

# Summary

**Event:** XIII Training Course in the Physics of Strongly Correlated Systems.

**Venue:** International Institute for Advanced Scientific Studies "E.R. Caianiello" (IIASS).

**Location:** Vietri sul Mare (Salerno, Italy).

**Period:** 6<sup>th</sup> to 17<sup>th</sup> October 2008.

## Organizing Institutions:

- Dipartimento di Fisica "E.R. Caianiello" – Università degli Studi di Salerno, Italy
- International Institute for Advanced Scientific Studies "E.R. Caianiello" (IIASS), Italy

## Organizing Committee:

- Prof. F. Mancini (Università degli Studi di Salerno and IIASS, Italy) (scientific coordinator)
- Prof. M. Marinaro (Università degli Studi di Salerno and IIASS, Italy)
- Dr. A. Avella (Università degli Studi di Salerno, Italy)

## International Advisory Board:

- Prof. A.S. Alexandrov (Loughborough University, Loughborough, UK)
- Prof. E. Bauer (Technische Universität, Wien, Austria)
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- Prof. W. Nolting (Humboldt-Universität zu Berlin, Berlin, Germany)
- Prof. A.M. Oles (Jagellonian University, Krakow, Poland)
- Prof. N.M. Plakida (Joint Institute for Nuclear Research, Dubna, Russia)
- Prof. M. Sigrist (ETH, Zurich, Switzerland)

## Lecturers:

- Prof. G. Aeppli (University College, London, United Kingdom).
- Prof. P. Littlewood (University of Cambridge, Cambridge, United Kingdom).
- Prof. M. Sigrist (ETH, Zurich, Switzerland).
- Prof. M. Troyer (ETH, Zurich, Switzerland).

## Sponsoring Institutions:

- Dipartimento di Fisica "E.R. Caianiello" & Scuola di Dottorato in Fisica – Università degli Studi di Salerno, Italy
- International Institute for Advanced Scientific Studies "E.R. Caianiello" (IIASS), Italy
- European Science Foundation (ESF)
- Regione Campania<sup>1</sup>, Italy
- Ministero dell'Università, Istruzione e Ricerca<sup>1</sup>, Italy

## Expenditures Balance:

• Lecturers <sup>2</sup> (travel, accomodation, honorary)	€ 8.955.00
• Participant fellowships <sup>3</sup> (fully or partially covering the accomodation expenses)	€ 16.585.00
• Logistic expenses (secretariat, stationery, Xerox, telephone, fax, postal expenses, coffee breaks)	€ 1.500.00
• Proceedings publication (estimate based on the last ten publications)	€ 3.200.00
Total	€ 30.240.00

## Funding Balance:

• Dipartimento di Fisica "E.R. Caianiello" & Scuola di Dottorato in Fisica	€ 13.680.00
• IIASS <sup>4</sup> (registration fees included: 30 × € 350.00)	€ 10.560.00
• Logistic expenses (secretariat, stationery, Xerox, telephone, fax, postal expenses, coffee breaks)	€ 1.500.00
• European Science Foundation (ESF)	€ 6,000.00
Total	€ 30.240.00

## Notes:

<sup>1</sup> Funds not yet and not surely awarded. If any fund will be awarded, it will partially compensate the costs beard by the Dipartimento di Fisica "E.R. Caianiello" and the Scuola di Dottorato in Fisica.

<sup>2</sup> Each of the four lecturers spent one week at the Course. The average expenditure per lecturer breaks down as follows: travel € 850.00, accommodation € 700.00, honorary € 700.00.

<sup>3</sup> The Course had 37 participants. 20 participants, among the youngest with the best CVs, received an average fellowship of € 830.00 each to cover their accommodation expenses. 7 participants had their registration fees waived on account of the reduced funding capabilities of their hosting institutions.

<sup>4</sup> IIASS also provided its main lecture hall well furnished with beamer, overhead projector, white- and blackboards and its computer room with more than 15 computers connected to the Internet.

# Description of the scientific content of and discussion at the event

**Professor Gabriel Aeppli**

*Department of Physics and Astronomy, University College London, United Kingdom*

## **Quantum Magnetism in Insulators.**

The course will emphasize new experimental tools including spallation neutron sources and free electron lasers.

