LOW TEMPERATURE PHYSICS

TIEFE TEMPERATUREN (TT)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms HSZ 02, HSZ 105, HSZ 301, HSZ 304, P1)

Internal Symposia within TT

TT10 Symposium: "Solid State Meets Quantum Optics"
Organization: P. Hänggi, S. Kohler (Universität Augsburg), A. Shnirman (Universität Karlsruhe)

TT 10.1	Mon	14:30	(HSZ 02)	**Circuit QED: Quantum Optics With Superconducting Electrical Circuits**, Steven Girvin
TT 10.2	Mon	15:00	(HSZ 02)	**Cooper-Pair Molasses: Cooling a Nanomechanical Resonator with Quantum Noise**, Keith Schwab, Akshay Naik, Olivier Buu, Matthew LaHaye, Aashish Clerk, Andrew Armour, Miles Blencowe
TT 10.3	Mon	15:30	(HSZ 02)	**Fermionic atoms in a crystal structure of light**, Tilman Esslinger
TT 10.4	Mon	16:30	(HSZ 02)	**Nonclassical States, Tomography, and Quantum Information in Circuit QED**, E. Solano, M. Mariantoni, M.J. Storcz, F.K. Wilhelm, W.D. Oliver, A. Emmert, A. Marx, R. Gross, H. Christ
TT 10.5	Mon	17:00	(HSZ 02)	**Integrated Atom Optics on a Bose-Einstein-Chip**, Claus Zimmermann

TT14 Symposium: "Molecular Electronics"
Organization: H. Schoeller (RWTH Aachen)

TT 14.1	Tue	09:30	(HSZ 02)	**Single-Molecule Transistor**, Hongkun Park
TT 14.2	Tue	10:00	(HSZ 02)	**Three-terminal transport through molecular junctions**, Herre van der Zant
TT 14.3	Tue	10:30	(HSZ 02)	**Transport through single molecules: vibrational and magnetic excitations**, Maarten Wegewijs, Christian Romeike, Herbert Schoeller, Walter Hofstetter
TT 14.4	Tue	11:15	(HSZ 02)	**Novel quantum transport effects in single-molecule junctions**, Felix von Oppen
TT 14.5	Tue	11:45	(HSZ 02)	**Electron Transport through Single Molecules**, Heiko B. Weber, Daniel Secker, Rolf Ochs, Mark Elbing, Ferdinand Evers, Max Köntopp, Marcel Mayor

TT22 Symposium: "Quantum Fluids"
Organization: R. Haley (University of Lancaster)

TT 22.1	Tue	15:00	(HSZ 304)	**A-B Transition and Anisotropic Scattering in Superfluid ^{3}He in Aerogel**, Yoonseok Lee
TT 22.2	Tue	15:30	(HSZ 304)	**Quantum Turbulence in superfluid ^{3}He**, Shaun Fisher
TT 22.3	Tue	16:00	(HSZ 304)	**The Transition in the Vortex Dynamics of Superfluid ^{3}He-B**, V.B. Eltsov, R. Blaauwgeers, R. de Graaf, J. Kopu, M. Krusius
TT 22.4	Tue	16:45	(HSZ 304)	**Stable textures and defects in slabs of superfluid 3He-A**, Paul Walmsley, Andrei Golov
TT 22.5	Tue	17:15	(HSZ 304)	**Molecular Spectroscopy in Helium Droplets at Low Temperatures**, Alkwin Slenczka

TT27 Symposium: "Twenty Years High-T_c Cuprates - Recent Progress"
Organization: D. Manske (MPI Stuttgart), L. Alff (TU Darmstadt), R. Hackl (WMI Garching)

TT 27.1	Thu	09:30	(HSZ 02)	**Vorticity in the phase diagram of cuprates: evidence from Nernst effect and torque magnetometry**, N. P. Ong
TT 27.2	Thu	10:00	(HSZ 02)	**Recent Photoemission Data from Layered Manganites and Cuprates**, Zhi-xun Shen
TT 27.3	Thu	10:30	(HSZ 02)	**"Kinks", Nodal Bilayer Splitting and Interband Scattering in YBCO**, Sergey Borisenko
TT 27.4	Thu	11:30	(HSZ 02)	**Universal magnetic spectrum in high-temperature superconductors**, Bernhard Keimer
TT 27.5	Thu	12:00	(HSZ 02)	**Spin-fluctuation mechanism of high-temperature superconductivity**, Andrey Chubukov
TT 27.6	Thu	12:30	(HSZ 02)	**The origin of anomalous transport in a high-temperature superconductor**, Nigel Hussey

Further Invited Talks

TT 5.1	Mon	09:30	(HSZ 304)	**Correlation effects on electronic transport through dots and wires**, Volker Meden
TT 6.1	Mon	10:30	(HSZ 105)	**Nuclear quadrupoles and magnetic-field effects in amorphous solids**, Alois Würger
TT 4.1	Mon	11:00	(HSZ 301)	**Current vs. Correlations: The Nonequilibrium Kondo Model**, Stefan Kehrein
TT 15.1	Tue	12:30	(HSZ 02)	**Electric field control of spin transport in carbon nanotubes**, Takis Kontos, Sangeeta Sahoo, Juerg Furer, Christian Hoffmann, Matthias Gräber, Audrey Cottet, Christian Schönenberger
TT 20.1	Tue	14:00	(HSZ 105)	**Theory of inelastic scattering from magnetic impurities**, Gergely Zarand, Laszlo Borda, Natan Andrei, Jan von Delft
TT 23.1	Wed	14:30	(HSZ 02)	**Electronic micro-refrigeration and thermometry**, Jukka Pekola, Alexander Savin, Matthias Meschke, Tero Heikkilä, Francesco Giazotto, Wiebke Guichard, Frank Hekking
TT 24.1	Wed	16:30	(HSZ 02)	**Cryogenic detectors**, Gabriel Chardin
TT 29.1	Thu	09:30	(HSZ 304)	**Decoherence of fermions subject to a quantum bath**, Florian Marquardt

Joint Symposia With Other Sections

SYSF Symposium: "Superfluidity", Monday morning (see SYSF)

SYMS Symposium: "Magnetic Switching", Monday afternoon (see SYMS)

SYNW Symposium: "Nano Wires", Wednesday afternoon (see SYNW)

SYIM Symposium: "Intrinsic Modes", Thursday afternoon (see SYIM)

Sessions

TT 1	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs**	Mon 09:30–11:15	HSZ 02	TT 1.1–1.7
TT 2	**Superconductivity: Conductor Development**	Mon 11:30–13:00	HSZ 02	TT 2.1–2.6
TT 3	**Correlated Electrons: Quantum-Critical Phenomena**	Mon 09:30–10:45	HSZ 301	TT 3.1–3.5
TT 4	**Correlated Electrons: Quantum Impurities, Kondo Physics**	Mon 11:00–13:00	HSZ 301	TT 4.1–4.7
TT 5	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1**	Mon 09:30–13:00	HSZ 304	TT 5.1–5.12
TT 6	**Solids At Low Temperature: Amorphous and Tunnel Systems, Glasses, ...**	Mon 10:30–13:00	HSZ 105	TT 6.1–6.9
TT 7	**Superconductivity & Solids At Low Temperature - Poster Session**	Mon 14:00–17:45	P1	TT 7.1–7.73
TT 8	**Correlated Electrons: Heavy Fermions**	Mon 14:30–17:45	HSZ 301	TT 8.1–8.12
TT 9	**Transport: Nanoelectronics III-Molecular Electronics**	Mon 14:00–17:45	HSZ 304	TT 9.1–9.14
TT 10	**Symposium Solid State Meets Quantum Optics**	Mon 14:30–17:30	HSZ 02	TT 10.1–10.5
TT 11	**Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence**	Tue 09:30–13:00	HSZ 301	TT 11.1–11.13
TT 12	**Correlated Electrons: Low-dimensional Systems - Models**	Tue 09:30–12:30	HSZ 304	TT 12.1–12.11
TT 13	**Correlated Electrons: Metal Insulator Transition 1**	Tue 11:45–13:00	HSZ 105	TT 13.1–13.5
TT 14	**Symposium Molecular Electronics**	Tue 09:30–12:15	HSZ 02	TT 14.1–14.5
TT 15	**Transport: Nanoelectronics II - Spintronics and Magnetotransport 1**	Tue 12:30–13:00	HSZ 02	TT 15.1–15.1
TT 16	**Solids At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ...**	Tue 09:30–11:30	HSZ 105	TT 16.1–16.8
TT 17	**Superconductivity: Thin Film Preparation**	Tue 14:00–14:45	HSZ 02	TT 17.1–17.3
TT 18	**Superconductivity: Borides, Borocarbides, Carbides, ...**	Tue 15:00–18:30	HSZ 02	TT 18.1–18.13
TT 19	**Correlated Electrons: Low-dimensional Materials**	Tue 14:00–19:00	HSZ 301	TT 19.1–19.19
TT 20	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2**	Tue 14:00–16:00	HSZ 105	TT 20.1–20.7
TT 21	**Transport: Nanoelectronics II - Spintronics and Magnetotransport 2**	Tue 16:15–19:00	HSZ 105	TT 21.1–21.10
TT 22	**Symposium Quantum Fluids**	Tue 15:00–17:45	HSZ 304	TT 22.1–22.5
TT 23	**Solids At Low Temperature: Cryogenics**	Wed 14:30–16:15	HSZ 02	TT 23.1–23.6
TT 24	**Superconductivity: Cryodetectors**	Wed 16:30–19:00	HSZ 02	TT 24.1–24.9
TT 25	**Correlated Electrons - Poster Session**	Wed 14:30–18:30	P1	TT 25.1–25.117
TT 26	**Transport - Poster Session**	Wed 14:30–18:30	P1	TT 26.1–26.42
TT 27	**Symposium Twenty Years High-T_c Cuprates - Recent Progress**	Thu 09:30–13:00	HSZ 02	TT 27.1–27.6
TT 28	**Correlated Electrons: General Theory**	Thu 10:00–13:00	HSZ 301	TT 28.1–28.11
TT 29	**Transport: Quantum Coherence and Quantum Information Systems 1**	Thu 09:30–12:45	HSZ 304	TT 29.1–29.11
TT 30	**Superconductivity: Twenty Years High-T_c Cuprates - Recent Progress**	Thu 14:00–18:45	HSZ 02	TT 30.1–30.18
TT 31	**Correlated Electrons: Metal Insulator Transition 2**	Thu 14:00–18:30	HSZ 301	TT 31.1–31.17
TT 32	**Transport: Quantum Coherence and Quantum Information Systems 2**	Thu 14:00–17:45	HSZ 304	TT 32.1–32.14
TT 33	**Superconductivity: Vortex Dynamics, Vortex Phases, Pinning**	Fri 10:15–12:30	HSZ 304	TT 33.1–33.9
TT 34	**Correlated Electrons: Spin Systems and Itinerant Magnets**	Fri 10:15–12:30	HSZ 301	TT 34.1–34.9

TT Time Table

PV: Plenary Talk ; ÖAV: Public Talk; HV: Invited Talk ; FV: Keynote Talk ; SY: Symposium
SC: Superconductivity ; CE: Correlated Electrons ; TR: Transport ; SLT: Solids at Low Temperature ; NE: Nanoelectronics

Monday 27/03/06

8:30 *PV Chan* HSZ 01

9:30-11:15 **TT1** HSZ 02
SC - Tunneling, Josephson Junctions, SQUIDs

11:30-13:00 **TT2** HSZ 02
SC - Conductor Development

9:30-10:45 **TT3** HSZ 301
CE - Quantum-Critical Phenomena

11:00-13:00 **TT4** HSZ 301
CE - Quantum Impurities, Kondo Physics
11:00 HV Kehrein

9:30-13:00 **TT5** HSZ 304
TR - NE I: Quantum Dots, Wires, Point Contacts 1
9:30 HV Meden

10:30-13:00 **TT6** HSZ 105
SLT - Amorphous and Tunnel Systems, Glasses, ...
10:30 FV Würger

14:00-17:45 **TT7** P1
SC & SLT - *Posters*

14:30-17:45 **TT8** HSZ 301
CE - Heavy Fermions

14:00-17:45 **TT9** HSZ 304
TR - NE III: Molecular Electronics

14:30-17:30 **TT10** HSZ 02
SY Solid State Meets Quantum Optics
14:30 HV Girvin
15:00 HV Schwab
15:30 FV Esslinger
16:30 FV Solano
17:00 FV Zimmermann

18:00 *PV Jarzynski* HSZ 01

Tuesday 28/03/06

8:30 *PV Loss* HSZ 01

9:30-13:00 **TT11** HSZ 301
SC - Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

9:30-12:30 **TT12** HSZ 304
CE - Low-dimensional Systems, Models

11:45-13:00 **TT13** HSZ 105
CE - Metal Insulator Transition 1

9:30-12:15 **TT14** HSZ 02
SY Molecular Electronics
9:30 HV Park
10:00 HV v.d.Zant
10:30 FV Wegewijs
11:15 FV v.Oppen
11:45 FV Weber

12:15-13:00 **TT15** HSZ 02
TR - NE II: Spintronics & Magnetotransport 1
12:30 HV Kontos

9:30-11:30 **TT16** HSZ 105
SLT - Quantum Liquids, BEC, Ultra-cold Atoms ...

