

Summary

Event: XIV 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: 5th to 16th October 2009.

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)
- 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)
- Prof. B. Coqblin (Université Paris-Sud, Orsay, France)
- Prof. C. Di Castro (Università degli Studi di Roma "La Sapienza", Roma, Italy)
- Prof. F. Guinea (Instituto de Ciencia de Materiales, Madrid, Spain)
- 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. V.I. Anisimov (Russian Academy of Sciences, Yekaterinburg, Russia).
- Prof. A.W. Sandvik (Boston University, Boston MA, USA).
- Prof. G. Sawatzky (University of British Columbia, Vancouver B.C., Canada).
- Prof. D. Vollhardt (University of Augsburg, Augsburg, Germany).

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): INTELBIOMAT Programme
- European Physical Society (EPS)
- Regione Campania¹, Italy
- Ministero dell'Università, Istruzione e Ricerca¹, Italy

Expenditures Balance:

• Lecturers ² (travel, accomodation, honorary)	€ 11,130.00
• Participant fellowships ³ (fully or partially covering the accomodation expenses)	€ 17,095.00
• 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	€ 32,925.00

Funding Balance:

• Dipartimento di Fisica "E.R. Caianiello" & Scuola di Dottorato in Fisica	€ 16,425.00
• IIASS ⁴ (registration fees included: 29 × € 350.00)	€ 10,150.00
• European Science Foundation (ESF): INTELBIOMAT Programme	€ 6,000.00
• European Physical Society (EPS)	€ 350.00
Total	€ 32,925.00

Notes:

¹ 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.

² Each of the four lecturers spent one week at the Course. The average expenditure per lecturer breaks down as follows: travel € 925.00, accomodation € 855.00, honorary € 1,000.00.

³ The Course had 38 participants. 21 participants, among the youngest with the best CVs, received an average fellowship of € 815.00 each to cover their accomodation expenses. 9 participants had their registration fees waived on account of the reduced funding capabilities of their hosting institutions.

⁴ IIASS also provided its main lecture hall well furnished with beamer, overhead projector, white- and black- boards 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 Vladimir I. Anisimov

Institute of Metal Physics Russian Academy of Sciences - Ural Division Yekaterinburg Russia

Electronic structure calculations for systems with strong Coulomb correlations

Lectures:

- 1. Correlation effect and electronic structure calculations**
 - a) Model Hamiltonians and *ab-initio* approaches
 - b) Density Functional Theory and its applications
- 2. Combining model approaches and Density Functional Theory**
 - a) Wannier functions and model Hamiltonian construction
 - b) Static mean-field approach: LDA+U method
- 3. LDA+U method applications to real materials**
 - a) Mott-insulators
 - b) Orbital, charge and spin ordering
- 4. LDA+DMFT method**
 - a) LDA+DMFT calculation scheme
 - b) Impurity solvers
- 5. LDA+DMFT method applications to real materials**
 - a) Strongly correlated metals
 - b) Metal-insulator transitions

References:

- K. Held , I. A. Nekrasov , G. Keller , V. Eyert , N. Blümer , A. K. McMahan , R. T. Scalettar , Th. Pruschke , V. I. Anisimov , D. Vollhardt, Realistic investigations of correlated electron systems with LDA + DMFT, *physica status solidi (b)*, 243, 2599 (2006).
- Electronic Structure Calculations using Dynamical Mean Field Theory, K. Held, *Adv. Phys.* 56, 829 (2007), arXiv:cond-mat/0511293.
- V. I. Anisimov, D. E. Kondakov, A. V. Kozhevnikov, I. A. Nekrasov, Z. V. Pchelkina, J. W. Allen, S.-K. Mo, H.-D. Kim, P. Metcalf, S. Suga, A. Sekiyama, G. Keller, I. Leonov, X. Ren, and D. Vollhardt, Full orbital calculation scheme for materials with strongly correlated electrons, *Phys. Rev.* 71, 125119 (2005).
- Edited by Vladimir Anisimov, "Strong Coulomb Correlations in Electronic Structure Calculations", Gordon and Breach Science Publishers, 2000.
- V.I.Anisimov, F.Aryasetiawan, A.I.Lichtenstein, First-principles calculations of the electronic structure and spectra of strongly correlated systems: the LDA+U method, *J.Phys.: Condens. Matter* 9, 767 (1997).