### **Lectures:**

1. Single impurities in semiconductors and insulators-analogies with atomic physics, hyperfine interactions, and free electron laser
2. 1-dimensional magnets, including direct evidence for fermionic quasiparticles in antiferromagnetic  $S=1/2$  chains, and quantum phase coherence and edge states in  $S=1$  chains
3. 2-dimensional magnets, including entanglement at short distances
4. 3-dimensional magnets-quantum phase transition, decoherence due to coupling to nuclear spin bath
5. Undoped and doped Kondo insulators

### **References:**

- General Background: "What Happens to Ordered Moments When They are no Longer Ordered?", G. Aeppli, *Physica B*, 318, p. 5-11, (2002). "Seeing the Spins in Solids", G. Aeppli, S. Hayden, T. Perring, *Physics World*, p. 33-37, (December 1997)
1. "Silicon as a model ion trap: Time domain measurements of donor Rydberg states" N. Q. Vinh, P. T. Greenland, K. Litvinenko, B. Redlich, A. F. G. van der Meer, S. A. Lynch, M. Warner, A. M. Stoneham, G. Aeppli, D. J. Paul, C. R. Pidgeon, B. N. Murdin *PNAS* 105 10649- 10653 (2008)
  2. "Direct Observation of Field-Induced Incommensurate Fluctuations in a One-Dimensional  $S = 1/2$  Antiferromagnet", D. C. Dender, P. R. Hammar, D. H. Reich, C. Broholm, G. Aeppli, *Phys. Rev. Lett.* 79(9), p. 1750-1753, (1997). "Mesoscopic Phase Coherence in a Quantum Spin Fluid" Guangyong Xu, C. Broholm, Yeong-AhSoh, G. Aeppli, J. F. DiTusa, Ying Chen, M. Kenzelmann, C. D. Frost, T. Ito, K. Oka, H. Takagi *Science* 317, p. 1049-1052 (2007)
  3. "Quantum dynamics and entanglement of spins on a square lattice" N. B. Christensen, H. M. Rønnow, D. F. McMorrow, A. Harrison, T. G. Perring, M. Enderle, R. Coldea, L. P. Regnault, G. Aeppli *PNAS* 104, 15264-15269
  4. "Quantum Critical Behavior for a Model Magnet", D. Bitko, T. F. Rosenbaum, G. Aeppli, *Phys. Rev. Lett.* 77(5), p. 940-943, (1996). "Tunable Quantum Tunneling of Magnetic Domain Walls" J. Brooke, T. F. Rosenbaum, G. Aeppli, *Nature* 413, p. 610 - 613 (2001). "Quantum phase transition in a spin bath", H. M. Ronnow, R. Parthasarathy, J. Jensen, G. Aeppli, T. F. Rosenbaum, and D. F. McMorrow, *Science* 308, p. 392-395 (2005)
  5. "Kondo Insulators", G. Aeppli, Z. Fisk, *Comments Cond. Matt. Phys.* 16, p. 155, (1992). "Unconventional Charge Gap Formation in Cubic FeSi", Z. Schlesinger, Z. Fisk, Hai-Tao Zhang, B. Maple, J. F. DiTusa and G. Aeppli, *Phys. Rev. Lett.* 71, p. 1748, (1993). "Magnetoresistance from Quantum Interference Effects in Ferromagnets", N. Manyala, Y. Sidis, J. F. DiTusa, G. Aeppli, D. P. Young, Z. Fisk, *Nature* 404, p. 581-584, (2000). "Doping a semiconductor to create an unconventional metal" N. Manyala, J.F. DiTusa, G.Aeppli, A.P.Ramirez *Nature* 454 976-980 (2008)

**Tutorials:** Journal Club.

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**Professor Peter Littlewood**

*Department of Physics, University of Cambridge, United Kingdom*

## **Novel quantum condensates in excitonic matter.**

This course will interleave discussion of a novel physical problem of a new kind of Bose-Einstein condensate with teaching of the fundamental theoretical tools of quantum condensed matter field theory.

### **Lectures:**

1. Introduction to the physical systems. The electron-hole gas, excitonic insulator; exciton-photon interactions, polaritons and the Dicke Model; exciton and polariton BEC.
2. Theoretical tools: Second quantization. Coherent states. Coherent state path integral. Examples of coherent state mean field theories: Dilute Bose gas. BCS superconductivity.
3. Exciton and polariton condensates in mean field theory. Field theory of polariton condensate; BEC-BCS crossover.
4. Theoretical Tools: Open systems and Keldysh formulation..Pair-breaking and the semiconductor laser.
5. Phase-breaking and open system dynamics. Review of experiment. Open questions and new systems.

## References:

The methodological aspects are covered in standard quantum field theory texts: Professor Littlewood's approach will be closest to the book of Altland and Simons [1]. A recent theoretically focussed review of polariton systems is [2].

1. A. Altland, and B.D. Simons; Condensed Matter Field Theory; Cambridge University Press (2006).
2. J. Keeling, F.M. Marchetti, M.H. Szymanska, and P.B. Littlewood; Collective coherence in planar semiconductor microcavities; Semiconductor Science and Technology 22, R1 (2007).

## Tutorials: Journal Club

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### Professor Manfred Sigrist

*Institut für Theoretische Physik, ETH Zürich, Switzerland*

#### Introduction to Unconventional Superconductivity.

## Lectures:

1. Generalized BCS Theory.
2. Phenomenological Approach and Symmetry Aspects.
3. Josephson and Tunneling Effects
4. Case Studies I.
5. Case Studies II.