13:15 *PV Götze* HSZ 04

14:00-14:45 **TT17** HSZ 02
SC - Thin Film Preparation

15:00-18:30 **TT18** HSZ 02
SC - Borides, Borocarbides, Carbides, ...

14:00-19:00 **TT19** HSZ 301
CE - Low-dimensional Materials

14:00-16:00 **TT20** HSZ 105
TR - NE I: Quantum Dots, Wires, Point Contacts 2
14:00 HV Zarand

16:15-19:00 **TT21** HSZ 105
TR - NE II: Spintronics & Magnetotransport 2

15:00-17:45 **TT22** HSZ 304
SY Quantum Fluids
15:00 HV Lee
15:30 FV Fisher
16:00 HV Eltsov
16:45 FV Walmsley
17:45 FV Slenczka

Wednesday 29/03/06

8:30 - 10:00 *PVs Zweck & Yacoby* HSZ 01
10:00 Festsitzung HSZ 01

14:30-16:15 **TT23** HSZ 02
SLT - Cryogenics
14:30 HV Pekola

16:30-19:00 **TT24** HSZ 02
SC - Cryodetectors
16:30 HV Chardin

14:30-18:30 **TT25** P1
CE - *Posters*

14:30-18:30 **TT26** P1
TR - *Posters*

20:00 *ÖAV Tolan*

Thursday 30/03/06

8:30 *PV Krausz* HSZ 01

9:30-13:00 **TT27** HSZ 02
SY Twenty Years High-T_c Cuprates - Recent Progress
9:30 HV Ong
10:00 HV Shen
10:30 FV Borisenko
11:30 FV Keimer
12:00 FV Chubukov
12:30 FV Hussey

10:00-13:00 **TT28** HSZ 301
CE - General Theory

9:30-12:45 **TT29** HSZ 304
TR - Quantum Coherence and Quantum Information Systems 1
9:30 HV Marquardt

13:15 *PV Sackmann* HSZ 01

14:00-18:45 **TT30** HSZ 02
SC - Twenty Years High-T_c Cuprates - Recent Progress

14:00-18:30 **TT31** HSZ 301
CE - Metal Insulator Transition 2

14:00-17:45 **TT32** HSZ 304
TR - Quantum Coherence and Quantum Information Systems 2

Annual General Meeting of the Section Low Temperature Physics

Thu 19:00–19:30 HSZ 304

Tagesordnung

1) Frühjahrstagung 2006, Statistics
2) Themenkreise, Symposien
3) Bericht: DPG und AKF Sitzungen
4) Frühjahrstagung 2007
5) Verschiedenes

Friday 31/03/06

8:30-10:00 *PVs Orrit & Dekker* HSZ 01

10:15-12:30 **TT33** HSZ 304
SC - Vortex Dynamics, Vortex Phases, Pinning

10:15-12:30 **TT34** HSZ 301
SC - Spin Systems & Itinerant Magnets

Sessions

– Invited, Keynote, Contributed Talks and Posters –

TT 1 Superconductivity: Tunnelling, Josephson Junctions, SQUIDs

Time: Monday 09:30–11:15 Room: HSZ 02

TT 1.1 Mon 09:30 HSZ 02

Intrinsic Josephson junction on misaligned Tl-2212 thin films with different tilt angle — •Michael Mans[1], Matthias Büenfeld[1], Henrik Schneidewind[2], Frank Schmidl[1], Marco Diegel[2], and Paul Seidel[1] — [1]Institute of Solid State Physics, Friedrich-Schiller-University Jena, Helmholtzweg 5, D 07743 Jena, Germany — [2]Institute for Physical High Technology (IPHT) Jena, P.O.B. 100239, D 07702 Jena, Germany

Tl-2212 films are grown in a two step process. An amorphous Ba-Ca-Cu-O precursor are sputtered by rf sputtering. Subsequent it will oxythallinized into the Tl-2212 phase. On misaligned $LaAlO_3$ substrates the Tl-2212 grows with Cu-O planes tilted to the surface. So it is possible to fabricate microbridges which contain serial arrays of intrinsic Josephson junctions. We present structural and electrical measurements on such arrays for different misalignment angles. The electrical behaviour will be discussed in respect to the possibility of phase synchronisation. The experimental data will be compared with theoretical calculations of serial arrays of Josephson junctions with and without shunts.

TT 1.2 Mon 09:45 HSZ 02

Enhanced Macroscopic Quantum Tunneling in $Bi_2Sr_2CaCu_2O_{8+\delta}$ Intrinsic Josephson Junction Stacks — •X.Y. Jin, J. Lisenfeld, Y. Koval, A. Lukashenko, A.V. Ustinov, and P. Müller — Physikalisches Institut III, Universität Erlangen-Nürnberg, Germany

We have investigated macroscopic quantum tunneling (MQT) in $Bi_2Sr_2CaCu_2O_{8+\delta}$ intrinsic Josephson junctions (IJJs) and performed spectroscopic measurements. Classical-to-quantum crossover temperatures T* of up to 700mK were found. Plasma frequencies ω_p of up to 1.13 THz have been observed. We discovered that T* of IJJ stacks is significantly enhanced in comparison to a single intrinsic junction having a comparable plasma frequency. This enhancement of MQT is due to the unique stacking structure of IJJs. The quality factor of the IJJ stacks is $Q \sim 50$ and the spectroscopic coherence time is $\tau \sim 1.3ns$. This will allow to observe Rabi oscillations at rather high temperatures.

TT 1.3 Mon 10:00 HSZ 02

Characterisation of Nb charge-phase qubit circuits at 4.2 — •J. Könemann, H. Zangerle, B. Mackrodt, R. Dolata, S.A. Bogoslovsky, M. Götz, and A.B. Zorin — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Due to their scalability superconducting circuits, based on small Josephson junctions, are promising candidates for qubits, which form the basis of a possible quantum computing processor. The Bloch transistor included in a superconducting loop can serve as a so-called charge-phase qubit. Our all-Nb circuits with junction area down to 80 nm by 80 nm and nominal critical current of individual junctions of 25-50 nA included the Bloch transistor inserted into a loop and on-chip inductor of the tank circuit. Due to appreciable charging energy of the island the critical current of the transistor was substantially suppressed. High temperature made this suppression stronger. We report the radio-frequency measurements of our Nb qubit circuits, which were possible at 4.2 K. Resonance and flux modulation curves were used to determine the characteristic parameters of the samples. From the phase modulation curves the critical current (as small as few nA) and almost harmonic phase dependence of supercurrent were found. These data are consistent with our estimation based on a multi-band quantum-statistical model.

TT 1.4 Mon 10:15 HSZ 02

Frozen-flux-quanta phase shifter for digital Josephson circuits — •Dmitry Balashov[1], M. Khabipov[1], D. Hagedorn[1], A. B. Zorin[1], F.-Im. Buchholz[1], J. Niemeyer[1], B. Dimov[2], Th. Ortlepp[2], and F. H. Uhlmann[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Technische Universität Ilmenau, 98684 Ilmenau, Germany

Superconducting Rapid Single Flux Quantum (RSFQ) digital circuits are very promising for integration with Josephson qubits of different types. The basic quantization condition of each RSFQ cell is given by $LI_c > \Phi_0$ (L is the loop inductance and $\Phi_0 \approx 2.07$ mV·ps is the single flux quantum). For qubit applications, the critical current I_c of the RSFQ circuits should be set to about several μA, which, in turn, requires large geometrical inductance of the loop to ensure a certain phase shift inside or between the cells. The replacement of large inductances by the novel passive phase shifting elements based on small integer numbers of flux quanta frozen in the superconducting loops provides the well-defined phase shift. We report on the experimental verification of operation of such compact passive phase shifter elements realised in standard niobium SIS-trilayer technology for two different critical current densities: $j_c = 100$ A/cm^2 ($I_c^{\min} = 10$ μA), and $j_c = 1$ kA/cm^2 ($I_c^{\min} = 125$ μA). The flux quanta injection to the phase shifter loops was managed by feeding proper current into specially designed control lines.

This work is supported by DFG (NI253/7-1, UH53/6-1) and the EU (RSFQubit).

TT 1.5 Mon 10:30 HSZ 02

Low frequency noise in shadow evaporated Josephson junctions — •Jonathan Eroms, L.C. van Schaarenburg, E. Driessen, K. Huizinga, J.H. Plantenberg, R.N. Schouten, A.H. Verbruggen, C.J.P.M. Harmans, and J.E. Mooij — Kavli Institute of Nanoscience Delft, TU Delft, The Netherlands

Shadow angle evaporation is a convenient technique to fabricate submicron size tunnel junctions for various applications in mesoscopic physics. Particularly, many realizations of superconducting qubits, both in the charge and flux regime, are manufactured in this way. Now that external sources of decoherence are well understood and increasingly well controlled, the intrinsic limitations of the junction technology become more important. We therefore measured the low frequency resistance fluctuations of a number of small Josephson junctions fabricated in the same manner as our flux qubits. While the low-frequency noise has a $1/f$ spectral density and drops sharply from room temperature down to about 5 K, the low temperature behavior down to 300 mK is always dominated by a small number of strong two-level fluctuators, and the noise strength saturates between 1 K and 600 mK. The consequences for qubit decoherence are discussed.

