

# Entanglement in Spin & Orbital Systems

18-22 June 2008, Cracow, Poland

Workshop organized by the ESF Program Highly Frustrated Magnetism

## Scientific report for the workshop

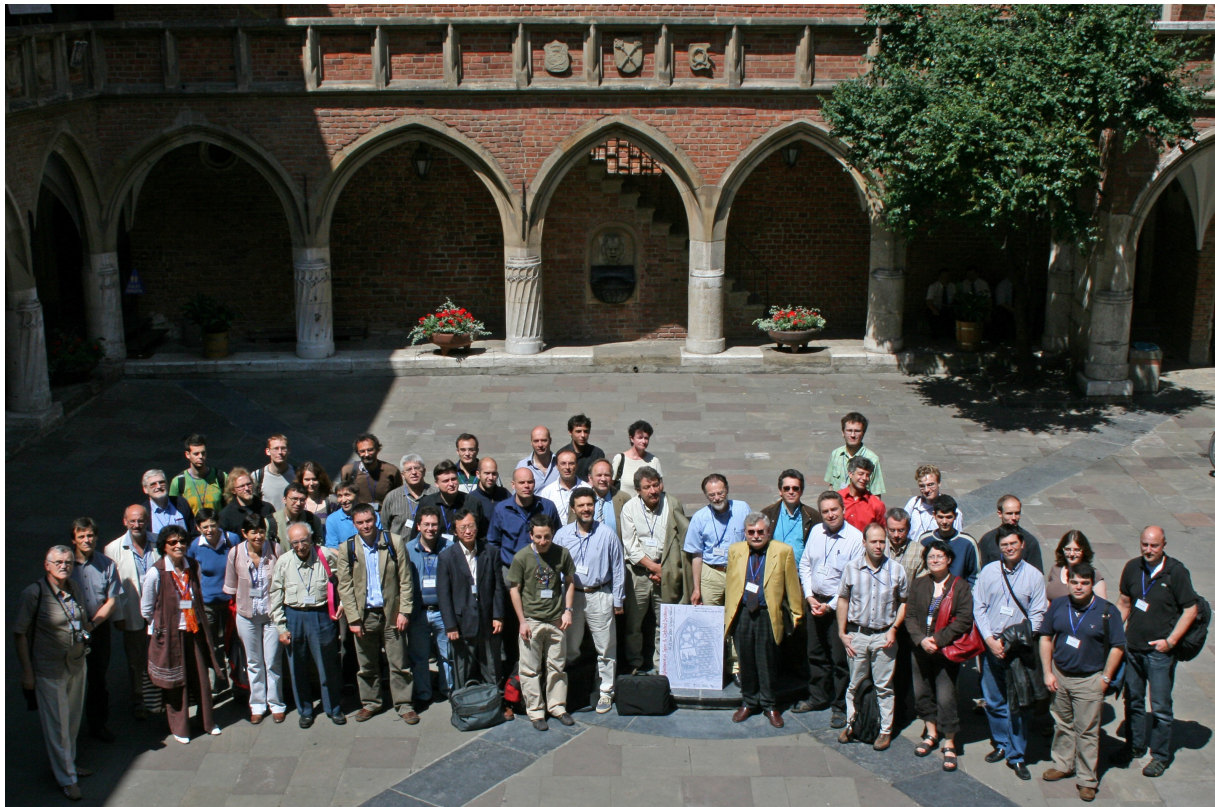
Peter Lemmens (Braunschweig), Andrzej M. Oles (Cracow), Karlo Penc (Budapest)

Local Organization: M. Bogucka, M. Raczkowski, K. Wohlfeld (Cracow)

Homepage: <http://confer.uj.edu.pl/hfm/>

### Summary

The workshop was organised within the scientific program Highly Frustrated Magnetism (HFM) supported by the European Science Foundation (ESF) and the Jagellonian University (Cracow). It was organized by: P. Lemmens (Braunschweig), A.M. Oles (Cracow), K. Penc (Budapest). The local organization of the workshop was performed by M. Bogucka (secretary) and M. Raczkowski, K. Wohlfeld from the Jagellonian University, Cracow, Poland.