## References:

1. V.P. Mineev, and K.V. Samokhin; Introduction to Unconventional Superconductivity; Gordon & Breach Publisher (1998).
2. M. Sigrist, and K. Ueda; Phenomenological Theory of Unconventional Superconductivity; Rev. Mod. Phys. 63, 239 (1991).
3. M. Sigrist; Introduction to Unconventional Superconductivity; AIP Conference Proceedings 789, 165 (2005).

## Tutorials:

1. Generalized BCS Theory: Bogolyubov-transformation and self-consistent equations.
  2. Generalize Ginzburg-Landau Theory: Free energy and phases of a two-component order parameter.
  3. Generalize Ginzburg-Landau Theory: Boundary properties of time reversal symmetry breaking phase.
  4. High-Tc-superconductivity: Simple model of an RVB state.
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### Professor Matthias Troyer

*Institut für Theoretische Physik, ETH Zürich, Switzerland*

#### Quantum Monte Carlo methods.

## Lectures:

1. Introduction to Monte Carlo simulations.
2. Classical and quantum cluster algorithms.
3. The worm algorithm.
4. Optimized ensembles for classical and quantum Monte Carlo simulations.
5. Continuous time QMC solvers for quantum impurity problems and DMFT.

## References:

1. D.P. Landau, and K. Binder; A Guide to Monte Carlo Simulations in Statistical Physics; Cambridge University Press (2005).
2. R.H. Swendsen, and J.-S. Wang; Phys. Rev. Lett. 58, 86 (1987). H.G. Evertz; Adv. Phys. 52, 1 (2003).
3. N.V. Prokof'ev et al.; Sov. Phys. - JETP 87, 310 (1998). A.W. Sandvik; Phys. Rev. B 59, 14157 (1999). O.F. Syljuasen, and A.W. Sandvik; Phys. Rev. E 66, 046701 (2002). F. Alet et al.; Phys. Rev. E 71, 036706 (2005).
4. F. Wang, and D.P. Landau; Phys. Rev. Lett. 86, 2050 (2001); Phys. Rev. E 64, 056101 (2001). M. Troyer et al.; Phys. Rev. Lett. 90, 120201 (2003). S. Trebst et al.; Phys. Rev. E 70, 046701 (2004). S. Wessel et al.; J. Stat. Mech. P12005 (2007).
5. A.N. Rubtsov; Phys. Rev. B 72 035122 (2005). P. Werner et al.; Phys. Rev. Lett. 97, 076405 (2006). P. Werner et al.; Phys. Rev. B 74, 155107 (2006). E. Gull et al.; Europhysics Letters 82, 57003 (2008).

## Tutorials: ALPS Monte Carlo codes

**Mr. Giacomo Coslovich**

*Università degli Studi di Trieste, Italy*

**Time-resolved ultrafast optical studies of High-Tc Superconductors**

**Abstract:** Pump-probe experiments give insight into the relaxation dynamics of electrons and phonons in solids. The physics behind this process is governed by electron-electron and electron-phonon interactions. Ultrafast optical spectroscopy is a suitable tool to study strongly correlated systems and in particular High-temperature superconductors, where the interplay of these interactions leads to a rich phase diagram. The subject of this seminar is the possibility to photo-induce a purely electronic phase transition from the superconducting state of a Bi-based underdoped cuprate by means of an ultrashort laser pulse. We report on the experimental evidence, by means of time-resolved reflectivity measurements, of an abrupt transition of the optical response at a critical fluence of  $I_{\text{pump}} \cong 70 \mu\text{J}/\text{cm}^2$  [1]. This value can be compared with the predictions of the available BCS models of non-equilibrium superconductivity [2,3,4]. A simple phenomenological model that accounts for the main observed features is proposed. The optical control of the electronic phase of a superconducting system opens the way towards the manipulation of matter based on the change of the thermodynamic potential along non-equilibrium pathways. This technique has possible application in other complex and strongly correlated materials. Further on, the possibility to follow the phase transition dynamics on the femtosecond timescale could help in the understanding of the key mechanisms at the base of the elusive superconducting and pseudogap phases in cuprates. [1] C. Giannetti, G. Coslovich, F. Cilento, G. Ferrini, H. Eisaki, N. Kaneko, M. Greven, F. Parmigiani, arXiv:0804.4822v1 (2008) [2] C. S. Owen and D. J. Scalapino, Phys. Rev. Lett. 28, 155 (1972) [3] W. H. Parker, Phys. Rev. B 12, 3667 (1975) [4] E. Nicol and J. Carbotte, Phys. Rev. B 67, 214506 (2003).