TT 1.6 Mon 10:45 HSZ 02

From 0 to π coupled Josephson junctions — •Martin Weides[1], Hermann Kohlstedt[1,2], Edward Goldobin[3], Dieter Koelle[3], and Reinhold Kleiner[3] — [1]Institute for Solid State Research, Research Centre Juelich, Germany — [2]Department of Material Science and Department of Physics, University of Berkeley, USA — [3]Physikalisches Institut - Experimentalphysik II, Universität Tübingen

We report on the successful fabrication of low- T_C SINFS Josephson junctions with 0 to π coupling transition as a function of d_F. Diluted ferromagnetic $Ni_{60}Cu_{40}$ is used as F-interlayer. Our technology [1] enables us to fabricate high quality junctions with low parameter spread. We studied [2] the dependence of I_c and β_C on the thickness of ferromagnet and on temperature for both coupling regimes. The influence of magnetic dead layer is investigated.
High $I_c \simeq 5$ A/cm^2 and $V_c \simeq 20$ mV for the π coupled state [2] are measured. For T below 3K the π coupled SINFS junction gets underdamped, indicating a rather weak Cooper pair breaking in the ferromagnetic layer. At the 0-π boundary half-integer vortices (semifluxons) may spontaneously appear. They are pinned at the 0-π-boundary and may have two different polarities with flux $\Phi = \pm\Phi_0/2$. The semifluxon represents the ground state of the system and therefore is extremely stable [3].
A patterning process of 0-π coupled SIFS junctions for the investigation of semifluxons was worked out and first results will be shown.
[1] Weides et al., to appear in Physica C
[2] Weides et al., to be submitted.
[3] E. Goldobin et al., PRB 66 (2002), 67 (2003), 69 (2004)

TT 1.7 Mon 11:00 HSZ 02

Decay of metastable states in annular Josephson junctions in the presence of external magnetic field — •Abdufarrukh A. Abdumalikov, Astria Price, Alexander Kemp, and Alexey V. Ustinov — Physikalisches Institut III, UniversitätErlangen-Nürnberg, Erlangen, Germany

We investigate numerically and experimentally thermal activation processes in annular Josephson junctions of different length L. Junctions with and without a trapped vortex are studied. The numerical analysis is performed using the perturbed sine-Gordon model with a thermal noise term. For long junctions ($L \sim 10\lambda_J$), the dependence of the switching current histogram width on the magnetic field agrees with the theoretical analysis of Refs. [1,2] based on the collective coordinate approach. For shorter junctions we find deviations from the prediction of this analysis. Experimental results and numerical simulations show fairly good agreement.

[1] M. Fistul et al., Physica B **284-288**, 585 (2000)
[2] M. Fistul et al., Phys. Rev. Lett. **91**, 257004 (2003)

TT 2 Superconductivity: Conductor Development

Time: Monday 11:30–13:00 Room: HSZ 02

TT 2.1 Mon 11:30 HSZ 02

First technical applications for thin MgB_2 superconducting wires — •Wilfried Goldacker, Sonja Schlachter, Bing Liu, and Bernhard Obst — Forschungszentrum Karlsruhe , P.O.Box 3640, 76021 Karlsruhe

Although superconducting wires of MgB_2 are still in an early stage of development, a row of appliactions are already in the focus. Due to the request for very thin MgB_2 wires for the application in the satellite (current lead application) and the liquid hydrogene technology (level meter), thin MgB_2 monofilamentary wires with application specific properties, as low thermal conductivity or high mechanical strength were developed, and in the case of a saellite already applied. These thin wires with diameters down to 50 microns can be regarded as a finite element for the requested multifilamentary superconducting wires. We present results about transport critical current densities of optimized composites, the achieved thermal stabilisation of the conductor upon quench and the possibilities of mechanical reinforcements.

TT 2.2 Mon 11:45 HSZ 02

Transport Properties of Grains and Low Angle Grain Boundaries in $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ — •Christof Schneider, Alexander Weber, Stefan Hembacher, Christian Schiller, Arno Kampf, Thilo Kopp, and Jochen Mannhart — Lehrstuhl für Experimentalphysik VI, Institut für Physik, Universität Augsburg, D-86135 Augsburg

One possibility to optimize for cable applications the critical current density of $YBa_2Cu_3O_{7-\delta}$ is to partially substitute Y^{3+} by Ca^{2+}. To systematically investigate the effects of Ca-doping on the transport properties of low angle grain boundaries, we prepared a set of $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ ($0 \leq x \leq 0.3$) thin films on monocrystalline and bicrystalline $SrTiO_3$. Characteristic trends are revealed by the $J_c(B,T)$-dependencies. The dependencies are in part highly surprising as will be presented and discussed.

This work was supported by the DFG through the SFB 484, by the BMBF via project No. 13N6918A and by the THIOX project of the ESF.

TT 2.3 Mon 12:00 HSZ 02

Grain boundaries in REBaCuO (RE=Er,Y,Yb) Ca-doped YBaCuO thin films: Mechanisms of current suppression and current enhancement — •Christian Jooss[1], Karsten Guth[2], Yimei Zhu[3], and Felip Sandiumenge[4] — [1]Institute of Materials Physics, University of Goettingen, Germany — [2]EUPEC GmbH — [3]Brookhaven National Laboratory, Upton NY 11973, USA — [4]CSIC, Universitat Autonoma de Barcelona, Spain

Recent results on low-angle grain boundaries in high-temperature superconductors give fascinating insight into their interplay of atomic structure, electronic properties and transport properties [1,2]. It was shown that Ca doping can reduce atomic strain and the related size of space charge layers and therefore can significantly improve the transport properties in a wide angular range. However, our experimental data suggests that this mechanism does not work for all types of grain boundaries. Furthermore, we present experiments on ErBaCuO and YbBaCuO bicrystalline films, where charge balance arguments suggests an increased hole density in the electronic conduction bands and, in the framework of specific models, an increased critical current density. The different types of experiments will be summarized to determine the atomic mechanism determining the grain boundary transport properties. [1] R. F. Klie, J. P. Buban, M. Varela, A. Franceschetti, C. Jooss, Y. Zhu, N. D. Browning, S. T. Pantelides, S. J. Pennycook, Nature 435 (2005) 475. [2] M. A. Schofield, M. Beleggia, Y. Zhu, K. Guth, Ch. Jooss, Phys. Rev. Lett. 92 (2004) 195502

TT 2.4 Mon 12:15 HSZ 02

Growth of thick high critical current $YBa_2Cu_3O_7$ films with Y_2O_3 nano-inclusions by HLPE — •Judith MacManus-Driscoll and Ahmed Kursumovic — Department of Materials Science and Metallurgy, University of Cambridge, Cambridge CB2 3QZ, UK

Liquid-mediated growth of $YBa_2Cu_3O_7$ has the potential to be high rate and low cost. However, the reported critical current densities (J_c) are generally lower than for films deposited by physical vapor deposition processes. We report the deposition of thick high-J_c films (>1 $MAcm^{-2}$ in self-field in 3 micron thick films) on (001) $SrTiO_3$ by high-rate hybrid liquid phase epitaxy (HLPE). In brief, HLPE involves deposition of a thin liquid flux layer, followed by introduction of YBCO to the layer from a vapour or particulate source. The high Y supersaturation achieved in the BaO-CuO flux made nucleation and growth of coherent, nano-sized Y_2O_3 possible. These particles are an additional source of flux pinning, and can explain the enhanced J_c observed in the lower field regime compared to standard PLD samples. Angular-dependent transport critical current measurements as a function of applied field are presented, as well as microstructural measurements by transmission electron microscopy.

TT 2.5 Mon 12:30 HSZ 02

Development of coated conductors with an elongated grain structure — •R. Hühne, J. Eickemeyer, D. Selbmann, J. Hänisch, L. Schultz, and B. Holzapfel — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The critical current density in RABiTS based coated conductors is limited by the network of small angle grain boundaries up to a texture dependent crossover field. However, YBCO layers with high aspect ratio grains should enable a more effective current transport due to an improved weak link behaviour at the elongated grain boundaries. Recently, cube textured substrates with an elongated grain structure were successfully prepared by specific processing of nickel tapes microalloyed with silver. The aspect ratio of the grains in these tapes was increased from about one to about four. Additionally, epitaxial NiO layers were grown a first buffer on the Ni-Ag substrate using surface oxidation epitaxy (SOE) resulting in a similar texture quality like the tape itself. YBCO layers were prepared afterwards by pulsed laser deposition on the Ni as well as on the NiO using a suitable buffer system. Inductive measurements revealed critical temperatures above 87 K and critical current densities J_c up to 1.6 MA/cm^2 at 77 K in zero magnetic field. The anisotropic current transport mechanism was experimentally proven in resistive measurements showing higher J_c-values along the grain elongation compared to the transverse direction.

TT 2.6 Mon 12:45 HSZ 02

Reel to Reel MOCVD of YBCO and buffer layers on textured metal tapes — •Oliver Stadel[1], Sergej Samoilenkov[1], Jürgen Schmidt[1], Ruslan Muydinov[1], Hartmut Keune[1], Georg Wahl[1], Oleg Gorbenko[2], Oleg Melnikov[2], Igor Korsakov[2], and Andrey Kaul[2] — [1]Institute of Surface Technology (IOT), Technical University Braunschweig, Bienroder Weg 53, 38108 Braunschweig, Germany — [2]Department of Chemistry, Moscow State University V 234, Moscow 119 899, Russia

We report the deposition of YBCO and oxide buffer layers on textured Ni tapes. We developed a new MOCVD technique for the deposition of epitaxial oxides on textured metal tapes. The oxygen partial pressure is controlled, so no NiO formation can take place, while the oxide

buffer layer is stable. This enable us to coat the textured metal tape with conductive and isolating oxides. A RTR MOCVD-system was used to coat textured metal tapes with oxide buffer layers and YBCO layers. These YBCO films were in plane and out of plane textured with FWHM 5-6° and 1,5-3° respectively. Additional textured Ni-tapes, which were buffered and delivered from partners of the German Virtual Institute, were coated with YBCO (jc > 1 MA/cm2 at 77 K).

Acknowledgement The authors thank the partners of the Virtual Institute "Chemically deposited YBCO Superconductors". We acknowledge the financial support by the Ministry of Science and Culture of Lower Saxony and the European Community in frame of the ESF/EFRE project SuperConTech and the Helmholtz Gemeinschaft e.V..

TT 3 Correlated Electrons: Quantum-Critical Phenomena

Time: Monday 09:30–10:45 Room: HSZ 301

TT 3.1 Mon 09:30 HSZ 301

Smeared Ferromagnetic Quantum Phase Transition in $CePd_{1-x}Rh_x$ — •Tanja Westerkamp, Robert Küchler, Adam Pikul, Nubia Caroca-Canales, Micha Deppe, Philipp Gegenwart, Julian Sereni, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Quantum phase transitions in Ce-based systems are presently a subject of strong interest. While there exists a number of compounds showing an antiferromagnetic quantum critical point (QCP), appropriate candidates for the study of the disappearance of a ferromagnetic (FM) state are very scarce. Theories favor a first-order transition in pure systems, while disorder might lead to a continuous second order QCP. In this respect the alloy $CePd_{1-x}Rh_x$ might be interesting, because it evolves from a FM Ce^{3+} state at $x = 0$ to a non-magnetic, valence fluctuating state at $x = 1$. A detailed investigation of this system by means of ac-susceptibility and specific heat at $T \geq 0.4$ K as well as thermal expansion at $T \geq 0.1$ K suggests a continuous suppression of the FM order. However, $T_C(x)$ shows an extended tale and the Grüneisen-ratio analysis raises doubts on a well defined QCP. Here, we report ac-susceptibility measurements down to very low temperatures $T \geq 0.02$ K at concentrations in the tale region of the phase diagram which characterize the nature of the quantum phase transition in this system.