Participants of the Workshop on 20 June 2008 at the courtyard of Collegium Maius (Grand College), the building where the Jagellonian University moved to in 1400

The initial planning for the workshop and first announcement happened during the HFM steering committee meeting in Trieste, Italy, August 2007. The focus on a restricted set of topics related to the entanglement and frustration in spin and orbital systems was motivated by numerous activities in this field over the last years. The purpose of the workshop was to exchange ideas, to promote collaborations, and to achieve a better understanding of this new emerging and active field. Indeed, several collaborations were started and new scientific projects emerged from the discussions among the participants.

The following topics were included in the talks and discussed during the workshop:

- entangled states in spin frustrated lattices
- frustration and entanglement in spin-orbital models and materials
- quantum phase transitions in spin and orbital systems
- experimental consequences of entangled states
- theoretical methods of investigating entangled states
- charge degrees of freedom in systems with entangled states

### **Meeting program and organization**

The workshop covered the above topics in dedicated sessions during three days. Most scientific contributions were presented as 30 minutes (but two longer 45 minutes) talks, including discussion. Poster session was also organized and included mainly the contributions presented by PhD students and postdocs attending the workshop. The posters were displayed during the two first days of the workshop (the posters were discussed during the poster session and during the breaks). The abstracts of the contributions were collected in the book of abstracts which was handed over to the participants at registration.

The workshop was a satellite conference to the European Conference *Physics of Magnetism'08* held in Poznań, Poland (June, 24 - June, 27 2008) and the workshop participants were encouraged to consider joining also this meeting.

The workshop was joined by 52 scientific participants, who presented 31 talks, 16 poster contributions, and took part in the panel discussion. The organizers tried to bring together a mix of young scientists on the level of PhD students, and postdocs together with senior researchers. The interdisciplinary approaches of the workshop lead to the additional advantage of a mutual exchange about all material related aspects.

All scientific activities as well as lunch and dinner were organized in the conference center of the Jagellonian University in Cracow. The conference centre situated in a peaceful wooded area ca. 5 km from the centre of Cracow. The guesthouse is integrated in the conference centre. This led to close contact and intensive discussions between the participants, and optimised the use of the time available.

The historic city of Cracow (Kraków) with its second oldest Jagellonian University in Central Europe was visited before or after the workshop by some of the participants. On 20 June 2008 an open session covering important aspects of entanglement in spin and orbital systems was held in the historic Aula of the Jagellonian University. After this session the 640-year-old building of the Jagiellonian University at the corner of the Jagiellonska and Sw. Anny streets, the Collegium Maius (Grand College), was visited by the participants (see photograph). The Jagellonian University moved to the Collegium Maius in 1400 when King Vladislav II Jagiello bought the house with funds his late wife, queen-saint Jadwiga, had earmarked for the renewal of Krakow's alma mater.

## Description of the scientific content

### Overview of the theory talks

Entanglement is of particular interest in highly frustrated spin systems without long-range magnetic ordering. These so called *spin liquids* are envisaged as a highly entangled linear combinations of resonating spin-1/2 singlet bonds. The simplest model capturing the essence of this state is the quantum dimer model. The recent developments in this fields were presented by G. Misguich "Entanglement Entropy in Quantum Dimer Models" and N. Shannon "Extended 'U(1)' Liquid Phase in a Three Dimensional Quantum Dimer". Also, the singlet dimer bonds can serve as a useful tool to measure entanglement in spin model, as shown by P. Tomczak in "A New Estimator of Block Entanglement for Heisenberg Antiferromagnets". Developments in the quantum information theory can lead to new efficient computational methods, as shown by J. Dziarmaga "Multi-scale Entanglement Renormalization Ansatz in Two Dimensions: Quantum Ising model".

