Report on the project “Magnetic Correlations in the Extended Kagome $\mathrm{YBaCo_4O_7}$”.

(visit to Theoretical Physics group in Oxford on 30/11/2010-6/12/2010)

The main task of the recent visit was to discuss the classification of the ground states in the $\mathrm{YBaCo_4O_7}$. This material is a geometrically frustrated antiferromagnet with a layered structure. It has been shown in recent experiments to have very unusual magnetic correlations, which are long range in the direction perpendicular to the layers but short range within each layer[1]. The model for this system is given by frustrated Heisenberg antiferromagnet with the Hamiltonian

$$H = J \sum_{inplane} \vec{S}_i \vec{S}_j + J' \sum_{interplane} \vec{S}_i \vec{S}_j .$$

and is composed of alternating Kagome and triangular spin planes in such a way that there is an antiferromagnetic exchange between the spins on the Kagome lattice as well as between the apical spins of the triangular lattice ($\vec{S}_4$,$\vec{S}_5$) with all three spins ($\vec{S}_1, \vec{S}_2, \vec{S}_3$) on every second triangle in the Kagome plane see Ref.[1]. Two apical spins and three triangular spins constitute a bypiramid, which is described by the Hamiltonian

$$H = -\frac{J}{2}\left[3 + 2(J'/J)^2\right] S^2 + \frac{J}{2}\{[\vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \frac{J'}{J}(\vec{S}_4 + \vec{S}_5)]^2 - 2\left(\frac{J'}{J}\right)^2 \vec{S}_4 \vec{S}_5\}.$$

In the ground states the total effective spin on the bypiramid is equal to zero $\vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \frac{J'}{J}(\vec{S}_4 + \vec{S}_5) = 0$ and the same is true for the total spin on the remaining triangles in the Kagome planes, which can be seen from the Hamiltonian for a single bypiramid.

Because of effectively ferromagnetic exchange between the apical spins, in the ground states, the ones which are running along the c-axis are aligned parallel within the same line of bypiramids, but they can have different directions for different lines. Apart from accidental degeneracies (in particular at the point $J = J'$) the system is made of copies of the planes wich are constructed from connected bypiramidal units. Using a simple counting argument one can show that, in general, for arbitrary alignement of apical spins the number of degrees of freedom is equal to the number of constraints.

In the limiting case of $J'/J = 3/2$ the ground state is planar, i.e. all spins lie in the plane such that the apical spin directions have a 120 degree pattern (as would be the ground state of classical spins on a triangular lattice) and the spins on the triangular units have total zero magnetization. The apical spins on the neighbouring sites can deviate from each other within a maximum solid angle, which is defined by the deviation from $3/2$, i.e. for small deviations the possible relative rotation of apical spins is small. Strikingly there is a manifold of ground states which are defined by directions of the apical spins.

The first task is to understand the general features of ground states and to find the way to classify them, at least for small deviations from $J' = J = 3/2$. After this had been done one should be able to understand the excitations in these, in general, disordered ground states.

The degrees of freedom of the system are given by rigid triangular and bypiramidal units with total zero magnetization (solid tops). This can be compared with a ferromagnet for which the order parameter leaves on the surface of a sphere S^2. The order parameter in our case have an $SO(3)$ rotational symmetry and can be characterized by, for example, three Euler angles or alternatively by a unit-size vector and the angle of rotation. Triangular units have in addition a discrete C_{3v} point group symmetry, which could lead to accidental degeneracies.

The expectation is to have a topological classification of the ground states with the states in different classes separated by energy barriers. For that we need to look at the homotopy groups of the order parameter space. The fundamental group is given by $\pi_1(SO(3)) = \mathbb{Z}_2$, so the system has stable defects (vortices), running along the c-axis, which are characterised by two-valued topological number $(0, 1)$. These point-defects are similar to ones which exist in a system of Heisenberg spins on a triangular lattice[4] (notice that they are zero-energy vortices in the ground states) or to "dysgirations" in the A-phase of $3He$.