TT 3.2 Mon 09:45 HSZ 301

Hidden Quantum Critical Point in $CeCoIn_{5-x}Sn_x$ Studied by Thermal Expansion and Grüneisen Ratio Divergence — •G. Donath[1], R. Küchler[1], P. Gegenwart[1], E.D. Bauer[2], J.L. Sarrao[2], and F. Steglich[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico, 87545 USA

The heavy fermion superconductor $CeCoIn_{5-x}Sn_x$ has attracted much interest because of a magnetic field-induced quantum critical point at H_{QCP} that coincides with the upper critical field H_{c2} for unconventional superconductivity. Most remarkably, it is not possible to separate both phenomena from each other. By contrast, H_{QCP} is pinned to H_{c2} if superconductivity is weakened by Sn substitution [1].
We present low-temperature thermal expansion measurements, $\alpha(T, B)$, for the various concentrations, $x = 0, 0.03, 0.06, 0.09, 0.12, 0.18$, and compare them with the predictions of the spin-density-wave theory for an antiferromagnetic quantum critical point.
Furthermore, the effect of Sn subsitution on the Grüneisen ratio $\Gamma(T) \propto \alpha/C$ (C: specific heat) is discussed.
[1] E.D. Bauer *et al.*, Phys. Rev. Lett. **94**, 047001 (2005)

TT 3.3 Mon 10:00 HSZ 301

Metamagnetic quantum criticality in $Sr_3Ru_2O_7$ studied by thermal expansion — •P. Gegenwart[1], F. Weickert[1], M. Garst[2], R.S. Perry[3,4,5], and Y. Maeno[4,5] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Theoretical Physics Institute, University of Minnesota, USA — [3]School of Physics and Astronomy, University of St. Andrews, Fife KY16 9SS, Scotland — [4]International Innovation Center, Kyoto University, Japan — [5]Department of Physics, Kyoto University, Japan

We report low-temperature thermal expansion measurements on the bilayer ruthenate $Sr_3Ru_2O_7$ as a function of magnetic field applied perpendicular to the Ruthenium-oxide planes. The field-dependence of the c-axis expansion coefficient indicates the accumulation of entropy close to 8 Tesla, related to an underlying quantum critical point. The latter is masked by two first-order metamagnetic transitions which bound a regime of enhanced entropy. Outside this region the singular thermal expansion behavior is compatible with the predictions for a two-dimensional metamagnetic quantum critical end point (work available at cond-mat/0507359).

Helpful discussions with S.A. Grigera, A.P. Mackenzie, A. Rosch and P. Wölfle are gratefully acknowledged. P.G. thanks the Deutsche Forschungsgemeinschaft (DFG grant GE 1640/1-1) and Royal Society (UK) for support of his stay at the St. Andrews University, M.G. is supported by DFG grant GA 1072/1-1.

TT 3.4 Mon 10:15 HSZ 301

Field-Induced Phase Transition in a Metalorganic Spin-Dimer System — •Y. Tsui[1], A. Brühl[1], K. Removic-Langer[1], V. Pashchenko[1], B. Wolf[1], M. Lang[1], G. Donath[2], A. Pikul[2], T. Kretz[3], H.-W. Lerner[3], M. Wagner[3], A. Salguero[4], T. Saha-Dasgupta[4], B. Rahaman[4], and R. Valenti[4] — [1]Physikalisches Institut, J.W. Goethe-Universität, Frankfurt, FOR-412, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Institut für Anorganische Chemie, J.W. Goethe-Universität, Frankfurt, FOR-412, Germany — [4]Institut für Theoretische Physik, J.W. Goethe-Universität, Frankfurt, FOR-412, Germany

We have investigated the field-induced magnetic order in a three-dimensional metalorganic spin-dimer system, $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91). The nature of the dimers and their couplings have been identified by first principles Density Functional Theory calculations. We have performed electron spin resonance, magnetic susceptibility, specific heat and thermal expansion measurements on both powder and single-crystal samples, in applied magnetic fields up to $12T$ and at temperatures down to $\sim 0.1K$. Clear indications of a field-induced phase transition have been observed when the applied magnet field is above a temperature-dependent critical field $B_c(T) \sim 3T$. A similar field-induced phase transition was also observed in an inorganic compound $TlCuCl_3$. In case of $TlCuCl_3$, the phase transition was interpreted as the Bose-Einstein condensation (BEC) of magnons. We propose TK91 as another possible model system to study the BEC of magnons.

TT 3.5 Mon 10:30 HSZ 301

Kondo lattice model with finite temperature Lanczos method — •Ivica Zerec, Burkhard Schmidt, and Peter Thalmeier — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden

The full Kondo lattice model (KLM) including localized spins and itinerant electrons is considered on finite size clusters using finite temperature Lanczos method (FTLM). The method is numerically exact for the finite size clusters. The study is focused on the weak coupling limit, where the competition between the RKKY interaction and the Kondo screening is analyzed by means of correlation functions and thermodynamic properties. Special attention is devoted to the finite size effects, which are important in that limit. From the analysis of the cluster calculations we derive a phase diagram in the T-J_K plane, where J_K is the coupling of local and conduction electron spins. It is compared to the phase diagram for the KLM without charge degrees of freedom and the Doniach phase diagram.

TT 4 Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Monday 11:00–13:00 Room: HSZ 301

Invited Talk

TT 4.1 Mon 11:00 HSZ 301

Current vs. Correlations: The Nonequilibrium Kondo Model — •Stefan Kehrein — LMU München, Department für Physik

Quantum dot experiments show new aspects of electron correlation physics that are inaccessible in bulk materials. One example is the realization of out-of-equilibrium situations far beyond the linear response regime. Such quantum many-body systems far away from equilibrium are theoretically not well-understood and are beginning to emerge as an exciting new frontier in quantum many-body physics. In this talk we examine the Kondo model as a paradigm for correlated impurity physics. While its equilibrium ground state with Kondo screening due to the formation of a many-body bound state is well-understood, much less is known about the steady state that develops when a constant voltage bias is applied across the impurity. In particular, the coherent Kondo screening processes turn out to be in competition with current-induced decoherence, and this competition determines the phase diagram of the nonequilibrium Kondo model. We will discuss various physical observables like the dynamic and static spin susceptibility and the T-matrix to get insights into this nonequilibrium steady state and to compare it with finite temperature equilibrium states. We will also see how the method of infinitesimal unitary transformations (flow equation method) serves as a suitable generalization of scaling concepts to such nonequilibrium situations [1].

[1] S. Kehrein, Phys. Rev. Lett. **95**, 056602 (2005)

TT 4.2 Mon 11:30 HSZ 301

Real Time RG for the non-equilibrium Kondo model: Cutoffs set by voltage and decoherence. — •Thomas Korb[1], Herbert Schoeller[1], and Jürgen König[2] — [1]Theoretische Physik A, RWTH Aachen, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum

While the equilibrium Kondo effect is well understood there is known less for the Kondo effect in non-equilibrium. The question was raised, if a finite voltage and current induced decoherence prevents the system from going into the strong coupling limit for $V > T_K$ and how to calculate the I-V [1,2]. In [2] a perturbative RG for the scaling of the verticies in non-equilibrium was developed, but the decoherence was included only on the basis of a perturbation calculation. A different approach was used in [3], where a flow equation analysis was performed on the expense to reside on a Hamiltonian description for the non-equilibrium. There it was found, that the scaling is cutted by balancing of second and third order contributions in the flow equations. We use the real time RG formalism developed in [4] to analyze the non-equilibrium Kondo effect. It is demonstrated how the cutoffs set by voltage and decoherence rate emerge naturally from a closed set of RG equations on the Keldysh contour (including dephasing of nondiagonal elements of the density matrix). Therefore we are able to calculate the I-V characteristic for $V > T_K$ within one scheme and within a full nonequilibrium formalism.

[1] P. Coleman *et al.*, Phys. Rev. Lett. 86, 4088 (2001).
[2] A. Rosch *et al.*, Phys. Rev. Lett. 90, 076804 (2003).
[3] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005).
[4] H. Schoeller and J. König, Phys. Rev. Lett. 84, 3686 (2000).

TT 4.3 Mon 11:45 HSZ 301

Transmission phase through a two-level quantum dot — •Theresa Hecht[1], Yuval Oreg[2], and Jan von Delft[1] — [1]Department für Physik, CeNS and Arnold Sommerfeld Center, Ludwig-Maximilians Universität München, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel

The recent measurements of Schuster *et al.* [1] of the transmission phase through a quantum dot embedded in one arm of an Aharonov Bohm interferometer contradict the simple models that were used to describe the phase evolution so far, see e.g. [2]. Inspired by this experiment, we study the transmission phase of a quantum dot embedded in one arm of a two path electron interferometer. Following [3], where it was shown that in a two-level quantum dot the generic and experimentally realistic condition $\Gamma_{upper} \neq \Gamma_{lower}$ always leads to an occupation inversion, $n_{upper} > n_{lower}$, we study a two-level Anderson model by means of Wilson's numerical renormalization group method. Relating the scattering phase and the occupation of the levels at $T = 0$ using the Friedel sum rule, we can explain that for $\Gamma_{upper} \neq \Gamma_{lower}$, the transmission always experiences a phase lapse of π as a function of gate voltage, independent of the parameters of the quantum dot or the parity of the levels. We investigate both the temperature and magnetic field dependence of the transmission amplitude through the dot.

[1] R. Schuster, E. Buks, M. Heiblum, D. Mahalu, V. Umansky, H. Shtrikman, Nature **385**, 417 (1997).
[2] U. Gerland *et al.*, Phys.Rev.Lett. **84**, 3710 (2000).
[3] M. Sindel, A. Silva, Y. Oreg, J.von Delft, PRB **72**, 125316 (2005).

TT 4.4 Mon 12:00 HSZ 301

Signatures of orbital two channel Kondo in the conductance of metallic nanowires? — •Procolo Lucignano[1], Giuseppe E. Santoro[1,2], Michele Fabrizio[1,2], and Erio Tosatti[1,2] — [1]SISSA and INFM Democritos National Simulation Center, Via Beirut 2-4, 34014 Trieste, Italy — [2]International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

We describe the transport properties of metallic nanowires by using a realistic generalization of the two level system kondo model[1]. The problem is attached by using numerical renormalization group method[2] and its results analyzed in the framework of conformal field theory[3]. Fractional values of the conductance have been observed in recent experiments. We show that for particular choices of the parameters, such fractional conductances can appear as a signature of a two channel kondo phase, for a reasonable window of temperatures[4].

[1] K. Vladar, A. Zawadowski, Phys. Rev. B **28** 1564 (1983).
[2] K. Wilson Rev. Mod. Phys. **47**, 773 (1975).
[3] I. Affleck, A. W. W. Ludwig, Nucl. Phys. B **352**, 849 (1991).
[4] P. Lucignano, G.E. Santoro, M. Fabrizio, E. Tosatti in preparation.

TT 4.5 Mon 12:15 HSZ 301

DMRG meets NRG — •Andreas Weichselbaum[1], Frank Verstraete[2], Ulrich Schollwöck[3], J. I. Cirac[4], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, 80333 München, Germany — [2]Institute for Quantum Information, Caltech, Pasadena, US. — [3]Institut für Theoretische Physik C, RWTH-Aachen, D-52056 Aachen, Germany — [4]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, D-85748, Germany

We present a unified framework of renormalization group methods, including Wilson's numerical renormalization group (NRG) and White's density-matrix renormalization group (DMRG), within the language of matrix product states. This allows to improve over Wilson's NRG for quantum impurity models by a variational method optimal in this framework. We illustrate it for the single-impurity Anderson model; moreover we use a variational method for evaluating Green's functions. The proposed method is more flexible in its description of off-resonance spectral properties, opening the way to time-dependent, out-of-equilibrium impurity problems. It also substantially improves computational efficiency for one-channel impurity problems, suggesting *linear* scaling of complexity for n-channel problems.