The effect of the spin liquid (or other correlated) ground state onto mobile carriers in these systems has been looked at by D. Poilblanc "Statistics of Holons in The Quantum Dimer Model", as well as by F. Becca "Magnetism and Superconductivity in the  $t$ - $t'$ - $J$  Model", by P. Prelovšek "Self-Localization of Composite Spin-Lattice Polarons", and by H. Fehske "Quantum Transport within a Background Medium: Fluctuations versus Correlations"

In the transition metal compounds the effect of the orbital degeneracy cannot be neglected. The interplay of spin and orbital degrees of freedom can lead to a very rich physics. Among others, the orbitals can contribute to stabilization of nearest neighbor spin singlet, thus providing an alternative way to the quantum dimer models, as shown in the talks of F. Mila "From Orbital Degeneracy to RVB Spin Liquids" and G. Jackeli "Classical Dimers in Orbitally Degenerate Honeycomb Antiferromagnet". The situation can be further complicated by magnetoelastic coupling as discussed by S. Di Matteo "Orbital Order in Titanium and Vanadium Spinels".

The central topic of the workshop, entanglement in spin and orbital systems, was covered in the talk by L.F. Feiner "Spin-Orbital Entanglement and Violation of the Goodenough--Kanamori Rules in  $t_{2g}$  Orbital Systems" which suggested also new ways of defining local and on-bond entanglement. The interrelation between the spin and orbital intersite correlations plays a central role in finite temperature properties of cubic vanadates, as highlighted by P. Horsch in his talk "Evolution of Spin-Orbital-Lattice Coupling in the  $RVO_3$  Perovskites". Similar ideas of entangled states in cobaltates were discussed by G. Khaliullin who concentrated on "The Origin of Strong Correlations in Layered Cobaltates".

Materials with coexisting (ferro)magnetic and (ferro)electric moment are called multiferroics and are being intensively studied in the last years. In these materials, the complex interplay of the geometric structure and spin ordering can lead to interesting physics. This has been discussed in the talks given by J. van den Brink "Multiferroicity Due to Entangled Spin, Charge and Orbital Order", M. Mostovoy "Toroidal and Other Magnetic Multipole Orders in Frustrated Spin Systems", and D.I. Khomskii "Spontaneous Currents and Polarization in Mott Insulators: Are Electrons Really Localized?".

Characterization of the materials and finding out the relevant degrees of freedom and the minimal model to describe the observed physics is a complex task. The evolution of the experimental techniques and the proper interpretation of measured data are necessary steps in this process. One of the new promising techniques is the resonant inelastic X-ray spectroscopy, discussed by F. Vernay "Theoretical Interpretation of RIXS Spectra: Another Route Towards Multiplets". In "Origin of Magnetic Interactions in  $\text{Ca}_3\text{ABO}_6$ " R. Frésard presented a case of a nontrivial effective Heisenberg model.

### **Experimental topics:**

According to the arguments given above experimental contributions were centred on systems with spin frustration of various competing interactions. An excellent review of the experimental topics related to spin-orbital entanglement in transition metal oxides was given by Y. Tokura. On the other side advanced experimental techniques, as resonant X-ray scattering and preparation techniques that lead to novel states of previously studied compounds were discussed.

Manganites with their complex interplay of electronic and lattice degrees of freedom are still an interesting topic. The talks from M. Hennion, F. Moussa, G. Ghiringhelli and B. Dąbrowski described the properties of these materials using neutron and X-Ray scattering, as function of doping and dimensionality. Manganites were contrasted with compounds that have  $t_{2g}$  electrons, e.g. the cubic vanadates by Y. Tokura and C. Ulrich. While cobaltates have been discussed due to the observation of superconductivity and complex transport phenomena. Here, P. Lemmens and Y. Pashkevich contributed with details on experimental investigations using Raman scattering and MSR. In the later talk a layered system with both pyramidal and octahedral coordinated transition metal sites with a sequence of antiferromagnetic and ferromagnetic instabilities as well as spin state ordering has been promoted.