Theory of correlated fermionic condensed matter

Lectures:

1. *Correlated electrons made simple.*
 - a) *What are electronic correlations and where do they show up?*
 - b) *Introduction to dynamical mean-field theory (DMFT) [1,2].*
2. *Electronic correlations - from models to materials.*
 - a) *DMFT and the Mott-Hubbard metal-insulator transition [1,2].*
 - b) *Merging DMFT with density functional theory (LDA+DMFT) [1,3].*
3. *Correlation-induced phenomena in electronic systems.*
 - a) *Correlation effects in transition metal oxides [3].*
 - b) *Kinks in the electronic dispersion [4].*
4. *Correlated electrons in the presence of disorder.*
 - a) *Non-interacting electrons with disorder: Anderson localization [5].*
 - b) *Mott-Hubbard transition versus Anderson localization [6].*
5. *Helium-3, Prototype of a correlated Fermi system [7].*
 - a) *Superfluid He-3: From very low temperatures to the big bang [8].*
 - b) *Common concepts in correlated Fermi systems.*

Public lecture (Friday afternoon):

"Magnetism: A Guided Tour from Ancient Greece to Modern Salerno"

References:

Books on many-body physics in general (occupation number formalism, Hubbard model, Green function, self-energy, finite temperature formalism, Fermi liquid theory) see, for example:
(i) Chapters 1,2,3,5,6 of J. W. Negele and H. Orland, "Quantum Many-Particle Systems" (Addison-Wesley, 1988), or
(ii) Chapters 6,7,8,9,10 of P. Coleman, "Many_Body Physics",
<http://www.physics.rutgers.edu/~coleman/mbody/pdf/bk.pdf>

[1] *Introduction to electronic correlations, dynamical mean-field theory (DMFT) and LDA+DMFT: "Strongly Correlated Materials: Insights from Dynamical Mean-Field Theory", G. Kotliar and D. Vollhardt, Physics Today 57, 53 (2004), see <http://www.physik.uni-augsburg.de/theo3/Publications/PT-Kotliar0304.pdf>*

[2] *Mean-field theories, the limit of high-dimensional lattices in statistical physics, and the construction of DMFT:*

(i) Chapters 1 and 4 of "Investigations of correlated electron systems using the limit of high dimensions", by D. Vollhardt, see http://www.physik.uni-augsburg.de/theo3/Research/research_jerusalem.vollha.de.shtml

(ii) *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions", A. Georges et al.; Rev. Mod. Phys., 68, 13 (1996).*

[3] *LDA+DMFT:*

"Realistic Investigations of correlated electron materials with LDA+DMFT", K. Held et al., Psi-k Newsletter 56, 65 (2003), see http://www.psi-k.org/newsletters/News_56/Highlight_56.pdf

[4] Kinks:

"Kinks in the dispersion of strongly correlated electrons" K. Byczuk et al.; *Nature Physics* 3, 168 (2007); see <http://www.physik.uni-augsburg.de/theo3/Publications/bibliography/10.1038/nphys538-manuscript.pdf>

[5] Disorder (Anderson localization):

"Localization Effects in Disordered Systems", D. Vollhardt, in *Festkoerperprobleme XXVII, Advances in Solid State Physics* (Vieweg, Wiesbaden, 1987), p. 63, see http://www.physik.uni-augsburg.de/theo3/Research/Localiz_effects-Festkoerperprob_1987.pdf

[6] Mott-Hubbard transition versus Anderson localization:

K. Byczuk, W. Hofstetter, and D. Vollhardt; *Phys. Rev. Lett.* 94, 056404 (2005); *Phys. Rev. Lett.* 102, 146403 (2009), see <http://www.physik.uni-augsburg.de/theo3/Publications/bibliography/10.1103/PhysRevLett.102.146403.pdf>

[7] Helium-3:

"Normal ^3He : An Almost Localized Fermi-Liquid", D. Vollhardt, *Rev. Mod. Phys.* 56, 99 (1984).

[8] Superfluid Helium-3:

"Superfluid Helium 3: Link between Condensed Matter Physics and Particle Physics", D. Vollhardt and P. Woelfle, *Acta Physica Polonica B* 31, 2837 (2000), [arXiv:cond-mat/0012052](https://arxiv.org/abs/cond-mat/0012052).

Computational studies of quantum spin systems

Summary:

These lectures will give an introduction to some of the computational techniques used to study quantum spin systems, primarily spin-1/2 models such as the Heisenberg model and extensions of it. Practical use of the methods will be illustrated by examples. In these applications, the main goal is to characterize different types of ordered and disordered ground states and quantum phase transitions between them.

Lectures:

1. Exact diagonalization studies
 - a) Use of symmetries for block-diagonalization
 - b) Studies of ground states and excitations with the Lanczos method
2. Stochastic series expansion (quantum Monte Carlo)
 - a) Algorithm for the spin-1/2 Heisenberg model
 - b) Studies of systems in one and two dimensions
3. Methods formulated in the valence-bond basis
 - a) The valence-bond basis and amplitude-product states
 - b) Variational and projector quantum Monte Carlo methods
4. Studies of quantum phase transitions
 - a) Finite-size scaling techniques
 - b) Neel to Valence-bond-solid transition
5. Disordered (random) systems
 - a) The diluted two-dimensional Heisenberg model
 - b) Low-energy dynamics; sum rules and triplet localization

Tutorials:

For the afternoon training sessions, the instructor will make available simple computer programs using the algorithms discussed in the lectures. These programs are written in Fortran 90. A good reference for this programming language is; *Fortran 90/95 for Scientists and Engineers*, by S. Chapman (McGraw Hill, 2004). Participants with their own laptops are urged to install a Fortran 90/95 compiler, e.g., "g95", available for free at www.g95.org.