TT 4.6 Mon 12:30 HSZ 301

Local moments formation in a t–J chain with an integrable impurity — •Guillaume Palacios and Holger Frahm — Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany

We consider an integrable model describing an Anderson-like impurity coupled to an open t–J chain. Both the hybridization (coupling between the bulk chain and the impurity) and the local spectrum can be controlled without breaking the integrability of the model.

In the strong hybridization limit, we show the appearance of boundary bound states in the energy spectrum which, as a function of the parameters, permits us to distinguish four phases, from zero to three bound states. We then compute the contribution of these bound states to the response of the system to a) a uniform magnetic field and b) a local field at the impurity site. The results obtained by means of Bethe Ansatz techniques and finite size analysis allow to make contact with the physics of local moments and the Kondo effect. Results for the impurity compressibility are also presented.

TT 4.7 Mon 12:45 HSZ 301

Two-stage Kondo effect in a spin-1 quantum dot. — •Babak Bayani[1], Piers Coleman[2], and Anna Posazhennikova[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Wolfgang-Gaede-Str.1, D-76128 Karlsruhe — [2]Center for Materials Theory, Rutgers University, Piscataway, NJ 08855, USA

We study the transport through a quntum dot (QD) with spin-1, connected to metallic leads. In practice a spin-1 QD is expected to undergo a two-stage Kondo effect, with a large temperature region, dominated by the underscreened Kondo physics. At zero temperature conductance of such a dot vanish due to interference effects of two channels. We show how this behaviour arises in the detalied many-body calculation, based on the Schwinger boson description of the spin on the dot.

TT 5 Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts - Part 1

Time: Monday 09:30–13:00 Room: HSZ 304

Invited Talk TT 5.1 Mon 09:30 HSZ 304

Correlation effects on electronic transport through dots and wires — •Volker Meden — Institut für Theoretische Physik, Universität Göttingen

We investigate how two-particle interactions affect the electronic transport trough several meso- and nanoscopic systems made of two building blocks: quasi one-dimensional quantum wires of interacting electrons and quantum dots with local Coulomb correlations. A recently developed functional renormalization group scheme is used that includes the essential aspects of Tomonaga-Luttinger liquid physics (one-dimensional wires) as well as of the physics of local correlations, with the Kondo effect being an important example. We describe the appearance of a variety of surprising correlation effects. (1) For a Y-junction of wires pierced by a magnetic flux we find a regime in which correlations restore time-reversal symmetry. (2) We investigate the interplay of Tomonaga-Luttinger physics and the Kondo effect in transport through a single site dot with interacting leads. Studied separately, the first leads to a sharp Lorentz-like resonance in the gate voltage dependence of the linear conductance while the latter implies a broad plateau-like resonance. (3) We find a pair of novel correlation induced resonances in the gate voltage dependence of the linear conductance through a parallel double-dot systems that results from the interplay of correlations and quantum interference. It should be observable in experiments on the basis of presently existing double-dot setups. An outlook on future application of the functional renormalization group scheme in mesoscopic physics is given.

TT 5.2 Mon 10:00 HSZ 304

Two-electron entanglement in double quantum dots with Coulomb and spin-orbit interaction — •S. Weiss, M. Thorwart, and R. Egger — Heinrich-Heine Universität Düsseldorf

We investigate the entanglement of two-particle electronic charge states in vertical double quantum dots in presence of the Coulomb and spin-orbit interaction. Upon using exact diagonalization, the spectrum and the eigenvectors of the Hamiltonian are obtained as a function of all the model parameters. The entanglement is quantified in terms of the Peres-Horodecki measure which follows immediately from the density operator of the system. Interestingly enough, we find a non-monotonous dependence of the entanglement on the Coulomb interaction strength. Depending on the tunneling amplitude between the two dots, we even find a suppression of the entanglement for large Coulomb interaction and for intermediate tunneling couplings. This counterintuitive behavior can be explained by the confinement of the electrons in the dots.

[1] S.Weiss, M. Thorwart and R. Egger, submitted.

TT 5.3 Mon 10:15 HSZ 304

Cotunneling and renormalization effects in the thermopower of a single-electron transistor — •Björn Kubala and Jürgen König — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We study thermal conductance and thermopower of a metallic single-electron transistor (SET) within a perturbative real-time theory. Like the conductance, the thermal conductance of an SET is governed by Coulomb blockade physics at low temperatures. The (Coulomb-) oscillations of thermopower with varying gate voltage have been studied, considering sequential [1] and cotunneling [2] processes.

We investigate thermopower by performing a systematic perturbative calculation of the (thermal) conductance including sequential tunneling and cotunneling as well as terms capturing the renormalization of system parameters by quantum fluctuations. As thermopower constitutes a direct measure of the average energy of transported particles, we predict, that the logarithmic reduction of the Coulomb blockade gap due to a multi-channel Kondo-effect can be accessed in thermopower measurements.

[1] A. A. M. Staring, L. W. Molenkamp, B. W. Alphenhaar, H. van Houten, O. J. A. Buyk, M. A. A. Mabesoone, C. W. J. Beenakker, and C. T. Foxon, Europhys. Lett. 22, **57** (1993).
[2] M. Turek and K. A. Matveev, Phys. Rev. B **65**, 115332 (2002).

TT 5.4 Mon 10:30 HSZ 304

Aharonov-Bohm Interferometry with Quantum Dots — •Stefan Legel[1], Jürgen König[2], and Gerd Schön[1,3] — [1]Universität Karlsruhe — [2]Ruhr-Universität Bochum — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie

We study electron transport through a closed Aharonov-Bohm interferometer containing two single-level quantum dots. We address the question how Coulomb interaction on the dots affects the coherence of the transport. The method of real-time transport theory enables us to treat these systems both in equilibrium as well as in non-equilibrium. A perturbation expansion in the coupling strength of the quantum dots to the leads allows us to make predictions for the signatures of quantum interference in the conductance of the considered systems in first and second order (so-called cotunneling) in the coupling strength.

TT 5.5 Mon 10:45 HSZ 304

Non-local effects in transport through coupled quantum dots — •Jasmin Aghassi[1,2], Axel Thielmann[1,2], Matthias Hettler[1], and Gerd Schön[1,2] — [1]Forschungszentrum Karlsruhe, INT, Postfach 3640, 76021 Karlsruhe — [2]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

We study current and shot noise in sequential tunneling through non-local systems such as two and three coupled quantum dots ("artificial molecules"). The dots are fully coherent among each other and weakly coupled to the electrodes via the interfacial dots. In the case of two coupled quantum dots various sources of asymmetry, i.e. non-resonant dots or asymmetric couplings lead eventually to super-Poissonian noise and negative differential counductance above the sequential tunneling threshold. In contrast, the three dot system displays interesting super-Poissonian behavior even in fully symmetric situations due to a complex spin-related mechanism. Fano factors may thus be largely enhanced up to values of 100. Such strong enhancement should allow direct experimental detection of shot noise in lateral quantum dot experiments. Within our diagrammatic approach we further discuss the influence of cotunneling processes on the transport characteristics in these non-local systems.

[1] J. Aghassi, A. Thielmann, M.H. Hettler, and G. Schön, cond-mat/0505345

TT 5.6 Mon 11:00 HSZ 304

Electron pumping in periodic fields — •Stefan Kurth[1], Angel Rubio[2], and E.K.U. Gross[1] — [1]Institute for Theoretical Physics, Free University Berlin, Berlin, Germany — [2]Donostia International Physics Center, San Sebastian/Donostia, Spain

Using our recently developed algorithm for the time-dependent description of transport(Phys. Rev. B **72**,035308 (2005)) we study pumping of electrons between two reservoirs at the same chemical potential. Pumping is achieved by applying a spatially inhomogeneous perturbation which is periodic in time. The flexibility of the algorithm, which is based on the time evolution of the Schrödinger equation, allows us to study pumping in the linear and nonlinear, adiabatic and non-adiabatic regimes. For perturbations with the shape of a travelling wave, electrons are transferred in packets moving with the minima of the wave.

— 15 min. break —

TT 5.7 Mon 11:30 HSZ 304

Adiabatic Pumping through Interacting Quantum Dots — •Janine Splettstoesser[1,2], Michele Governale[1,2], Jürgen König[2], and Rosario Fazio[1] — [1]Scuola Normale Superiore, Piazza dei Cavalieri, I-56126 Pisa — [2]Institut für Theoretische Physik, Ruhr-Universität Bochum, D-44780 Bochum

By periodically changing in time some parameters of a conductor a DC current can be produced without applying a bias voltage. This effect is known as *pumping*. In case of non-interacting electrons Brouwer's formula provides a general framework for the computation of the pumped charge [1]. The situation is profoundly different for pumping through interacting systems. In fact, there are only few works that address this problem with methods suited to tackle specific systems/regimes. We present a general formalism to study adiabatic pumping through interacting quantum dots. We derive a formula that relates the pumped charge to the local, instantaneous Green's function of the dot. This formula is then applied to the infinite-U Anderson model both for weak and strong tunnel-coupling strengths [2].

[1] P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).
[2] J. Splettstoesser, M. Governale, J. König, R.Fazio, cond-mat/0506080 (2005), to be published in PRL.

TT 5.8 Mon 11:45 HSZ 304

Non-adiabatic electron pumping: Maximal current with minimal noise — •Sigmund Kohler, Michael Strass, and Peter Hänggi — Institut für Physik, Universität Augsburg, 89135 Augsburg

The noise properties of pump currents through an open double quantum dot setup with non-adiabatic ac driving are investigated. Driving frequencies close to the internal resonances of the double-dot system mark the optimal working points at which the pump current assumes a maximum while its noise power exhibits a remarkably low minimum. Within a rotating-wave approximation, we derive for the current and its noise power analytical expressions, which allow to optimize the pump. For an inter-dot tunneling larger than the coupling between the dots and the electrodes, we find that the current noise is significantly below the shot noise level [1]. The analytical results are compared against numerically exact results from a Floquet transport theory [2]. The role of electron-electron interactions is studied within a master equation formalism.

[1] M. Strass, P. Hänggi, S. Kohler, Phys. Rev. Lett. **95**, 130601 (2005).
[2] S. Kohler, J. Lehmann, P. Hänggi, Phys. Rep. **406**, 379 (2005).

TT 5.9 Mon 12:00 HSZ 304

Coulomb blockade (CB) and Andreev reflection (AR) in a series of two quantum-point contacts (QPCs) — •Ursula Schröter, Olivier Schecker, and Elke Scheer — FB Physik, Universität Konstanz, 78457 Konstanz

Merging a Green's functions method and a rate equation technique we developed a model to calculate current-voltage characteristics (IVs) of a series of two QPCs in the normal and the superconducting state. Between the two junctions is a bulk-like metallic island of, however, such small capacitance that the potential shifts considerably with each single excess charge. Our method is valid for arbitrary transmissions of the transport channels in both contacts and multiple AR are included. Interaction between transport processes in both junctions is assumed via the island charging only, but our approach allows extension to maintaining coherence over the whole system.

Based on wave-function overlaps our calculations for QPCs predict qualitatively different behavior from models relying purely on energy conservation and typically used to describe tunnel diodes, even in the low transmission regime. Different conditions have to be fulfilled for particular transport processes to occur. These multiple conditions involve the island charging energy and, in the superconducting state, the gap of the material. Steps in the IVs can be explained in an intuitive energy-level picture. Furthermore we find that multiple AR in the first junction are not necessarily suppressed due to CB by the presence of a second junction of low transmission.