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**Mr. Tomislav Ivek**

*Institute of Physics, Zagreb, Croatia*

**Collective Charge Excitations below the Metal to-Insulator Transition in BaVS<sub>3</sub>**

**Abstract:** Collective Charge Excitations below the Metal-to-Insulator Transition in BaVS<sub>3</sub> T. Ivek\*, T.Vuletić\*, S. Tomić\*, A. Akrap<sup>^</sup>, H. Berger<sup>^</sup>, L. Forró<sup>^</sup> \*Institut za fiziku, Zagreb, Croatia <sup>^</sup>Ecole Polytechnique Fédérale, Lausanne, Switzerland The perovskite-type sulfide the barium vanadium sulfide (BaVS<sub>3</sub>) consists of parallel VS<sub>3</sub> spin chains separated by Ba atoms, which yields a quasi-one-dimensional structure. There are two electrons per unit cell which are shared between a broad A1g band derived from vanadium d<sub>22</sub> orbitals overlapping along the chain direction, and a quasi-degenerate narrow Eg<sub>1</sub> band originating from e(t<sub>2g</sub>) orbitals with isotropic interactions via V-S-S-V bonds [1]. The spin degrees of freedom of the localized electrons together with coupling of itinerant and localized electrons give rise to a novel and complex physics, resulting in a MI transition [2,3] at about 70 K and a magnetic transition at about 30 K. In spite of a great deal of experimental efforts, no definite understanding has been reached yet on the detailed nature of the MI phase transition and the ground state in BaVS<sub>3</sub>. We have characterized charge response in BaVS<sub>3</sub> single crystals by dc resistivity and low frequency dielectric spectroscopy [4]. A broad relaxation mode in MHz range with a huge dielectric constant  $\sim 10^6$  emerges at the metal-to-insulator phase transition TMI  $\sim 67$  K, weakens with lowering temperature and eventually levels off below the magnetic transition Tchi  $\sim 30$  K. The mean relaxation time is thermally activated in a manner similar to the dc resistivity. These features are interpreted as signatures of short-wavelength charge excitations characteristic for the orbital ordering which sets in at TMI and develops a long-range order below Tchi. References: [1] F. Lechermann et al., Phys. Rev. B 76, 085101 (2007). [2] S. Fagot et al., Phys. Rev. Lett. 90, 196401 (2003). [3] S. Fagot et al., Phys. Rev. B 73, 033102 (2006). [4] T. Ivek et al., accepted for publication in Phys. Rev. B, arXiv:0706.2079v4 (2008).

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**Dr. Kyungwan Kim**

*Department of Physics, University of Fribourg, Switzerland*

**Optical response of insulating CuO<sub>4</sub> plaquette network**

**Abstract:** The high temperature superconductivity of cuprates appears with charge doping in insulating parent materials. Those insulating cuprates become insulator thanks to the strong Coulomb repulsion at Cu d orbitals. They have charge gap between filled oxygen 2p and empty Cu 3d states categorized as charge transfer insulators. Although only Cu 3d and O 2p states are involved in low energy optical transitions, optical excitation spectra of insulating cuprates show rich structures depending on the form of CuO<sub>4</sub> networks. One dimensional chain systems with corner sharing plaquettes and edge sharing plaquettes provide basic characters of these transitions. Comparison of available spectra with one dimensional chain compound Sr<sub>2</sub>CuO<sub>3</sub> shows that excitonic effect is strong in insulating cuprates with CuO<sub>2</sub> planes.

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**Mr. Guido Klingschat**

*Institute for Theoretical Physics and Astrophysics, University of Würzburg, Germany*

**SU(3)-Hubbard model with (strong) attractive coupling**

**Abstract:** Recently, a quantum phase transition from a color superfluid to a colorless phase with conglomerates of 3 fermions on a single site ('trions') has been proposed to occur in the attractive SU(3)-Hubbard model [Rapp et al., Phys. Rev. Lett. 98, 160405 (2007)]. Here we analyze the properties of the trionic phase using exact diagonalization. We determine the spectral function of single particle and trionic excitations, and compute spatial correlations. This way we can characterize the effective quasiparticles of the strong coupling phase.

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**Dr. Nicola Magnani**

*European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, Germany*

**Hidden Order and Low-Energy Excitations in Neptunium Dioxide**

**Abstract:** We investigate the nature of the hidden order parameter of NpO<sub>2</sub>, which had been identified with a staggered arrangement of  $\Gamma_5$  magnetic multipoles. By analyzing the existing experimental data, we show that the most likely driving order parameter is not provided by octupoles, as usually assumed, but rather by the rank-5 triakontadipoles. Calculations of the coupled dynamics of spins,  $\Gamma_5$  quadrupoles, and  $\Gamma_5$  triakontadipoles in the ordered phase enable us to analyze the resulting structure of low-energy excitations. We show that the powder inelastic neutron scattering cross section should contain, in addition to the already-observed peak at 6.5 meV, a second weaker peak at about 14 meV. As a test, we have performed polarized inelastic neutron scattering experiments in the ordered phase of neptunium dioxide. The observation of magnetic scattering between 11 and 18 meV can indeed be attributed to a transition between two states with the same expectation value of the electric quadrupole, but opposite values of the magnetic triakontadipole. In contrast to resonant X-ray scattering, which detects the secondary order parameter (electric quadrupoles) associated with the 25 K phase transition, the results reported here are a direct manifestation of the primary (magnetic) order parameter.