References:

1. E. Dagotto, *Rev. Mod. Phys.* 66, 763 (1994).
2. A. W. Sandvik, *Phys. Rev. B* 59, R14157 (1999); O. F. Syljuasen and A. W. Sandvik, *Phys. Rev. E* 66, 046701 (2002).
3. A. W. Sandvik, *Phys. Rev. Lett.* 95, 207203 (2005); J. Lou and A. W. Sandvik, *Phys. Rev. B* 76, 104432 (2007).
4. S. Sachdev, *Nature Physics* 4, 173 (2008); A. W. Sandvik, *Phys. Rev. Lett.* 98, 227202 (2007); J. Lou, A. W. Sandvik, and N. Kawashima, *arXiv:0908.0740*.
5. A. W. Sandvik, *Phys. Rev. B* 66, 024418 (2002); L. Wang and A. W. Sandvik, *Phys. Rev. Lett.* 97, 117204 (2006).

Professor George Sawatzky

Department of Physics and Astronomy, University of British Columbia, Vancouver B.C., Canada

Electronic structure of strongly correlated complex oxide systems

Lectures:

- 1.** *Basics of the electronic structure of strongly correlated electron system: why not DFT*
- 2.** *Why are 3d transition metal and rare earths special and experimental tools to demonstrate this*
- 3.** *Description of some models and of correlated systems and some exotic effects expected*
- 4.** *Parameter determination and the standard theories of screening and the effects in real materials with nonuniform polarizabilities leading to unconventional "screening"*
- 5.** *Interplay between orbital-spin, charge and lattice degrees of freedom – highT_c's Fe pnictides, surfaces and interfaces.*

06/10/2009

Mr. Sergey Artyukhin

Zernike Institute for Advanced Materials, University of Groningen, Netherlands

Ferromagnetic insulator state in iron-doped FeTiO₃

The solid solution of two antiferromagnetic compounds, FeTiO₃ and Fe₂O₃, exhibits an unusual insulating ferromagnetic state appearing around room temperature. FeTiO₃ is formed by alternating ferromagnetic planes of magnetic Fe and nonmagnetic Ti ions. In the solid solution some Ti atoms are substituted by Fe dopants, which frustrates the antiferromagnetic spin ordering by inducing a local ferromagnetic coupling between neighboring magnetic layers. The result is a large non-collinear modulation of spins around Fe dopants. We study properties of these spin polarons and their effect on magnetic properties of (1-x)FeTiO₃- xFe₂O₃. The polarons carry a large magnetization, which at low doping leads to superparamagnetic behavior, while at larger doping the overlapping spin polarons induce a transition into a ferrimagnetic state. The phase diagram of (1-x)FeTiO₃- xFe₂O₃ obtained by Monte Carlo simulations agrees well with experimental observations

06/10/2009

Mr. Wojciech Brzezicki

M. Smoluchowski Institute of Physics, Jagiellonian University, Cracov, Poland

Quantum compass model on a chain, ladder and finite square clusters.

I show the exact solutions for the quantum compass model on a chain and ladder which are based on mapping to quantum Ising models in certain subspaces. I discuss the ground - state and thermodynamic properties of both models. I show the application of the Kernel Polynomial Method to finite compass clusters of the size 4x4 and 5x5. I show the transformation which maps 5x5 compass model to 10 classes of 4x4 models which can be solved by KPM for the ground - state and thermodynamic properties.

07/10/2009

Dr. Giacomo Coslovich

Università degli Studi di Trieste, Italy

Discontinuities in the ultrafast electronic response of High-Tc Superconductors

Ultrafast optical spectroscopy has been used in the past as a tool to study the strength of electron-electron and electron-phonon interactions in strongly correlated systems and High-temperature superconductors. Recently, the possibility to impulsively photo-induce a collapse of the superconducting state in these materials by means of an ultrashort laser pulse has attracted growing attention [1,2,3]. Non-linear laser intensity dependencies and discontinuities in the ultrafast electronic response are the key experimental features of this new physics, which is barely understood yet. In this seminar we consider the case of Bi2212 superconductors at different dopings and temperatures. We present both experimental results of the ultrafast electronic response and simulations of the non-equilibrium behavior of a superconducting BCS gap. In the simulations the electronic structure of the Bi2212 sample is considered and several models of the non-equilibrium electron distribution functions are assumed. 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 dynamics of such non-equilibrium phase transitions 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] P. Kusar, V. V. Kabanov, J. Demsar, T. Mertelj, S. Sugai and D. Mihailovic, "Controlled Vaporization of the Superconducting Condensate in Cuprate Superconductors by Femtosecond Photoexcitation", PRL 101, 227001 (2008)