TT 5.10 Mon 12:15 HSZ 304

Transport of interacting electrons through quantum point contacts — •Andreas Lassl, Peter Schlagheck, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

We investigate the influence of interaction effects on the electronic transport properties of two-dimensional nanostructures. For our numerical studies we use a self-consistent iteration scheme based on the nonequilibrium Green function formalism. This allows us to include electron-electron interactions on the level of a mean-field description for the spin-dependent conductance. For transport through point contacts we show how short-range interactions can cause an asymmetry in the transmission of different spin directions leading to anomalous conductance steps which resemble the so-called "0.7 anomaly"[1].

[1] K.J. Thomas, J.T. Nicholls, M.Y. Simmons, M. Pepper, D.R. Mace, D.A. Ritchie, Phys. Rev. Lett. **77**, 135 (1996)

TT 5.11 Mon 12:30 HSZ 304

Transport through Interacting Quantum Wires with Impurities: Influence of Tunneling Barriers on Power Laws. — •Severin Jakobs[1], Tilman Enss[2], Volker Meden[3], and Herbert Schoeller[1] — [1]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Germany — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [3]Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen, Germany

We theoretically analyze the conductance through an interacting quantum wire with impurities, and its dependence on temperature and voltage. The wire is modelled by a tight-binding-chain including nearest neighbour interaction. For calculating the transport properties, we use a functional renormalization group method recently developed for the analysis of linear transport through quantum wires [1], and a generalization of this technique to nonlinear transport. We find that the power laws predicted by bosonization for the current vs. temperature or the current vs. voltage [2] are eliminated if tunneling barriers separate the wire from the leads. This behaviour can be traced back to the scaling of the height and width of the single peaks of transmission.

[1] V.Meden et al., Phys.Rev.B **65**, 045318 (2002)
[2] C.L.Kane, M.P.A.Fisher, Phys.Rev.B **46**, 15233 (1992)

TT 5.12 Mon 12:45 HSZ 304

Photo-assisted transport in the Luttinger Liquid with weak disorder — •Dmitry Bagrets — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128, Karlsruhe, Germany

We consider a photo-assisted transport through a one-dimensional interacting wire (Luttinger Liquid) with a weak disorder. The photo-assisted conductance, current shot noise and generally the full counting statistics (FCS) of charge transfer are evaluated under the presence of alternating bias voltage of the form $V(t) = V_{dc} + V_{ac}\cos(\Omega t)$, Ω being a driven frequency. The Coulomb interaction is treated exactly, while the backscattering due to impurities is considered in the second order Born approximation. The FCS of backscattering current is a bidirectional Poissonian process. In the limit of large Ω and dc applied voltage V_{dc} as compared to the Thouless energy of the wire the differential conductance and photo-assisted shot noise exhibit a series of power low singularities of the form $\sim |n\Omega - eV_{dc}|^{g-1}$ as a function of dc voltage, where $g < 1$ is the interaction constant in the wire. The experimental verification of this phenomenon is feasible in the 10-20 GHz range of Ω with the use of V-groove and cleaved edge overgrowth GaAs nanowires.

TT 6 Solids At Low Temperature: Amorphous and Tunnel Systems, Glasses, ...

Time: Monday 10:30–13:00 Room: HSZ 105

Keynote Talk TT 6.1 Mon 10:30 HSZ 105

Nuclear quadrupoles and magnetic-field effects in amorphous solids — •Alois Würger — CPMOH, CNRS - Université Bordeaux 1, 351 cours der la Libération, 33405 Talence, France

In recent years, the low-temperature dielectric properties of various insulating glasses (silica based materials, glycerol, mixed crystals) have been shown to depend on an applied magnetic field B [1]. The amplitude of dielectric echoes of tunnel systems oscillates with B, with a period of about 20 milliTesla, and attains the maximum value above 1 Tesla. At temperatures below 1 Kelvin, both the real and imaginary parts of the dielectric function vary with the magnetic field.

These findings are not accounted for by standard theory for diamagnetic and insulating solids. Several models have been proposed that are

based on the Aharanov-Bohm phase of atoms on circular trajectories, or on nuclear spins [2]. We show that experiments clearly speak in favor of the latter, and point out the crucial role of nuclear quadrupole moments.

In particular, we discuss the magnetic-field dependence of the dielectric function. There is strong evidence that it arises from Debye relaxation.

[1] P. Strehlow et al., PRL 84, 1938 (2000); S. Ludwig et al., PRL 88, 075501 (2002); C. Enss and S. Ludwig, PRL 89, 075501 (2002); R. Haueisen and G. Weiss, Physica B 316, 555 (2004); P. Nagel et al., PRL 92, 245511 (2004);

[2] S. Kettemann, P. Fulde, P. Strehlow, PRL 83, 4325 (1999); A. Würger, PRL 88, 075502 (2002); A. Würger, A. Fleischmann, C. Enss, PRL 89, 237601 (2002)

TT 6.2 Mon 11:00 HSZ 105

Investigating the microscopic nature of tunnelling processes in amorphous glycerol — •Masoomeh Bazrafshan[1], Marek Bartkowiak[1], Herbert Zimmermann[2], Andreas Fleischmann[1], and Christian Enss[1] — [1]a) Kichhoff-Institut fuer Physik, Universitaet Heidelberg, Germany — [2]b) Max-Planck-Institut fuer medizinische Forschung, Heidelberg, Germany

At temperatures below a few kelvin the properties of amorphous solids are dominated by atomic tunnelling systems. Over the past few years it was shown that the unexpected magnetic field effects, observed in many non-magnetic multicomponent glasses, originate from a coupling of the tunnelling motion to nuclear quadrupole moments present in the system. In dielectric polarisation echo experiments a strong magnetic field dependence of the echo amplitude as well as a periodic modulation of the echo decay, the so-called quantum beating, can be observed. The frequency of the quantum beating corresponds to the energy splitting of the quadrupole levels.

In this work we present dielectric echo measurements on partially deuterated glycerol, a system wich allows to introduce nuclear quadrupoles at specific sites of the molecule. By comparison with numerical calculations of the transition amplitudes we are able to suggest possible microscopic scenarios for tunnelling processes in amorphous glycerol. We believe that this work will provide important input for the development of a microscopic theory of glasses.

TT 6.3 Mon 11:15 HSZ 105

Low temperature breakdown of coherent tunneling in amorphous solids by the nuclear quadrupole interaction — •Alexander Burin[1], Peter Fulde[2], and Ilya Polishchuk[3] — [1]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA — [2]Max-Planck-Institut fur Physik Komplexer Systeme, D-01187*Dresden, Germany — [3]RRC Kurchatov Institute, Kurchatov Sq. 1, 123182 Moscow, Russia

We consider the effect of the internal nuclear quadrupole interaction on quantum tunneling of complex multi-atomic two-level systems. Two distinct regimes of strong and weak interactions are found. They depend on the relationship between the characteristic energy of the internal interaction λ_*, which is directly proportional to the number of tunneling atoms per tunneling system, and a bare tunneling coupling strength Δ_0. When $\Delta_0 > \lambda_*$, the internal interaction is negligible and tunneling remains coherent, being defined by the strength of Δ_0. When $\Delta_0 < \lambda_*$, coherent tunneling breaks down and the effective tunneling amplitude decreases by an exponentially small overlap factor $\eta^* \ll 1$ between the internal ground states of the left and right well, affecting thermal and kinetic properties of tunneling systems. The theory is applied to interpret the anomalous behavior of the resonant dielectric susceptibility in amorphous solids for $T \leq 5mK$ in terms of the nuclear quadrupole interaction. We suggest clarifying experiments using external magnetic fields to test the theories predictions and to shed some light on the internal structure of tunneling systems in amorphous solids.

TT 6.4 Mon 11:30 HSZ 105

Effect of Nuclear Quadrupole Interaction on the Relaxation in Amorphous Solids — •Ilya Polishchuk — Kurchatov Institute, 123182 Moscow, Russia

Recently it has been experimentally demonstrated that certain glasses display an unexpected magnetic field dependence of the dielectric constant. In particular, the echo technique experiments have shown that the echo amplitude depends on the magnetic field. The analysis of these experiments results in the conclusion that the effect seems to be related to the nuclear degrees of freedom of tunneling systems. The interactions of a nuclear quadrupole electrical moment with the crystal field and of a nuclear magnetic moment with magnetic field transform the two-level tunneling systems inherent in amorphous dielectrics into many-level tunneling systems. The fact that these features show up at temperatures T ¡ 100mK, where the properties of amorphous materials are governed by the long-range dipole - dipole interaction between tunneling systems, suggests that this interaction is responsible for the magnetic field dependent relaxation. We have developed a theory of many-body relaxation in an ensemble of interacting many-level tunneling systems and show that the relaxation rate is controlled by the magnetic field. The results obtained correlate with the available experimental data. Our approach strongly supports the idea that the nuclear quadrupole interaction is just the key for understanding the unusual behavior of glasses in a magnetic field.

TT 6.5 Mon 11:45 HSZ 105

The Mystery of Quantitative Universality - Resolved? — •Reimer Kühn — King's College London, UK

We present a simple explanation of the mysterious so-called quantitative universality of glassy low-temperature physics in terms of solutions of microscopic glass-models obtained earlier.

TT 6.6 Mon 12:00 HSZ 105

Thermal Conductivity of Glasses and the "Boson Peak" — •Walter Schirmacher — Technische Universität München, Phys. Dept. E13, D-85747 Garching

A theory for the anomalous vibrational and thermal properties of disordered solids based on the model assumption of randomly fluctuating transverse elastic constants is presented. Mean-field expressions for the vibrational density of states and the energy diffusivity are derived with field theoretical techniques. As in previous approaches of this type the boson peak (enhancement of the low-frequency density of states) is explained as a result of the frozen-in disorder and compares well with the experimental findings. The plateau in the temperature variation of the thermal conductivity and the behavior beyond the plateau is shown to arise from the enhanced scattering in the boson peak regime and to be essentially a harmonic phenomenon.

TT 6.7 Mon 12:15 HSZ 105

Properties of transition-metal nanoclusters on biological substrates — •T. Herrmannsdörfer[1], A. D. Bianchi[1], T. P. Papageorgiou[1], F. Pobell[1], J. Wosnitza[1], S. Selenska-Pobell[2], K. Pollmann[2], M. Merroun[2], and J. Raff[2] — [1]Institut Hochfeld-Magnetlabor Dresden (HLD) and — [2]Institut für Radiochemie, Forschungszentrum Rossendorf, P.O.-Box 51 01 19, D-01314 Dresden, Germany

Micro- and nanogranular materials can reveal strongly altered properties compared to their bulk counterparts. In particular, their magnetic and superconducting behaviour can be drastically changed. We have investigated transition-metal clusters with a well defined size of 1 to 1.5nm which are isolated and separated from each other. These metal nanoclusters have been deposited on a regular square lattice of a biological template. In more detail, this template is a purified self-assembling paracrystalline surface layer (S-layer) of *Bacillus sphaericus* JG-A12 which exhibits square symmetry and is composed of identical protein monomers. These S-layer proteins are capable of selective and reversible binding of high amounts of metals, making the metallic nanocluster covered S-layer also interesting for technological applications. The transition-metal nanoclusters were investigated using EXAFS spectroscopy and SQUID magnetometry. The magnetization of Pd and Pt nanoclusters at $0 \leq B \leq 7$ T and 1.8 K $\leq T \leq 350$ K reveal interesting magnetic properties. The Stoner enhancement factor of the d conduction-electron susceptibility of the nanoclusters is clearly reduced compared to the one of the bulk transition metals.