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**Dr. Victor Yushankhai**

*Laboratory of Theoretical Physics, JINR, Dubna, Russia*

**Self-consistent renormalization theory of spin fluctuations in paramagnetic spinel LiV<sub>2</sub>O<sub>4</sub>**

**Abstract:** The appearance of a rather peculiar paramagnetic ground state in LiV<sub>2</sub>O<sub>4</sub> is likely related directly to the geometrical frustration of the magnetic V ion lattice. The observed in the inelastic neutron scattering and NMR measurements, the evolution of critical spin fluctuations with temperature and pressure is described in terms of properly parametrized self-consistent renormalization (SCR) theory.

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**Mr. Alexander Mai**

*Institute of Theoretical Physics, Dresden Technical University, Germany*

**Valence Transition and Superconductivity in the Two-Dimensional Extended Periodic Anderson Model**

**Abstract:** The periodic Anderson model (PAM) describes the interplay of itinerant conduction and strongly correlated localized f electrons on a microscopic scale and can be used to investigate heavy fermion behavior and its breakdown. Using an extension of the Projector-based Renormalization Method (PRM) we study the valence transition as a function of the local f-energy  $\epsilon_f$  and the orbital degeneracy  $\nu_f$ . It is claimed in the literature that in the presence of an additional local Coulomb repulsion  $U_{fc}$  between f- and conduction electrons the system is susceptible to superconductivity in the valence transition regime. Therefore we extend the model in order to calculate superconducting order parameters originating from either an enhanced electron phonon mechanism or an additional  $U_{fc}$  contribution.

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**Mr. Matthias Nyfeler**

*Institut for Theoretical Physics, Bern, Switzerland*

#### **From an Antiferromagnet to a Valence Bond Solid: Evidence for a First Order Phase Transition**

**Abstract:** Using a loop-cluster algorithm we investigate the spin 1/2 Heisenberg antiferromagnet on a square lattice with exchange coupling J and an additional four-spin interaction of strength Q. We confirm the existence of a phase transition separating antiferromagnetism at  $J/Q > J_c/Q$  from a valence bond solid (VBS) state at  $J/Q < J_c/Q$ . Although our Monte Carlo data are consistent with those of previous studies, we do not confirm the existence of a deconfined quantum critical point. Instead, using a flowgram method on lattices as large as 802, we find evidence for a weak first order phase transition. We also present a detailed study of the antiferromagnetic phase. For  $J/Q > J_c/Q$  the staggered magnetization, the spin stiffness, and the spinwave velocity of the antiferromagnet are determined by fitting Monte Carlo data to analytic results from the systematic low-energy effective field theory for magnons. Finally, we also investigate the physics of the VBS state at  $J/Q < J_c/Q$ , and we show that long but finite antiferromagnetic correlations are still present.

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**Dr. Marina Poltavskaya**

*Dept. of Mathematical Modeling of Physical Processes, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine*

#### **Two-Time Green Functions in the Theory of Low-Dimensional Spin-1/2 Magnets**

**Abstract:** Analytical approaches based on the two-time Green function formalism proved to be very effective in calculating the thermodynamic properties of one- and two-dimensional quantum Heisenberg magnets. These methods give quantitative results in the wide temperature and magnetic field ranges and are appropriate for both ferromagnetic and antiferromagnetic exchanges. They are based on one or another decoupling scheme for higher Green functions, which result in a closed set of self-consistent equations for thermodynamic averages. Random phase approximation is the simplest variant of such scheme with decoupling at the first step. It usually gives satisfactory results for magnetization and spin susceptibility at high magnetic fields. More complicated schemes are based on the decoupling of higher Green functions at the second step with introducing vertex parameters to be found. These schemes give quantitative results for both magnetic (magnetization, spin susceptibility) and thermodynamic (correlation functions, energy, heat capacity, correlation length) functions of low-dimensional quantum magnets in the external magnetic field and without it. The basic properties of two-time Green functions will be reviewed. The equations for the Green functions of low-dimensional spin-1/2 ferromagnet in the external magnetic field will be derived within the random phase approximation. For this system the scheme with the decoupling at the second step will be outlined. The characteristic features of the Green function theory in the case of antiferromagnetic exchange will be discussed

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**Mr. Yao Yao**

*Department of Physics, Fudan University, Shanghai, China*

#### **Controllable spin-current blockade in a Hubbard chain**

**Abstract:** We investigate the spin/charge transport in a one-dimensional strongly correlated system by using the adaptive time-dependent density-matrix renormalization group method. The model we consider is a non-half-filled Hubbard chain with a bond of controllable spin-dependent electron hoppings, which is found to cause a blockade of spin current with little influence on charge current. We have considered (1) the spread of a wave packet of both spin and charge in the Hubbard chain and (2) the spin and charge currents induced by a spin-dependent voltage bias that is applied to the ideal leads attached at the ends of this Hubbard chain. It is found that the spin-charge separation plays a crucial role in the spin-current blockade, and one may utilize this phenomenon to observe the spin-charge separation directly.

