both our code and ALPS agree on the magnetization curves for classical Shastry-Sutherland lattices. Pseudo-plateaux do not seem to require fine tuning on the value of the ratio between the exchange constants of the Shastry-Sutherland lattice (see Fig. 1).

- A better undestanding of the ground state properties was obtained numerically (see Fig. 2). This was done for the special ratio of the coupling constants that also allows some analytical treatment. This result gives a precise idea of the energy barriers between soft modes lines previously calculated. Those barriers are extremely low which means low temperature properties will appear at lower temperature than thought.
- We found a signature of a phase transition in the specific heat (around $T \propto J/10$). More work is needed to understand this phenomenon. Moreover very low temperatures simulations will require modifications of the Monte Carlo codes [1]. More work will have to be done in order to continue the study of the specific heat.

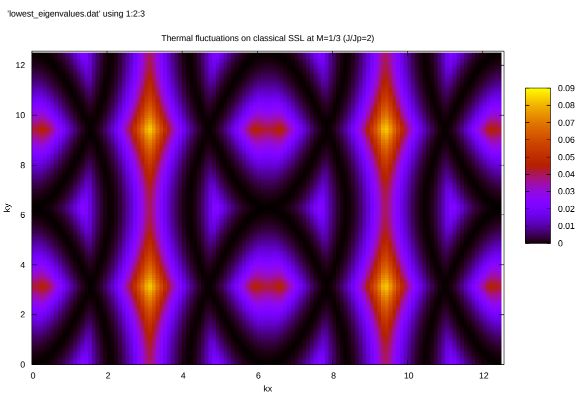

Figure 2: Ground state for the ratio $J/J' = 2$ with thermal fluctuations.

Future collaboration with host institution (if applicable)

The collaboration on this project will continue between the three institutes (Goettingen, Strasbourg and Toulouse).

Projected publications/articles resulting or to result from your grant

So far more work is needed before publishing.

References

[1] S. Yoshii, T. Yamamoto, M. Hagiwara, T. Takeuchi, A. Shigekawa, S. Michimura, F. Iga, T. Takabake and K. Kindo J. Magn. and Magn. Mat. **0**, 1-0 (2006)

[2] T. Inami, K. Ohwada, Y. H. Matsuda, Z. W. Ouyang, H. Nojiri, D. Okuyama, T. Matsumura, Y. Murakami arXiv:0709.0977, (2007)

[3] J. Villain, R. Bidaux, J. P. Carton, and R. J. Conte, J. Phys. (Paris) **41**, 1263 (1980).

[4] J.M.D. Champion and P.C.W. Holdsworth J. Phys. Cond. Mat. **16**, S665 (2004)

[5] The ALPS Project (Algorithms and Libraries for Physics Simulations), http://alps.comp-phys.org

[1] Unfortunately we did not achieve quantitave agreement for the specific heat between our code and ALPS. We suspect that the ALPS code has problems in the present case, although the precise reason remains to be understood. Analysis of this problem was one reason we did not investigate lattice distortions yet.