Superconductivity and the electronic properties of the novel Fe pnictides have been addressed by I. Eremin, both from experimental as well as from theoretical side. He gave an excellent overview of the experimental situation and theory in the newly discovered family of iron pnictides and pointed out possible frustration effects. Experimental properties of high temperature superconductors and spin entangled states were also discussed.

Finally, also more general topics have been addressed. P. Radaelli demonstrated on several compounds how competing interactions lead to fascinating properties from spin liquid states to multiferrocity. The latter property given by a mutual coupling of polar distortions and magnetic moments has also been highlighted by R.K. Kremer.

### **Poster session:**

Posters were presented by young scientists who used this opportunity to present their results and to receive comments from the experts. In most cases the posters covered details of analytic or numerical methods used for obtaining the results presented in the talks. Therefore, the poster session played a very important role in explaining novel methods and making them comprehensive and popular among the workshop participants.

### **Impact of the event**

As discussed in the preceding paragraphs, the workshop provided a unique opportunity for discussions and exchange of scientific information among the leading experts in the field of frustration and entanglement in systems with spin and orbital degrees of freedom. Although this workshop served mainly to develop new concepts and to launch new collaborations by the experts in the field, we made an effort to accept a number of young scientists (PhD students and postdocs) active in this field, who could rapidly learn and present their results as posters. Given the well-focussed topic of the workshop, it was possible to accommodate all of the applications for participation from the people working in this field (application to the workshop was open to everyone who could present a meaningful contribution to the program).

The excellent local organization of the workshop and all events was possible due to the efforts by M. Bogucka two young scientists from Cracow, K. Wohlfeld and M. Raczkowski. The importance of the meeting was also highlighted by a number of emails received after the meeting. In spite of rather short duration of the workshop, its importance for the future developments of new ideas in this field was remarkable and cannot be overestimated.

**Financial report for the workshop  
“Entanglement in Spin & Orbital Systems”  
Cracow, 18 - 22 June 2008**

The travel expenses of Prof. Yoshinori Tokura were partly covered by ESF (supplement to travel costs of 800 €). Otherwise, the organizers covered all local costs including accomodation, meals and transportation in Cracow.

**Actual Expenses:**

Travel:	800.00 €
Local transportation:	815.24 €
Accommodation:	8 000.00 €
Meals:	7 200.00 €
Local administrative costs:	2 666.78 €
Conference materials:	1 057.02 €
Renting the lecture hall:	479.80 €
<b>TOTAL EXPENDITURE:</b>	<b>21 018.84 €</b>
CO-SPONSORSHIP (CNRS):	1 700.00 €
CO-SPONSORSHIP (JU in Cracow)	1 818.84 €
<b><u>Expenses on account of ESF:</u></b>	<b><u>17 500.00 €</u></b>

## **Participants**

In total 53 people attended the workshop (52 scientists and workshop secretary), including 7 women and 46 men who presented 31 oral, 16 poster contributions and four contributions to the panel discussion summarizing the workshop.

### **Geographical distribution of the participants:**

<b>European Union</b>	<b>44</b>
<b>Switzerland</b>	<b>5</b>
<b>other European countries</b>	<b>2</b>
<b>from outside Europe</b>	<b>2</b>

Belarus	1
France	7
Germany	10
Great Britain	2
Italy	3
Japan	1
The Netherlands	4
Poland	12
Slovakia	1
Slovenia	2
Switzerland	5
Hungary	3
Ukraine	1
USA	1

### **Educational background of the participants:**

PhD students:	8
Postdocs:	6
Senior researchers:	38

### **List of participants:**

From the ESF-HFM steering committee C. Lacroix, P. Lemmens, F. Mila, A.M. Oles, and K. Penc did attend the meeting, pointing to the relevance of the topic.