[2] C. Giannetti, G. Coslovich, F. Cilento, G. Ferrini, H. Eisaki, N. Kaneko, M. Greven, F. Parmigiani: "Discontinuity of the ultrafast electronic response of underdoped superconducting $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ strongly excited by ultrashort light pulses", PRB 79, 224502 (2009)

[3] T. Mertelj, V. V. Kabanov, C. Gadermaier, N. D. Zhigadlo, S. Katrych, J. Karpinski and D. Mihailovic, "Distinct Pseudogap and Quasiparticle Relaxation Dynamics in the Superconducting State of Nearly Optimally Doped $\text{SmFeAsO}_{0.8}\text{F}_{0.2}$ Single Crystals", PRL 102, 117002 (2009)

07/10/2009

Dr. Andrea Di Ciolo

Institut für Theoretische Physik, Goethe Universität Frankfurt, Frankfurt am Main, Germany

Evaluation of observables using Gutzwiller wave functions

I will discuss about the determination of response functions and projected excitations of Gutzwiller wave functions. According to my expertise, I will also deliver a short survey of the state of art of the generalized Gutzwiller approaches for strongly correlated systems (Time-Dependent Gutzwiller Approximation, Renormalized Mean Feld Theory ...).

08/10/2009

Mr. Mark Fischer

Institute for Theoretical Physics, ETH Zürich, Switzerland

Effects of spin-orbit coupling on the metamagnetic transition in $\text{Sr}_3\text{Ru}_2\text{O}_7$

Ultra-clean crystals of $\text{Sr}_3\text{Ru}_2\text{O}_7$ undergo a metamagnetic transition at low temperatures. This transition shows a strong anisotropy in the applied field direction with the critical field H^* ranging from $\sim 5.1\text{T}$ for $H_{\perp c}$ to $\sim 8\text{T}$ for $H_{\parallel c}$. In addition, studies on ultra-pure samples revealed a splitting of the metamagnetic transition into at least two magnetization anomalies for fields in c -direction. It has been suggested that a nematic phase emerges between the magnetization jumps. The aim of our study is to explain the field anisotropy of these phenomena. Based on a microscopic tight-binding model, we introduce the metamagnetic transition by means of a van Hove singularity scenario and we describe the low-temperature phase as a nematic state favored by forward scattering processes. The rotation of the O -octahedra around the c -axis observed in this material introduces a staggered spin-orbit coupling within the planes and naturally leads to an anisotropy of the magnetic response in accordance to observation. Moreover, the spin-orbit coupling shows a strong influence on both, the critical field H^* and the occurrence of the nematic phase.

08/10/2009

Miss Olga Howczak

M. Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland

de Haas-van Alphen magnetization oscillations and spin-dependent masses in a two-dimensional Fermi liquid of correlated quasiparticles

We consider the magnetic properties of two-dimensional Fermi liquid of quasiparticles with spin dependent masses in periodic crystal potential. To determine thermodynamic properties of this

Hofstadter like model we use quantum transfer-matrix method developed by T. Xiang and collaborators. The de Haas-van Alphen oscillation of magnetization is calculated at finite temperatures.

09/10/2009

Dr. Anna Kauch

Center for Electronic Correlations and Magnetism,
Institute of Physics, University of Augsburg, Germany

Strong coupling approximation of the Bosonic Dynamical Mean-Field Theory equations

The bosonic dynamical mean-field theory (B-DMFT), recently formulated by Byczuk and Vollhardt (Phys. Rev. B 77, 235106 (2008)), provides a comprehensive and thermodynamically consistent description of correlated lattice bosons. Within the B-DMFT normal and Bose-Einstein condensed bosons are treated on equal footing. In the B-DMFT the lattice bosonic problem is replaced by a single impurity coupled to two bosonic baths (corresponding to normal and condensed bosons, respectively). This yields a set of B-DMFT equations which have to be solved self-consistently. We propose here an approximate method to solve the B-DMFT equations for the bosonic Hubbard model by performing a renormalized strong-coupling perturbation expansion (linked-cluster expansion) around the atomic limit. We investigate the validity of this approach by comparing our results to the known phase diagram of the Hubbard model.