In order to discuss higher dimensional defects let us first consider a single two-dimensional spin-plane (Kagome + apical spins). As we mentioned earlier at $J'/J = 3/2$ the ground state is planar. A small deviation from this value of anisotropy will lead to ground states with some of them having only small corrugations out of the plane. Let us assume that such ground states exist (we will call the class of these ground states a base class) and try to build other classes of ground states from this base. Consider a ground state which at infinity is described locally by the spin configuration in the base class. Then we can compactify the plane into a sphere S^2 and look at the maps from S^2 to $SO(3)$. The defects in this case will be classified according to second homotopy group $\pi_2(SO(3)) = 0$. This group is trivial and the system cannot have zero-energy instantons (skyrmions) for a single spin-plane. However this simple topological argument has to be checked as here we do not take into account interplane couplings. The third homotopy group $\pi_3(SO(3)) = \mathbb{Z}$ tells us that there can be nontrivial static point-like topological excitations - similar to Shankar's monopoles. There is also a possibility to have dynamic excitations of this sort for a single plane in $2+1$ dimensions (?) as well as Z_2 vortices in 3+1, as $\pi_4(SO(3)) = \mathbb{Z}_2$. Apart from these the system can also have domain walls in the (a,b) plane. For the excitations near these ground states one can make an observation that a given choice of the directions of apical spins breaks completely the $O(3)$ rotational symmetry of the Hamiltonian, which leads to appearance of three phonon branches with, in general, different sound velocities.

Further plans:

1. Need to derive a nonlinear σ model in our case along the lines of the paper Ref.[2] and describe quantitatively, if possible, topological excitations.

2. Calculate excitation spectra for different classes of ground states.

3. Understand experimental signatures. The ground states in different classes should have different susceptibilities, and this could explain the difference seen experimentally between field cooled and zero-field cooled susceptibility.

4. Introduce quantum fluctuations. Study simplified models of weakly-coupled chains of bypiramids. Study Ising version of the model via classical to quantum mapping. Disorder-free glassiness.

---

[1] P. Manuel, L. C. Chapon, P. G. Radaelli, H. Zheng, and J. F. Mitchell, "Magnetic Correlations in the Extended Kagome $YBaCo_4O_7$ Probed by Single-Crystal Neutron Scattering", Phys. Rev. Lett. 103, 037202 (2009).

[2] T. Dombre, N. Read, "Nonlinear σ models for triangular quantum antiferromagnets", Phys. Rev. B **39**, 6797 (1989).

[3] M. Nakahara, "Geometry, Topology and Physics, Second Edition", IOP publishing, (2003); N. D. Mermin "The topological theory of defects in ordered media", Rev. Mod. Phys. **51**, 591 (1979).

[4] H. Kawamura and S. Miyashita, "Phase transition of the two-dimensional heisenberg antiferromagnet on the triangular lattice", J. Phys. Soc. Jpn. **53**, 4138 (1984).

There's no better way to fly.
Lufthansa

Reservation code:
4MZUW2

Ticket details & travel information

Travel dates for: KOVRIZHIN / DMITRY MRDR
Ticket number: 220-2305513004 *
Form of Payment:

* You have access to the passenger receipt by clicking the ticket number up to 30 days after commencement of travel.

Your flight itinerary

Flight	Date	from	to	Departure	Arrival	Reservation
LH 3406 operated by: BMI	30 November	DRESDEN DE	LONDON GB HEATHROW TERMINAL 1	16:10 h	17:05 h	Economy Class (T) confirmed
LH 3407 operated by: BMI	17 December	LONDON GB HEATHROW TERMINAL 1	DRESDEN DE	12:45 h	15:35 h	Economy Class (V) confirmed

Total Price of your Ticket

Price		Taxes & Fees		Passengers		Total	
94.00	+	103.59	x	1 Adult	=	EUR	197.59
				Ticket Service Charge	=	EUR	10.00
				Total Price for all passengers	=	EUR	207.59

Flight information

- An electronic ticket has been issued for you. Your boarding pass will be available at www.lufthansa.com up to 23 hours prior to departure. For identification please have your booking reference and your miles&more or credit card which you used at the time of booking ready. Alternatively you can also use the check in terminals at the airport to print your boarding
- In advance of your journey, please note the current free baggage allowance included in your ticket price and the applicable hand baggage regulations.
- It is not necessary to reconfirm any Lufthansa flight booking after ticket purchase.