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**Mr. Matous Ringel**

*Department of Condensed Matter Theory, Institute of Physics of the Academy of Science of CR, Prague, Czech Republic*

#### **Magnetic properties of impurities with strongly correlated electrons**

**Abstract:** We study the single impurity Anderson model in an external magnetic field. There are no exact results for the spectral function in this situation. Using a resummation of the diagrammatic expansion we demonstrate that the strong coupling regime in a weak magnetic field is Kondo-like with a quasiparticle resonant peak split into two. We find two exponentially small Kondo scales (temperatures), one for transverse and one for longitudinal spin fluctuations. We show that the salient features of the spectral function in the Kondo regime can be seen already within an extended random phase approximation. To reveal the dependence of the Kondo scales on the bare electron interaction, however, one has to use a two-particle self-consistency with renormalized vertices. We use the parquet approach to derive the dependence of the Kondo scales on magnetic field.

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**Mr. Marc Warner**

*London Centre for Nanotechnology, University College London, United Kingdom*

#### **Towards Organic Quantum Computation?**

**Abstract:** Quantum computers show tremendous promise to revolutionise any field in which the modelling of a quantum mechanical system is currently performed using classical computation. This includes vast swathes of physics, chemistry, biology and medicine. We present the first steps towards the creation a phthalocyanine organic quantum computer. Thin films of spin diluted copper phthalocyanine (CuPc) were prepared on a kapton substrate by organic molecular beam deposition. The spin of the electron on the copper atom serves as the quantum bit (qubit). The CuPc can be templated, where the molecular plane of the CuPc molecules are forced to lie parallel to the substrate, by coating the substrate with a layer of PTCD. Alternatively the substrate can be left uncoated, under which circumstances the plane of the molecule lies perpendicular to the substrate. The work presented consists of the characterization of these samples using continuous wave (CW) EPR, measurements of the coherence times and the demonstration of Rabi oscillations with pulsed EPR. The results from the CW rotation patterns of the templated spin diluted CuPc samples showed clearly that the CuPc and metal free phthalocyanine form a good approximation of a single crystal. The varying spin dilution shows the effects of couplings between phthalocyanines broadening the linewidths of the spectra. Finally the dephasing time ( $T_2$ ) measurements of order  $1\mu s$  show that quantum information processing is a possibility in these systems.

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**Mr. Krzysztof Wohlfeld**

*Condensed Matter Theory, Jagellonian University, Cracow, Poland*

#### **Novel Spin-Orbital Polarons in Cubic Vanadates**

**Abstract:** When a single hole is introduced into the insulating plane of undoped cubic vanadates (such as e.g.  $LaV_0.3S_3$ ) it cannot move freely as it can disturb the alternating orbital (AO) and antiferromagnetic (AF) order present in the system. Instead, its motion is strongly renormalized due to the polaron-like coupling between the hole and the collective excitations of the AO state (orbitons) and the AF state (magnons). Here, we investigate this phenomenon using self-consistent Born approximation and show how these novel spin-orbital polarons differ from the well-known spin polarons in the high-Tc cuprates or from the orbital polarons in the manganites or fluorides.

## Assessment of the results and impact of the event on the future direction of the field

The principal aim of the School was to introduce the young researchers to a number of aspects of the theory of strongly correlated systems, presenting the theoretical framework as well as some experimental and numerical results. The importance of this field has been growing during the latest years, mainly after the discovery of the high- $T_c$  superconductors. This is a consequence of the very interesting and unusual properties exhibited by these systems (e.g., cuprates, manganites, vanadates, ruthenates, etc.) that could potentially lead to relevant technological applications. Furthermore, this field is of central importance to the study of puzzling and current problems such as the variety of metal-insulator transitions, the anomalous behaviors of heavy-fermion and mixed valence compounds, the oddities of quantum magnetism, the coexistence of several ordered phases such as the ferro- and the antiferro- magnetic phases and the superconducting one, the competition between itinerancy and localization, the effect of disorder, the hierarchy of the interactions, the quantitative description of real materials. On the experimental side, many results are being consolidated; this is due to the improvement in the quality of the samples, which has eliminated many of the uncertainties in the interpretation of data. On the contrary, the theoretical frame is still far from being satisfactory.