09/10/2009

Dr. Ivan Leonov

Center for Electronic Correlations and Magnetism,
Institute of Physics, University of Augsburg, Germany

Structural transformations caused by electronic correlations

The electronic structure of materials can often be described quite accurately by density functional theory in the local density approximation (LDA) or the generalized gradient approximation (GGA). However, these methods usually fail to predict the correct electronic and structural properties of materials where electronic correlations play a role. Extensions of LDA, e.g., LDA + U and self-interaction correction LDA, can improve the results, e.g., the band gap value and local moment, but only for solids with long-range order. Hence the computation of electronic, magnetic, and structural properties of strongly correlated paramagnetic materials remains a great challenge. Here, we present a computational scheme [1] for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural transformation, caused by electronic correlations. It combines *ab initio* band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. With this approach, we address electronic and structural properties of paramagnetic perovskites $KCuF_3$, K_2CuF_4 , and $LaMnO_3$, the prototypical materials for orbital ordering and cooperative Jahn-Teller distortion.

[1] I. Leonov, N. Binggeli, Dm. Korotin, V. I. Anisimov, N. Stojic, and D. Vollhardt, Phys. Rev. Lett. 101, 096405 (2008).

12/10/2009

Mr. Jan Kaczmarczyk

Condensed Matter Theory and Nanophysics Department,
Jagiellonian University, Cracow, Poland

Superconductivity in a correlated system of quasiparticles with spin-dependent masses

I will discuss a paired state of quasiparticles with spin dependent masses, which were observed recently in the CeCoIn₅ system. In the same strongly-correlated system the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase appears. I will show that the spin-dependent masses essentially extend the regime of applied field and temperatures under which the FFLO phase is stable. We believe that the mechanism of stabilization of the FFLO phase by the spin-dependent masses is generic. Therefore, FFLO phases should be searched for in the same systems in which spin-dependent masses were observed and vice versa. I will compare results of our model calculations with the experiment.

12/10/2009

Mr. Zhou Li

Department of Physics, University of Alberta, Edmonton, Canada

Refinements of Lanczos method to solve the Holstein Model

We proposed two simple refinements of Lanczos method to solve the Holstein model. 1. By starting from the unperturbed state in the strong-coupling limit instead of the bare electron state, we speed up the convergence considerably in the intermediate and strong coupling regime. 2. By starting from the well converged strong coupling regime, each step we lower the value of electron phonon coupling (or phonon energy) with a small amount, use as a starting wave function the previous solution, truncate to include components with some minimal amplitude (so that a few hundred basis states at most are used), then converge the solution for this value of electron phonon coupling. This process can be continued until the desired range is covered. As is known, in the adiabatic limit, there is phase transition from a small polaron localized state to a free electron delocalized state, in dimensions two and higher. Nonetheless, as is known through other considerations, for any nonzero phonon frequency, the crossover is smooth. By using these two refinements, we have obtained numerical exact results for a wide range of parameters. In particular, we obtain well converged results over all coupling strengths and for low phonon frequencies. The results for low frequencies in particular illustrate a rather abrupt crossover to a regime where multi-phonon processes are prevalent.

[1] J. Bonca, S.A. Trugman and I. Batistic, *Phys.Rev.B* 60, 1633 (1999).

[2] H. Fehske and S.A. Trugman, "Polarons in Advanced Materials", edited by A.S. Alexandrov, Springer Series in Material Sciences 103 pp. 393-461, Springer Verlag, Dordrecht (2007).

13/10/2009

Dr. Giovanni Mazzeolla

Dipartimento di Fisica "Galileo Galilei", Universita' degli Studi di Padova, Italy

Atomic Josephson junction with two bosonic species

We study an atomic Josephson junction (AJJ) in presence of two interacting Bose-Einstein condensates (BECs) confined in a double well trap. We assume that bosons of different species interact with each other. The macroscopic wave functions of the two components obey to a system of two 3D coupled Gross-Pitaevskii equations (GPE). We write the Lagrangian of the system, and from this we derive a system of coupled ordinary differential equations (ODE), for which the coupled pendula represent the mechanic analogous. These differential equations control the dynamical behavior of the fractional imbalance and of the relative phase of each bosonic component. We perform the stability analysis around the points which preserve the symmetry and get an analytical formula for the oscillation frequency around the stable points. Such a formula could be used as an indirect measure of the inter-species s-wave scattering length. We also study the oscillations of each fractional imbalance around zero and non zero - the macroscopic quantum self-trapping (MQST) - time averaged values. For

different values of the inter-species interaction amplitude, we carry out this study both by directly solving the two GPE and by solving the corresponding coupled pendula equations. We show that, under certain conditions, the predictions of these two approaches are in good agreement. Moreover, we calculate the crossover value of the inter-species interaction amplitude which signs the onset of MQST.