Luuk Ament, The Netherlands  
Sergei Barilo, Belarus  
Federico Becca, Italy  
Monika Bogucka, Poland  
Sandor Bordacs, Hungary  
Jeroen van den Brink, The Netherlands  
Wojciech Brzezicki, Poland

Lukasz Cinzio, Poland  
Bogdan Dabrowski, USA  
Jacek Dziarmaga, Poland  
Ilya Eremin, Germany  
Holger Fehske, Germany  
Louis Felix Feiner, The Netherlands  
Raymond Fresard, France  
Giacomo Ghiringhelli, Italy  
Martine Hennion, France  
Peter Horsch, Germany  
George Jackeli, Germany  
Giniyat Khaliullin, Germany  
Daniel I. Khomskii, Germany  
Reinhard K. Kremer, Germany  
Claudine Lacroix, France  
Peter Lemmens, Germany  
Salvatore R. Manmana, Switzerland  
Sergio Di Matteo, France  
Frederic Mila, Switzerland  
Gregoire Misguich, France  
Maxim Mostovoy, The Netherlands  
Fernande Moussa, France  
Geran Jan Nilsen, Switzerland  
Canio Noce, Italy  
Andrzej M. Oles, Poland  
Yurii Pashkevich, Ukraine  
Karlo Penc, Hungary  
Didier Poilblanc, France  
Peter Prelovsek, Slovenia  
Marcin Raczkowski, Poland  
Paolo G. Radaelli, UK  
Marek Rams, Poland  
Judith Romhanyi, Hungary  
Krzysztof Rosciszewski, Poland  
Nic Shannon, UK  
Samir El Shawish, Slovenia  
Olga Sikora, Germany  
Jozef Spalek, Poland  
Andrzej Szytula, Poland  
Yoshinori Tokura, Japan  
Piotr Tomczak, Poland  
Tamas Toth, Switzerland  
Clemens Ulrich, Germany  
Krzysztof Wohlfeld, Poland  
Francois Vernay, Switzerland  
Anna Zorkovska, Slovakia



**Program of the HFM workshop**  
**“Entanglement in Spin & Orbital Systems”**  
**Cracow, 18 - 22 June 2008**

**18 June (Wednesday)**

Arrival in the evening

20:00 - Get together and dinner at the conference centre

**19 June (Thursday)**

Breakfast in the guesthouse

**8:55 Welcome and opening**

**9:00-11:00 Entanglement in spin systems**

- G. Misguich "Entanglement Entropy in Quantum Dimer Models" [»pdf](#)
- P. Tomczak "A New Estimator of Block Entanglement for Heisenberg Antiferromagnets" [»pdf](#)
- J. Dziarmaga "Multi-scale Entanglement Renormalization Ansatz in Two Dimensions: Quantum Ising model" [»ppt](#)
- R. Frésard "Origin of Magnetic Interactions in  $\text{Ca}_3\text{ABO}_6$ " [»pdf](#)

**11:00-11:30 Coffee break**

**11:30-13:00 Manganites**

- M. Hennen "Quantized Spin Waves in 2D Step Levels Probe the Metallic State of  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ " [»ppt](#)
- F. Moussa "Intra- and Interlayer Exchange Tuned by Magnetic Field in the Bilayer Manganite  $(\text{La}_{0.4}\text{Pr}_{0.6})_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$  Probed by Inelastic Neutron Scattering" [»ppt](#)
- G. Ghiringhelli "Looking for Low Energy Orbital Excitations in  $\text{LaMnO}_3$  Using Resonant Inelastic Soft X-ray Scattering"

**13:00-14:30 Lunch in the conference centre**

**14-30-16:00 Poster session / discussions**

**16:00-16:30 Coffee break**

**16:30-18:00 Multiferroics**

- J. van den Brink "Multiferroicity Due to Entangled Spin, Charge and Orbital Order" [»ppt](#)
- R. K. Kremer "Search for Multiferroicity in New Spin Spiral Chain Cu Systems"
- M. Mostovoy "Toroidal and Other Magnetic Multipole Orders in Frustrated Spin Systems"