The course is not organized as usual workshops or schools where many formal lectures are delivered in a quite short period of time and no real contact develops between the many lecturers and the audience. Instead, as the main aim of this course is on training, TC on SCS are organized on two weeks with only two senior researchers per week. Our main idea is to put together few seniors and not many young researchers in a closed environment for a quite long period of time within an informal atmosphere. In the morning, each senior researcher will deliver a lecture, whereas the afternoon sessions are devoted to training and all efforts should be put on introducing the young researchers to specific problems, on guiding them in their solution, on helping them to become more familiar with different approaches and on starting new collaborations. The participants will also be encouraged to present their own activity. Our past experience with the previous courses suggests that the lecturers themselves should shape, under our supervision, the afternoon sessions according to the specificities of the subject of their lectures (coding in the computer room, problem solving, round table, brainstorming, journal club, ...).

The School was held over two weeks, with morning and afternoon sessions. The main courses were scheduled from Monday to Friday, two per week. Two plenary lectures were given during the morning. The lectures started at 9:00 a.m. and lasted two hours each, with a coffee break of 30 minutes, thus each mini-course was allocated 10 hours. The afternoon training sessions started at 3:00 p.m. and lasted around three hours. The afternoon activities aimed principally to increase discussions among the young researchers and between the young researchers and the lecturers. During the first afternoon each participant introduced himself and his scientific activity to the audience and some of them were given the possibility to deliver a 25 minutes seminar in the following afternoon sessions. The senior scientists run the other afternoon activities through Training Sessions, including tutorials and computer-based practice where appropriate. The young researchers could therefore profit from the training of the senior scientists not only from the content of the traditional courses, but also from the afternoon discussions. It is worth recalling that the concentration of the activities in a small village (Vietri sul Mare, Salerno) where both the Institute and the Hotel are located (200 meters away from each other), strongly enhanced the opportunities of informal contacts and discussions.

The purposes of this Training Courses included the promotion of scientific excellence by contributing to the advancement of science through exchange, and to create the conditions for experienced researchers to impart their knowledge and experience to young researchers at doctoral and post-doctoral level. Indeed, young scientists from various European countries were present, and 4 out of the 4 lecturers were European. As a matter of fact, this Training Course provided an opportunity for both the senior and the younger researchers to create a network of scientific relations and possible collaborations. Joint work to write down the lecture notes has been achieved in some cases, leading to further scientific cooperation. To advertise the Training Course and to encourage the participation of the researchers an Announcement and the Poster was sent to more than 300 Universities, Institutes and Laboratories, all over Europe. The Announcement was also personally sent to more than 2000 Professors and researchers in many European Universities and to Coordinators of Italian Ph.D. programmes in Physics. Moreover, the Announcement has been electronically published on the electronic Conference information services of the Institute of Physics, of AIP, and many others. From the standpoint of the world scientific community, the outcome of this Training Course is going to be spread by means of the publication of the

lectures and of the afternoon seminars by the American Institute of Physics (AIP) in a book edited by the organizers (in preparation).

In the past years we organized the following events (<http://scs.sa.infn.it/TC>):

**I TC: 18th to 30th November 1996.**

Lecturers: K. Hallberg, N.M. Plakida, J. Spalek

**II TC: 13th to 25th October 1997.**

Lecturers: F. Guinea, K. Maki, A. Moreo

**III TC: 14th to 26th September 1998.**

Lecturers: G. Kotliar, M. Randeria, J. Ranninger, S. Sorella

**IV TC: 11th to 22th October 1999.**

Lecturers: A.F. Barabanov, W. Nolting, A.M. Oles, A. Ruckenstein

**V TC: 30th Oct. to 10th Nov. 2000.**

Lecturers: S. Alexandrov, L. Maritato, N.M. Plakida, A.M. Tsvelik

**VI TC: 8th to 19th October 2001.**

Lecturers: P. Coleman, C. Di Castro, P. Prelovsek, C.M. Varma.

Web page: <http://scs.sa.infn.it/TCVI>

**VII TC: 14th to 25th October 2002.**

Lecturers: N. Andrei, F.F. Assaad, J.T. Devreese, Y. Izyumov, J. Tempere.

Web page: <http://scs.sa.infn.it/TCVII>

**VIII TC: 6th to 17th October 2003.**

Lecturers: A. Georges, M. Imada, M.L. Kubic, A. Muramatsu.

Web page: <http://scs.sa.infn.it/TCVIII>

**IX TC: 4th to 15th October 2004.**

Lecturers: K. Maki, H. Matsumoto, R. Noack, M. Sigrist.

Web page: <http://scs.sa.infn.it/TCIX>

**X TC: 3rd to 14th October 2005.**

Lecturers: B. Coqblin, T. Giamarchi, W. Metzner, W. von der Linden.

Web page: <http://scs.sa.infn.it/TCX>

**XI TC: 2nd to 13th October 2006.**

Lecturers: M. Fabrizio, D. Poilblanc, R. T. Scalettar, D. van der Marel.

Web page: <http://scs.sa.infn.it/TCXI>

**XII TC: 1st to 12th October 2007.**

Lecturers: S. Haas, M. Jarrell, H. v. Löhneysen, V. Zlatic.