13/10/2009

Mr. Rubem Mondaini

Solid State Physics Department, Federal University of Rio de Janeiro, Brazil

Electronic correlations in disordered honeycomb lattices

In the past few years, much attention has been given to the study of honeycomb lattices. Beyond the experimental motivation due to the recent fabrication of graphene sheets, this importance also arises from the fact that the honeycomb lattice has many interesting properties. In usual square-lattice systems, any nonzero interaction energy U between the electrons drives a Mott metal-insulator and paramagnetic-antiferromagnetic phase transitions. In the honeycomb lattice, it is necessary a finite energy U_c to drive both transitions. Moreover it is interesting to study such systems with a disorder term. Anderson showed that below a critical density any system with disorder could not possess conductivity. The approach used in this work is the Hubbard-Anderson model, where we can define different onsite energies chosen randomly within a symmetric range. This configures a disorder term and it can be measured by the magnitude of the range. To perform the simulations we employ the determinant quantum monte carlo (DQMC) method. In this work, the aim is to study how magnetic correlations are affected by disorder at near half-filling. We will present results for spin correlations as a function of temperature, lattice size and correlation strength U for different degrees of disorder.

14/10/2009

Miss Aroon O'Brien

Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Charge fractionalization in a model of spinless fermions on a kagome lattice

The study of the magnetic properties of geometrically frustrated spin systems is an area of intense interest. However, the charge degrees of freedom of such structures are less understood. Previous work on checkerboard lattice models has revealed the existence of fractional charges [1]. These charges were later shown to be confined [2]. We study a model of spinless fermions on finite kagome clusters, which gives rise to charge fractionalization in a similar manner. The 2D nature of the kagome lattice raises the question as to whether the fractional charges have anyonic statistics. Furthermore, kagome lattice models have established and emerging analogies in experiment [3]. In our model, the fractional charge excitations occur at $1/3$ filling. We present an investigation of the statistics and dynamics of these fractional charges through an analysis of the dynamical properties of hardcore bosonic and spinless fermionic spectral functions. Furthermore we discuss a complementary dimer model analysis.

[1] P. Fulde, K. Pence, N. Shannon, *Ann. Phys.*, V11, 892 (2002)

[2] F. Pollmann. and P. Fulde, *Europhys. Lett.*, v75, 133 (2006)

[3] arXiv: 0906.3042v1 [cond-mat.quant-gas] 16 Jun 2009.

15/10/2009

Miss Dorota Rudzinska

Institute of Physics, University of Technology, Wroclaw, Poland

Broader view on superconducting phase in presence of a

momentum-dependent impurity scattering potential.

Controlled impurity doping is an useful tool in the identification of a symmetry of a superconducting ground state. We intensively studied behavior of order parameter (OP) and local density of states (LDOS) in s-wave superconductors in vicinity of scattering center [1-7] and analyzed these quantities from two points of view. Namely in real and complementary in reciprocal space. The k-space image carries interesting information about feature of the system like in case of LDOS [8,9]. Followed this trace we also investigate Fourier transform of order parameter. Our calculation are done in linear approximation and more extended form in T-matrix approximation but only for 'on-site' potential.

- [1] A.L. Fetter, Phys. Rev. 140, A1921 (1965).
- [2] T. Xiang, J.M. Wheatley, Phys. Rev. B 51, 11721 (1995).
- [3] G. Litak, Physica B 359-361, 566 (2005).
- [4] A. Ghosal, M.Randeria, N. Trivedi, Phys. Rev. Lett. 81, 3940 (1998).
- [5] G. Harań, PRB 65, 216501 (2002)
- [6] A. Maciąg, P. Pisarski, G. Harań, Physica C 387, 73 (2003)
- [7] D. Rudzińska, P. Pisarski, G. Harań Acta Phys. Pol. A 114, 149 (2008).
- [8] L. Capriotti, D.J. Scalapino, R.D Sedgewick, Phys. Rev. B. 68, 014508 (2003).
- [9] P.Pisarski,G.Harań, Phys. Status Solidi B 242, 426 (2005).

15/10/2009

Mr. Philipp Wissgott

Solid State Physics, UT Vienna, Austria

Thermopower of Na_{0.7}CoO₂ studied by LDA+DMFT

Recently, cobaltates Na_xCoO₂ have attracted much interest due to their high thermopower and for the appearance of superconductivity in the H₂O intercalated compounds. This talk describes a combined Local Density Approximation(LDA) and Dynamical Mean Field Theory (DMFT) study to investigate the strength of correlation effects in the representative compound Na_{0.7}CoO₂. The bandstructure shows mostly a1g characteristics around the Fermi edge. Therefore, an effective one band model is considered, where a single-band tight-binding fit has been applied to the LDA bandstructure. To account for the stoichiometric factor xNa=0.7, we extend the existing DMFT code to include disorder by means of the Coherent Potential Approximation. Computational results can be separated in sodium and vacancy contributions, which allows for a detailed correlation analysis. From the DMFT self energy, the thermopower for various temperatures is computed by Linear Response Theory and compared with experiment.