TT 6.8 Mon 12:30 HSZ 105

Thermal conductivity of suspended silicon nanowire at low temperature — •Olivier Bourgeois, Thierry Fournier, and Jacques Chaussy — CRTBT-CNRS, laboratoire associé à l'UJF et à l'INPG, 25 avenue des Martyrs, BP 166, 38042 Grenoble, Cedex 9, France

We report sensitive thermal conductivity measurement (down to few femtoW/K) at low temperature by means of the 3ω method of silicon suspended nanowires. The silicon nanowires have a square shape cross sections and are made by e-beam lithography. They are suspended between two electrically isolated pads, and hence thermally isolated from the heat bath. A thin film of niobium nitride, a highly resistive thermometric element, is deposited on top of the wire in order to measure the thermal

conductivity using the 3ω method. The geometry of the nanowire section is designed to match the order of magnitude of the dominant phonon wave length in silicon at low temperature which is expected to be of the order of 100 nm at 1K. The width of the nanowires varies between 100 nm and 200 nm for a thickness 130 nm and a length ranging from 5μm to 10 μm. The mean free path of the phonons is much larger than the length of the wire, hence these nanowires can be considered as ballistic quasi 1D thermal conductors at sufficientlt low temperature. Under these conditions, the thermal conductivity of the Si nanowire is expected to be strongly influenced by the reduced dimensions. Below 0.9K a clear deviation from the classical cubic law is observed in the 200nm wide wires which is associated to the universal behavior of the thermal conductance.

TT 6.9 Mon 12:45 HSZ 105

Low-temperature investigation of phase transition in $SrTiO_3$ (001) single-crystal plate — •Alexander A. Levin, Dirk. C. Meyer, and Peter Paufler — Institut für Strukturphysik, TU Dresden

A (001) $SrTiO_3$ single-crystal plate is investigated in a temperature range 300 K...25 K by means of wide-angle X-ray scattering (WAXS) under vacuum conditions. Depending on the quality of surface preparation, the plates exhibited different structural characteristics and low-temperature phase-transition and domain behaviour.

At the polished surface of the single-crystal plate, in a cooling cycle a cubic (C-phase, space group Pm-3m) - tetragonal (T-phase, space group I4/mcm) phase transformation is recorded at a temperature of approx. 107.5 K close to the known C-T-phase transition temperature of bulk $SrTiO_3$ (105 K - 108 K). When cooling, the formation of domains of T-phase with different orientation ([110] and [001]) was observed starting from a temperature of 80 K. The volume fraction of the orientation domains mentioned above changed step-wise with decrease of temperature.

The non-polished surface remained in a single-domain state down to a temperature of 25 K. Considerable decrease of the profile parameters of the X-ray reflection of non-distorted cubic phase were recorded below a temperature of about 90 K referred to C-T phase transition. The lowering the temperature of C-T transition can be attributed to non-bulk plate constraint conditions and coexistence of ideal perovskite and distorted regions in the non-polished side of the plate.

This work is supported by DFG, FOR 520.

TT 7 Superconductivity & Solids At Low Temperature - Poster Session

Time: Monday 14:00–17:45 Room: P1

TT 7.1 Mon 14:00 P1

SupraTrans - a superconductively levitated transport system — •Christoph Beyer, Oliver de Haas, and Ludwig Schultz — IFW Dresden, PF 270116, D-01171 Dresden, Germany

Based on investigations on a toy sized model levitation train [1], a full working demonstrator for a superconductively levitated transport system has been developed. The levitation and guidance system is based on flux pinning in melt-textured bulk $YBa_2Cu_3O_{7-x}$ (YBCO) that stabilizes the vertical and lateral positions of the vehicle above the magnetic track. The track is made of Nd-Fe-B permanent magnets mounted within soft-magnetic iron yokes acting as flux collectors. The actual vehicle contains 4 cryostats. Using 10 rectangular shaped bulk YBCO blocks with dimensions of $35 \times 90 \times 15$ mm^3 in each of them a maximum total load of nearly 800 kg at 77 K has been achieved. More details about the capability of the system will be given in the contribution. The concept also includes a fast electromagnetic turnout switch to establish a highly branched transportation network. An experimental setup has been created for the toy sized model train and will complete the SupraTrans demonstrator.
[1] L. Schultz et al.; Z. Metallkd. 93, 1057

TT 7.2 Mon 14:00 P1

Rare Earth Nickel Borocarbide Thin Films and Related Compounds — •Tim Niemeier, Ruben Hühne, Günter Behr, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, 01171 Dresden

Epitaxial thin films of YNi_2B_2C and related rare earth borocarbide compounds have been found to be a suitable alternative to single crystal growth for the characterisation of usual superconducting properties such as T_c, H_{c2} and J_c . Comparable results concerning the anisotropy require a good texture quality. For YNi_2B_2C, a new buffer layer architecture was developed, which improves both epitaxial growth and texture quality. The films were grown by pulsed laser deposition from stoichiometric and multicomponent molten targets under ultra-high vacuum conditions. Bare as well as buffered ceramic single crystals were used as substrates. Additionally, thin films of modified phase compositions such as $Y(Pt_xNi_{1-x})_2B_2C$ were investigated and the influence of disorder on the superconducting properties was studied. The critical temperature, the critical current density and also the properties of the upper critical field were determined and compared to polycrystal data.

TT 7.3 Mon 14:00 P1

Superconducting and magnetic properties of $RENi_2B_2C$ (RE=Y, Tb, Ho, Tm) single crystals — •Dmitri Souptel[1], Gunter Behr[1], Wolfgang Loser[1], Gunter Fuchs[1], Tilmann Leisegang[2], and Dirk Meyer[2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstr. 20, 01171 Dresden — [2]Technische Universität Dresden, Institut für Strukturphysik D-01062 Dresden

High-quality single crystals of $RENi_2B_2C$ (RE=Y, Tb, Ho, Tm) intermetallic compounds have been grown by a floating zone technique with optical heating [1, 2]. Crystals are crack free, without traces of 2nd phases and single crystalline in the volumes of 6 mm in diameter and 25-40 mm in length. The high crystal perfection was confirmed by x-ray, metallographic and neutron methods. Physical properties depend strongly on small composition variation and the temperature of heat treatment. For instance $HoNi_2B_2C$ show a variety of properties: plain superconductivity (T_c about 8 K), re-entrant superconductivity (T_c about 8 K and loss of superconductivity between 4 - 6 K due to incommensurate magnetic ordering) and normal conducting behaviour. Origins of different superconducting properties and their anisotropic behaviour are related to crystal composition, lattice parameters and changes of lattice site occupancies of the composing elements.
[1] D. Souptel et al., J. Cryst. Growth 276 (3-4) (2005) 652-662 [2] D. Souptel et al., J. Cryst. Growth 275 (1-2) (2005) e91-e95

TT 7.4 Mon 14:00 P1

Magnetic quantum oscillations in the normal and superconducting state of nonmagnetic borocarbides — •O. Ignatchik[1], B. Bergk[2], M. Jäckel[2], J. Wosnitza[1], D. Souptel[3], G. Behr[3], and P. C. Canfield[4] — [1]Dresden High Magnetic Field Laboratory, Forschungszentrum Rossendorf, 01314 Dresden — [2]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden — [3]Leibniz-Institut für Festkörper- und Werkstofforschung, D-01069 Dresden — [4]Condensed Matter Physics, Ames Laboratory, Ames, Iowa 50011, USA

We report on de Haas-van Alphen (dHvA) investigations of the nonmagnetic borocarbides YNi_2B_2C and $LuNi_2B_2C$. The measurements were carried out on high-quality single crystals by the torque method in magnetic fields up to 30 T. In the normal state the Fermi-surface topology has been analysed. In comparison with band-structure calculations several deviations are determined. Below the upper critical field, B_{c2}, in the vortex state an additional damping of the dHvA amplitudes appears. This damping is caused by the evolution from of the superconducting gap parameter. Concerning these topics we observe strong differences between differently grown crystals. The crystals produced by a zone-melting method show an abrupt vanishing of the dHvA signal at the upper critical field B_{c2}. In contrast, the flux grown crystals display a broader phase transition combined with a continuous decrease of the dHvA amplitude.

TT 7.5 Mon 14:00 P1

First-Principles Electronic Structure Study of Layered TB_2C_2 Compounds (T = Y, La, Lu) — •Alim Ormeci and Helge Rosner — MPI for Chemical Physics of Solids, Dresden, Germany

Metal borocarbides TB_2C_2, where T = Y and rare earth (R) metals, are layered compounds with metal atom layers alternating with the (B_2C_2) layers. The RB_2C_2 compounds crystallize in the tetragonal LaB_2C_2-

type structure with symmetry $P4/mbm$ (SG 127). CaB_2C_2 also has the same crystal structure and is isoelectronic to MgB_2. However, due to heteropolar B-C bonds it is an insulator. The compound YB_2C_2, on the other hand, is a metal and a superconductor. Although there are some ambiguities about its crystal structure [1], it can be regarded as an electron-doped version of CaB_2C_2. Consequently, both the crystal and electronic structure of YB_2C_2, as well as the electron-phonon interactions in the (B_2C_2) layers are of interest.

We use the FPLO method to investigate the above mentioned aspects in YB_2C_2. In particular, we find that YB_2C_2 has the LaB_2C_2-type structure in agreement with the FP-LAPW results [1]. Furthermore, we study the effects of (i) possible disorder in the B-C network, and (ii) different stacking orders on the electronic properties. LaB_2C_2 and LuB_2C_2 are included in the study for comparative reasons.

[1] S. Khmelevskyi, et al. Supercond. Sci. Technol. **18** 422 (2005)

TT 7.6 Mon 14:00 P1

$CaSi_2$, the "antibonding sister" of MgB_2 — •Claire Loison and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

After the suprising superconductivity of MgB_2 at 40 K, the superconductivity of other solids with the layered AlB_2-type has been discovered recently: $CaSi_2$, CaAlSi, SrAlSi ($T_c \sim$ 14 K, 8 K and 4 K respectively). At the same time, similar layered compounds, like the intercalated graphites YbC_6 and CaC_6 are discovered to superconduct at temperatures substancially higher than previously known for other intercalated graphites (6.5 K and 11 K respectively). Here, we study the electronic structure and the electron-phonon coupling of the superconducting phase of $CaSi_2$ using density functional theory, and compare it to MgB_2. The crystal structure of superconducting $CaSi_2$ is also of the AlB_2-type, with a slight buckling in the silicon planes. Superconductivity mechanism is similar in MgB_2 and $CaSi_2$, except that in $CaSi_2$ the *antibonding* σ^*-bands of the silicon layers are main contributor to the electron-phonon coupling, whereas in $CaSi_2$, it is the *bonding* 2p-σ-bands of boron. We investigate the influence of the buckling, which can be controled experimentally by the pressure, on the electron-phonon coupling. Finally, we discuss the possibility to find other superconductors in the familly of metal disilicides ASi_2 with A = Ba Ca, Lu, Sc, Yb.

TT 7.7 Mon 14:00 P1

Influence of aluminium substitution on the heat transport in single crystalline MgB_2 — •A.V. Sologubenko[1,2], N.D. Zhigadlo[2], S. M. Kazakov[2], J. Karpinski[2], and H.R. Ott[2] — [1]II. Physikalisches Institut, University of Cologne, 50937 Cologne, Germany — [2]Laboratorium für Festkörperphysik, ETH Hönggerberg, CH-8093 Zürich, Switzerland

We report data on the thermal conductivity $\kappa(T, H)$ of single-crystalline superconducting $Mg_{1-y}Al_yB_2$ ($y = 0.02, 0.07$) in the normal and mixed states at temperatures between 0.5 and 50 K, and in external magnetic fields H up to 50 kOe. The results are analyzed in terms of a combined phononic ($\kappa_{\rm ph}$) and quasiparticle (κ_e) heat transport and compared with our earlier results on pure and carbon-doped MgB_2. The substitution of Al for Mg leads to a considerable reduction of the field-induced κ_e, while $\kappa_{\rm ph}$ seems to be much less sensitive to impurities. The analysis of the $\kappa_e(H)$ data leads to the conclusion that the introduction of aluminium results in comparable enhancement of the intraband scattering in both the σ- and the π-band. This is in contrast to the carbon substitution for boron, which enhances mostly the intraband scattering in the σ-band. The interband scattering is rather weak in both cases.