Web page: <http://scs.sa.infn.it/TCXII>

# Final programme of the meeting

I Week

Prof. M. Sigrist: *Introduction to Unconventional Superconductivity.*

Prof. M. Troyer: *Quantum Monte Carlo methods.*

## 6 October

08:00 - 08:50	Registration.
08:50 - 09:00	Opening of the Training Course.
09:00 - 11:00	Prof. M. Troyer: 1 <sup>st</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. M. Sigrist: 1 <sup>st</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:20	Participant presentations.
16:20 - 16:30	Break.
16:30 - 18:30	Prof. M. Sigrist - Prof. M. Troyer: Training Session.

## 7 October

09:00 - 11:00	Prof. M. Troyer: 2 <sup>nd</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. M. Sigrist: 2 <sup>nd</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. G. Coslovich: <i>Time-resolved ultrafast optical studies of High-T<sub>c</sub> Superconductors.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. M. Sigrist - Prof. M. Troyer: Training Session.

## 8 October

09:00 - 11:00	Prof. M. Troyer: 3 <sup>rd</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. M. Sigrist: 3 <sup>rd</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. T. Ivek: <i>Collective Charge Excitations below the Metal-to-Insulator Transition in BaVS<sub>3</sub>.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. M. Sigrist - Prof. M. Troyer: Training Session.

## 9 October

09:00 - 11:00	Prof. M. Troyer: 4 <sup>th</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. M. Sigrist: 4 <sup>th</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Dr. K. Kim: <i>Optical response of insulating CuO<sub>4</sub> plaquett network.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. M. Sigrist - Prof. M. Troyer: Training Session.

## 10 October

09:00 - 11:00	Prof. M. Troyer: 5 <sup>th</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. M. Sigrist: 5 <sup>th</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. G. Klingschat: <i>SU(3)-Hubbard model with (strong) attractive coupling.</i>
16:00 - 16:30	Dr. N. Magnani: <i>Hidden Order and Low-Energy Excitations in Neptunium Dioxide.</i>
16:30 - 16:40	Break.
16:40 - 18:30	Prof. M. Sigrist - Prof. M. Troyer: Training Session.

Prof. G. Aeppli: *Collective quantum effects in simple insulators.*

Prof. P. Littlewood: *Novel quantum condensates in excitonic matter.*

**13 October**

09:00 - 11:00	Prof. G. Aeppli: 1 <sup>st</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. P. Littlewood: 1 <sup>st</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:20	Dr. V. Yushankhai: <i>Self-consistent renormalization theory of spin fluctuations in paramagnetic spinel <math>\text{LiV}_2\text{O}_4</math>.</i>
16:20 - 16:30	Break.
16:30 - 18:30	Prof. G. Aeppli - Prof. P. Littlewood: Training Session.

**14 October**

09:00 - 11:00	Prof. G. Aeppli: 2 <sup>nd</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. P. Littlewood: 2 <sup>nd</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. A. Mai: <i>Valence Transition and Superconductivity in the Two-Dimensional Extended Periodic Anderson Model.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. G. Aeppli - Prof. P. Littlewood: Training Session.

**15 October**

09:00 - 11:00	Prof. G. Aeppli: 3 <sup>rd</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. P. Littlewood: 3 <sup>rd</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. M. Nyfeler: <i>From an Antiferromagnet to a Valence Bond Solid: Evidence for a First Order Phase Transition.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. G. Aeppli - Prof. P. Littlewood: Training Session.

**16 October**

09:00 - 11:00	Prof. G. Aeppli: 4 <sup>th</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. P. Littlewood: 4 <sup>th</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Dr. M. Poltavskaya: <i>Two-Time Green Functions in the Theory of Low-Dimensional Spin-1/2 Magnets.</i>
16:00 - 16:15	Break.
16:15 - 18:30	Prof. G. Aeppli - Prof. P. Littlewood: Training Session.

**17 October**

09:00 - 11:00	Prof. G. Aeppli: 5 <sup>th</sup> Lesson.
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. P. Littlewood: 5 <sup>th</sup> Lesson.
13:30 - 15:30	Lunch.
15:30 - 16:00	Mr. M. Ringel: <i>Magnetic properties of impurities with strongly correlated electrons.</i>
16:00 - 16:30	Mr. Y. Yao: <i>Controllable spin-current blockade in a Hubbard chain</i>
16:30 - 16:40	Break.
16:40 - 17:20	Mr. M. Warner: <i>Towards Organic Quantum Computation?</i>
17:20 - 17:50	Mr. K. Wohlfeld: <i>Novel Spin-Orbital Polarons in Cubic Vanadates.</i>
17:50 - 18:00	Break.
18:00 - 18:30	Prof. G. Aeppli - Prof. P. Littlewood: Training Session.
18:30 - 18:45	Closing of the Training Course.