16/10/2009

Mr. Andrej Schwabe

Physics Department, University of Hamburg, Germany

Interacting Spin Waves in the Ferromagnetic Kondo Lattice Model

We present an approach for the ferromagnetic, three-dimensional, translational symmetric Kondo lattice model which allows to derive both magnon energies and linewidths (lifetimes) and study the properties of the ferromagnetic phase. Our approach consists of mapping the Kondo lattice model onto an effective Heisenberg model by the help of the "modified RKKY interaction" and the "interpolating self-energy approach". The Heisenberg model is approximatively solved by applying the Dyson-Maleev transformation and using the "spectral density approach" with a broadened magnon spectral density.

16/10/2009

Dr. Bretislav Sopik

Institute of Physics, Academy of Sciences, Prague, Czech Republic

Conserving T-matrix theory of superconductivity

A selfconsistent T-matrix theory of many-Fermion systems is proposed. In the normal state the theory agrees with the Galitskii-Feynmann approximation, in the superconducting state it has the form of the renormalized Kadanoff-Martin approximation. The two-particle propagator satisfies the Baym-Kadanoff symmetry condition which guarantees that the theory conserves the number of particles, momentum and energy. The theory is developed for retarded interactions leading to the Eliashberg theory in the approximation of a single pairing channel. Let us note, we hope to have finished a numerical discussion of T-matrix behaviour close to T_c using proposed theory during the end of summer.

16/10/2009

Miss Hanna Terletska

Florida State University, National High Magnetic Field Laboratory, Tallahassee, USA

Fingerprints of intrinsic phase separation

We theoretically study the properties of a recently observed [1] inhomogeneous phase preceding the metal-insulator transition in a magnetically-doped two-dimensional electron gas (2DEG). We show that, due to competition between (ferromagnetic) double-exchange and (anti-ferromagnetic) super-exchange, at very low carrier density such a system is unstable toward intrinsic phase separation (PS). Here, ferromagnetic carrier-rich (metallic) "droplets" emerge within a magnetically disordered carrier-poor (insulating) matrix. Our calculations indicate that this regime should display very unusual transport, featuring colossal magneto-resistance with exceptionally weak density dependence - in striking agreement with experiments [1] on CdMnTe quantum wells. Such exotic transport properties - we argue - should be considered as "fingerprints" for intrinsic phase separation, a behavior very different from situations where phase coexistence is driven by disorder due to extrinsic impurities or defects.

[1] J. Jaroszynski et.al, Phys. Rev. B 76, 045322 (2007).

16/10/2009

Dr. Luca Tocchio

Institute for Theoretical Physics, University of Frankfurt , Germany

Spin-liquid and magnetic phases in the anisotropic triangular lattice: the case of organic charge-transfer salts

The two-dimensional Hubbard model on the anisotropic triangular lattice, with two different hopping amplitudes t and t' , is relevant to describe the low-energy physics of k -(ET)₂X, a family of organic salts. The ground-state properties of this model are studied by using Monte Carlo techniques, on the basis of a recent definition of backflow correlations for strongly-correlated lattice systems. The results show that there is no magnetic order for reasonably large values of the electron-electron interaction U and frustrating ratio $t'/t = 0.85$, suitable to describe the non-magnetic compound with $X = \text{Cu}_2(\text{CN})_3$. On the contrary, Néel order takes place for weaker frustrations, i.e., $t'/t = 0.4 \div 0.6$, suitable for other compounds

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 22nd 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>

XIII TC: 6th to 17th October 2008.

Lecturers: G. Aeppli, P. Littlewood, M. Sigrist, M. Troyer.

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

Final programme of the meeting

I Week

Prof. V. I. Anisimov: *Electronic structure calculations for systems with strong Coulomb correlations.*

Prof. D. Vollhardt: *Theory of correlated fermionic and bosonic condensed matter.*

5 October

08:00 - 08:50	Registration.
08:50 - 09:00	Opening of the Training Course.
09:00 - 11:00	Prof. D. Vollhardt: 1st Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. V. I. Anisimov: 1st Lecture
13:30 - 15:30	Lunch.
15:30 - 17:20	Participant presentations.
17:20 - 17:30	Break.
17:30 - 18:30	Prof. V. I. Anisimov - Prof. D. Vollhardt: Training Session

6 October

09:00 - 11:00	Prof. V. I. Anisimov: 2nd Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. D. Vollhardt: 2nd Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Mr. S. Artyukhin: <i>Ferromagnetic insulator state in iron-doped FeTiO₃.</i>
15:55 - 16:20	Mr. W. M. Brzezicki: <i>Quantum compass model on a chain, ladder and finite square clusters.</i>
16:20 - 16:30	Break.
16:30 - 18:30	Prof. V. I. Anisimov - Prof. D. Vollhardt: Training Session

7 October

09:00 - 11:00	Prof. D. Vollhardt: 3rd Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. V. I. Anisimov: 3rd Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Dr. G. Coslovich: <i>Discontinuities in the ultrafast electronic response of High-Tc Superconductors.</i>
15:55 - 16:20	Dr. A. Di Ciolo: <i>Evaluation of observables using Gutzwiller wave functions.</i>
16:20 - 16:30	Break.
16:30 - 18:30	Prof. V. I. Anisimov - Prof. D. Vollhardt: Training Session.