Reservation code: 4MZUW2

pass.
In case you are travelling with an airline other than Lufthansa please contact them for their respective check in conditions.

- As the airfare you have chosen may be a special fare, please note that restrictions may apply regarding rebooking and refund. If rebooking and refunds are possible please be aware that charges may apply. For refunds of taxes and charges only, Lufthansa applies a refund service charge (RSC) of EUR 30,00. For rebooking with different travel dates please be aware to consider the applicable advance purchase periods, minimum and maximum stays and restrictions regarding the departure times. For further questions regarding the fare conditions of your booked airfare please contact your local Lufthansa representative who will be happy to assist you.
- Please acquaint yourself with the applicable health and entry requirements.

Flight services

- **You've booked a Rail&Fly Ticket?**
  Please note the terms and conditions regarding the use of Rail&Fly in conjunction with a Lufthansa Ticket!
  The Rail&Fly ticket is only valid in conjunction with a valid plane ticket / flight confirmation for a flight on the same or previous day.
  The Rail&Fly ticket is non-rebookable, non-refundable and valid, with the exception of auto trains, on all DB (German Railways) trains as well as specially designated bus lines.
  Please note that surcharges apply to the ICE Sprinter, DB night trains, and CityNightLine.
- **Always up-to-date**
  Don't miss our latest offers - register now for our online newsletter!
- **Are you earning miles yet for your flights with Miles & More?**
  Don't waste another mile - instead, register online now to start earning miles with Miles & More.
- **Lufthansa on your mobile**
  Enter lufthansa.com into your mobile phone´s internet browser. From the mobile Lufthansa portal you have access to various services like check-in, online timetable, arrival and departure information and more.
- **Organising your online bookings will become even easier.**
  You receive your travel information today together with calender dates in the form of icalender files.
  These files can be used to automatically transfer your travel information to your electronic organizer. You will find information regarding this subject here.
  Important Information!
  Please be aware that the data being transferred to your electronic calender could be corrupted by your personal PC preferences and in this case might need manual correction when imported.

There's no better way to fly.
Lufthansa

Reservation code:
4MZUW2

Thank you for your booking and have a pleasant journey.
Kind regards

Lufthansa German Airlines

Carriage is subject to Lufthansa's Condition of Carriage. Lufthansa German Airlines is not liable for any changes of the transmitted data undertaken by you or a third party. No liability can be accepted for the accuracy of the information included in this document.
Please note that all flight times are local times.

Oxford University
Department of Physics, The Rudolf Peierls Centre for Theoretical Physics

1 KEBLE ROAD · OXFORD OX1 3NP
Telephone: Department +44 1865 273999
Direct Access No. +44 1865 273973
FAX: +44 1865 273947
EMAIL: j.chalker1@physics.ox.ac.uk

Chantal Durant
European Science Foundation (ESF)
1 quai Lezay Marnesia
BP 90015
67080 Strasbourg Cedex
France

30th December 2010

Dear Colleagues,

This letter is to confirm that Dr Dmitry Kovrizhin from the Max-Planck Institute for the Physics of Complex Systems, Dresden visited me at the Physics Department, University of Oxford, from 30/11/2010 to 6/12/2010. During this time we collaborated on research into the physics of highly frustrated magnetism, and more specifically *magnetic correlations in extended kagome compounds*, as described in detail in a separate report provided by Dr Kovrizhin.

I understand that Dr Kovrizhin's visit to Oxford will be financed by the European Science Foundation under the activity title Highly Frustrated Magnetism through a Short Visit Grant, reference number 3852.

Yours sincerely,

Professor J. T. Chalker