**19:00-20:00 Dinner in the conference centre**

## **20 June (Friday)**

Breakfast in the guesthouse

**8:30 Coach to Collegium Novum in the old town**

**9:15-11:15 Spin-orbital systems**

**(open session with more attendants in Collegium Novum)**

- Y. Tokura "Spin-Orbital-Charge Coupled Dynamics in  $t_{2g}$ -Electron Systems" [»ppt](#)
- D.I. Khomskii "Spontaneous Currents and Polarization in Mott Insulators: Are Electrons Really Localized?" [»ppt](#)
- P. Radaelli "Frustration and Functionality in Complex Oxides" [»ppt](#)

**11:30-13:30 Visit to Collegium Maius - the museum of the Jagellonian University  
and short walk through the center of Cracow**

**13:45 Coach to the conference centre**

**14:00-15:30 Lunch in the conference centre**

**15:30-17:00 Entanglement in the cubic vanadates**

- L.F. Feiner "Spin-Orbital Entanglement and Violation of the Goodenough-Kanamori Rules in  $t_{2g}$  Orbital Systems" [»ppt](#)
- P. Horsch "Evolution of Spin-Orbital-Lattice Coupling in the  $RVO_3$  Perovskites" [»ppt](#)
- C. Ulrich "Evolution of the 'Orbital Peierls State' with Doping" [»ppt](#)

**17:00-17:30 Coffee break**

**17:30-19:00 Entanglement in the cobaltates**

- G. Khaliullin "The Origin of Strong Correlations in Layered Cobaltates" [»ppt](#)
- P. Lemmens "Anomalous Electronic Scattering Rates, Phonon Anomalies and the Phase Diagram of the Cobaltates  $Na_xCoO_2 \cdot yH_2O$ "
- Y. Pashkevich "Spin-orbital Entanglement in Layered Cobaltites  $RBaCo_2O_{5.5}$  with  $R=Y, Tb, Dy, \text{ and } Ho$ "

**19:00-20:00 Dinner in the conference centre**

## **21 June (Saturday)**

Breakfast in the guesthouse

### **9:00-11:00 Doped systems**

- F. Becca "Magnetism and Superconductivity in the  $t-t'-J$  Model" [».pdf](#)
- P. Prelovšek "Self-Localization of Composite Spin-Lattice Polarons" [».ppt](#)
- B. Dąbrowski "Oxygen Vacancy Order and Magnetic Frustration in  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3-d}$ "
- I. Eremin "Doping Dependent Evolution of Magnetism and Superconductivity in Iron Pnictides: Itinerant electrons and Possible Frustration Effects" [».ppt](#)

### **11:00-11:30 Coffee break**

### **11:30-13:00 Complex systems**

- F. Vernay "Theoretical Interpretation of RIXS Spectra: Another Route Towards Multiplets"
- C. Noce "Investigating Spin / Orbital / Lattice Interplay: the Case of Ca-Based Ruthenates" [».ppt](#)
- H. Fehske "Quantum Transport within a Background Medium: Fluctuations versus Correlations" [».pdf](#)

### **13:00-14:30 Lunch in the conference centre**

### **14:30-17:00 Dimer models**

- F. Mila "From Orbital Degeneracy to RVB Spin Liquids" [».pdf](#)
- D. Poilblanc "Statistics of Holons in The Quantum Dimer Model" [».pdf](#)
- N. Shannon "Extended 'U(1)' Liquid Phase in a Three Dimensional Quantum Dimer Model" [».pdf](#)
- S. Di Matteo "Orbital Order in Titanium and Vanadium Spinels" [».ppt](#)
- G. Jackeli "Classical Dimers in Orbitaly Degenerate Honeycomb Antiferromagnet" [».ppt](#)

### **17:00-17:30 Coffee break**

### **17:30-18:30 Panel discussion "Topics in frustrated systems"**

Speakers: Y. Tokura, F. Mila, D.I. Khomskii, P. Radaelli

### **19:30 Conference dinner in the conference centre**

## **22 June (Sunday)**

Breakfast in the guesthouse

Departure