8 October

09:00 - 11:00	Prof. V. I. Anisimov: 4th Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. D. Vollhardt: 4th Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Mr. M. H. Fischer: <i>Effects of spin-orbit coupling on the metamagnetic transition in Sr₃Ru₂O₇.</i>
15:55 - 16:20	Miss O. Howczak: <i>de Haas-van Alphen magnetization oscillations and spin-dependent masses in a two-dimensional Fermi liquid of correlated quasiparticles.</i>
16:20 - 16:30	Break.
16:30 - 18:30	Prof. V. I. Anisimov - Prof. D. Vollhardt: Training Session.

9 October

09:00 - 10:00	Prof. D. Vollhardt: 5th Lecture
10:00 - 10:30	Dr. A. K. Kauch: <i>Strong coupling approximation of the Bosonic Dynamical Mean-Field Theory equations.</i>
10:30 - 11:00	Dr. I. Leonov: <i>Structural transformations caused by electronic correlations.</i>
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. V. I. Anisimov: 5th Lecture
13:30 - 15:30	Lunch.
17:00 - 18:00	Prof. D. Vollhardt: <i>Public Lecture on: "Magnetism: A Guided Tour from Ancient Greece to Modern Salerno"</i>

II Week

Prof. A. W. Sandvik: Computational studies of quantum spin systems.

Prof. G. Sawatzky: Electronic structure of strongly correlated complex oxide systems.

12 October

09:00 - 11:00	Prof. G. Sawatzky: 1st Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. A. W. Sandvik: 1st Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Mr. J. S. Kaczmarczyk: Superconductivity in a correlated system of quasiparticles with spin-dependent masses.
15:55 - 16:20	Mr. Z. Li: Refinements of Lanczos method to solve the Holstein Model.
16:20 - 16:30	Break.
16:30 - 18:30	Prof. A. W. Sandvik - Prof. G. Sawatzky: Training Session.

13 October

09:00 - 11:00	Prof. G. Sawatzky: 2nd Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. A. W. Sandvik: 2nd Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Dr. G. Mazzaarella: Atomic Josephson junction with two bosonic species.
15:55 - 16:20	Mr. R. Mondaini: Electronic correlations in disordered honeycomb lattices
16:20 - 16:30	Break.
16:30 - 18:30	Prof. A. W. Sandvik - Prof. G. Sawatzky: Training Session.

14 October

09:00 - 11:00	Prof. G. Sawatzky: 3rd Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. A. W. Sandvik: 3rd Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Miss A. O'Brien: Charge fractionalization in a model of spinless fermions on a kagome lattice.
15:55 - 16:30	Break.
16:30 - 18:30	Prof. A. W. Sandvik - Prof. G. Sawatzky: Training Session

15 October

09:00 - 11:00	Prof. G. Sawatzky: 4th Lecture
11:00 - 11:30	Coffee Break.
11:30 - 13:30	Prof. A. W. Sandvik: 4th Lecture
13:30 - 15:30	Lunch.
15:30 - 15:55	Miss D. H. Rudzinska: Broader view on superconducting phase in presence of a momentum-dependent impurity scattering potential.
15:55 - 16:20	Mr. P. Wisgott: Thermopower of $\text{Na}_{0.7}\text{CoO}_2$ studied by LDA+DMFT.
16:20 - 16:30	Break.
16:30 - 18:30	Prof. A. W. Sandvik - Prof. G. Sawatzky: Training Session..

16 October

09:00 - 11:00	Prof. A. W. Sandvik: 5th Lecture
11:00 - 11:15	Coffee Break.
11:15 - 11:40	Mr. A. Schwabe: Interacting Spin Waves in the Ferromagnetic Kondo Lattice Model.
11:40 - 12:05	Dr. B. Sopik: Conserving T-matrix theory of superconductivity.
12:05 - 12:20	Coffee Break.
12:20 - 12:45	Miss H. Terletska: Fingerprints of intrinsic phase separation.
12:45 - 13:10	Dr. L. F. Tocchio: Spin-liquid and magnetic phases in the anisotropic triangular lattice: the case of organic charge-transfer salts.
13:10 - 13:30	Closing of the Training Course.
13:30 - 15:30	Lunch.