TT 7.8 Mon 14:00 P1

Microwave properties of MgB_2 thin films prepared in situ by thermal evaporation combined with sputtering — •Rudolf Schneider, Alexander G. Zaitsev, Roland Hott, Fritz Ratzel, and Jochen Geerk — Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe, Germany

Superconducting MgB_2 thin films were prepared *in situ* using a combination of rf magnetron sputtering of B and thermal evaporation of Mg. The films exhibited T_c of up to 36 K. Microwave measurements were performed on 14×14 mm^2 films using both Cu-shielded and Nb-shielded sapphire puck resonators at the frequency of 18.8 GHz. The hf surface resistance (R_s) and the change of the hf surface reactance (ΔX_s) were determined. The films exhibited low R_s matching the literature results for high-quality MgB_2 films. Below 3 K R_s reached 3-5 $\mu\Omega$ which was the resolution limit of our measurement. The temperature dependence of both R_s and ΔX_s were in good agreement with BCS theory. From the R_s(T) dependence we obtained an energy gap $\Delta(0) \approx$ 3 meV. The measured variation of the London penetration depth with temperature, $\Delta\lambda_L$(T), was also in good agreement with the BCS model. Using the BCS relation between the energy gap and the penetration depth we fitted our experimental $\Delta\lambda_L$(T) data and obtained $\lambda_L(0)$ values which ranged for different films from 85 to 100 nm.

TT 7.9 Mon 14:00 P1

Effect of impurity additions on the superconducting properties of in situ-processed MgB_2 — •Marko Herrmann[1], Margitta Schubert[1], Wolfgang Häßler[1], Bernhard Holzapfel[1], and Ludwig Schultz[1,2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dresden University of Technology, Department of Physics, Institute for Physics of Solids, D-01062 Dresden, Germany

The MgB_2 powder was prepared by mechanical alloying of Mg, amorphous Boron and the additive. For studying the influence of the additive on the superconducting properties its amount was varied up to 20 m-%. Single elements as carbon as well as compounds like SiC were used as dopants. The result of the milling process was a partially reacted nano-sized precursor powder with a high reactivity which was hot pressed to bulk samples. Starting from the undoped MgB_2 with a critical temperature of 36 K and best current densities of 10 kA/cm^2 at 7.5 K and 4 T, the changes of the superconducting properties with the kind and amount of additive are described in detail.

TT 7.10 Mon 14:00 P1

TEM cross-section analysis of $La_2Zr_2O_7$ buffer layers for YBCO-coated conductors prepared by chemical solution deposition — •Leopoldo Molina[1], Sebastian Engel[2], Kerstin Knoth[2], Bernhard Holzapfel[2], and Oliver Eibl[1] — [1]Institute of Applied Physics, University of Tuebingen, Auf der Morgenstelle 10, D-72076 Tuebingen, Germany — [2]IFW Dresden, Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

Chemical solution deposition is a promising method to fabricate low cost buffer layers for YBCO-coated conductors. In this study we present transmission electron microscopy (TEM) analysis of cross-sectional and plan-view prepared $La_2Zr_2O_7$ buffer layers on biaxially textured Ni-W substrates for YBCO-coated conductors prepared by chemical solution deposition methods. The $La_2Zr_2O_7$ buffer layers were deposited on 100 μm thick Ni-W substrate and were heat treated at 900°C and 1050°C. TEM cross-section samples were prepared by conventional mechanical polishing and ion milling techniques. By means of transmission electron microscopy the grain size, the buffer layer thickness, the void size and void density and the orientation of LZO with respect to the Ni substrate was determined. The Ni-W substrate interface with the $La_2Zr_2O_7$ buffer layer was also investigated. Using two-beam imaging conditions bright-field, dark-field and energy spectroscopic images (ESI) were acquired. Chemical composition determination of the films and substrate was done by energy dispersive X-ray microanalysis (EDX).

TT 7.11 Mon 14:00 P1

Optimisation of $La_2Zr_2O_7$ buffer layers and CeO_2 cap layers on Ni RABiTS for YBCO coated conductors using chemical solution deposition — •Sebastian Engel, Kerstin Knoth, Thomas Thersleff, Heike Schlörb, Ruben Hühne, Ludwig Schultz, and Bernahrd Holzapfel — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

Chemical Solution Deposition (CSD) has been used to prepare biaxially textured cerium oxide cap layers and $La_2Zr_2O_7$ (LZO) buffer layers on Ni RABiTS. For the cerium oxide cap layer, a precursor solution consisting of dissolved Ce(III)-acetate in propionic acid, 2,5-pentandion, and 2-propanol was used. The LZO precursor solution was prepared by dissolving La-, and Zr-2,4-pentanedionates in propionic acid. Both, prepared buffer and cap layers were dip-coated and subsequently heat-treated at various temperatures between T = 900°C and 1100°C under different gas flow conditions. The surface texture quality was analysed with Reflection High Energy Electron Diffraction (RHEED) and Electron Back Scattering Diffraction (EBSD). EBSD maps show nearly 100 % biaxially textured surfaces for the optimised LZO buffer layers and cerium oxide cap layer. Further surface properties were investigated by atomic force microscopy and secondary electron microscopy. 300nm thick $YBa_2Cu_3O_{7-\delta}$ test structures were prepared on this buffer layer system

CeO_2 (CSD)/LZO (CSD)/ Ni-5 % W tape by pulsed laser deposition and characterised by resistivity measurements at 77 K in magnetic fields up to 9 T.

TT 7.12 Mon 14:00 P1

All CSD $YBa_2Cu_3O_{7-\delta}$ coated conductor on cube textured Ni-W substrates — •Kerstin Knoth, Sebastian Engel, Ruben Hühne, Steffen Oswald, Brigitte Schlobach, Steffen Strehle, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Chemical Solution Deposition (CSD) was used as a low cost method to prepare an all CSD $YBa_2Cu_3O_{7-\delta}$ (YBCO) coated conductor having a YBCO/CeO_2/$La_2Zr_2O_7$ (LZO)/Ni-5at%W architecture. The LZO and CeO_2 precursor solutions were prepared using new solution routes, whereas the trifluoroacetate (TFA) process was used for the preparation of the YBCO layer. A highly textured LZO/CeO_2 architecture was obtained on Ni-W after annealing at $T_A = 900\,°C$ in a reducing atmosphere. The TFA-YBCO layer was deposited afterwards and annealed at $T_A = 780\,°C$. The characterization of the CSD YBCO coated conductor was done using X-Ray Diffraction (XRD), Reflection High Energy Electron Diffraction (RHEED), SEM, AFM, X-Ray Photoelectron Spectroscopy (XPS) and cross sectional analysis using the Focussed Ion Beam (FIB) technique. The TFA-YBCO(200 nm)/CeO_2(60 nm)/LZO(400 nm)/Ni-W coated conductor showed a T_c of 91.0 K with a ΔT_c of 1.2 K. The critical current density J_c was below 1.0 MA/cm^2 compared to a PLD-YBCO/PLD-CeO_2/LZO(400 nm)/Ni-W test sample (PLD - Pulsed Laser Deposition) with $J_c = 1.0$ MA/cm^2. Nevertheless, these results are very promising towards the realization of an all CSD YBCO coated conductor.

TT 7.13 Mon 14:00 P1

Effect of H_2S treatment on the orientation and texture sharpness of MgO buffer layers on highly cube textured Ni-4at.%W tapes as a template for YBCO coated conductors — •Rainer Nast[1], Bernhard Obst[1], Oliver Stadel[2], and Wilfried Goldacker[1] — [1]Forschungszentrum Karlsruhe, Institut für Technische Physik, Postfach 3640, D-76021 Karlsruhe — [2]TU Braunschweig, Institut für Oberflächentechnik (IOT), Bienroder Weg 53, D-38108 Braunschweig

To achieve high current carrying capabilities in YBCO coated conductors based on cube textured metal substrates, the texture and stability of the buffer/metal interface is a necessary requirement. In this work cube textured Ni-4at.%W substrate tapes were subjected to different H_2S treatments and the texture development of post-deposited MgO buffer layers was studied. The in-plane orientation and the texture sharpness of the MgO layers was found to depend strongly on the heat treatment time in Ar-10 ppm H_2S. Increasing the time from 5 to 60 min at 800°C changes the in-plane orientation from 45° over 0° to 45° at 15 min and the texture sharpens continuously to an FWHM (220) of $< 6°$.

TT 7.14 Mon 14:00 P1

Physical properties of chemically deposited $La_2Zr_2O_7$ and CeO_2 buffer layers on cube textured Ni-4 at.% W substrates — •Gunter Kotzyba, Bernhard Obst, Rainer Nast, and Wilfried Goldacker — Forschungszentrum Karlsruhe, Institut für Technische Physik, P.O. Box 3640, 76021 Karlsruhe

The chemical solution deposition route for YBCO-coated conductors is of interest as a promising way to develop a low cost conductor. Thin films of $La_2Zr_2O_7$ and CeO_2 were prepared on Ni-4 at.% W by dip coating. The layers serve as buffer for depositing superconducting YBCO on top of it. We systematically investigated the dependence of the thickness on the viscosity and the concentration of the La (III) and Ce (IV) precursor solutions by means of a cone plate rheometer and an ICP OES. The roughness was analysed with a profilometer, the thickness determination was done by X-ray microanalysis. EBSD mappings show very good cube in-plane and out-of-plane texture.

TT 7.15 Mon 14:00 P1

dc and rf transport in normal and superconducting HTS, MgB_2, and Nb networks — •Jürgen Halbritter — Forschungszentrum Karlsruhe, Postfach 36 40

Island/grain boundaries occur naturally in film growth or sintering. The hindrance of electric transport by boundary resistances $R_{bn}(Wcm^2)$ in distances $a_J(\leq 10mm)$ is easy to measure in normal conducting transport in such granular networks. The resistivity $r(T) = R_{bn}/a_J + p(\rho^i(T) + \rho^i(0))$ is fitted to observations with percolation factors $p > 1$ by current diverting $a_J\rho^i(300K)$ boundaries with $R_{bn} \geq a_J\rho^i(300K)$ where $\rho^i(T) + \rho^i(0)$ is due to the grain interior (IG) and R_{bn}/a_J and p describes the effects of boundaries (GB) and the network. In the superconducting transport GB may act as Josephson junctions (JJ) with $j_{cJ}(A/cm^2)$ as current density. For superconducting networks is a simple separation in IG and GB not possible. But low I_c values, $p > 1$ and large R_{bn} values are clear indications for growth boundary limitations. Analysis of $I_c(T, B, q, \omega)$ as junction of temperature, field B, angle q and frequency ω give crucial information about GB and flux low or pinning of Josephson (JF) or Abrikosov fluxons (AF) in the network. The combination of normal and superconducting analysis is of crucial importance for dc, ac and rf engineering applications and for the understanding of the related material science.

TT 7.16 Mon 14:00 P1

Electronic structure calculations for YBCO/metal interfaces — •Udo Schwingenschlögl and Cosima Schuster — Institut für Physik, Universität Augsburg, 86135 Augsburg

Transport properties of heterostructures consisting of a metal and a correlated superconductor are of great importance for electronic devices based on HTSC. Using electronic structure calulations within density functional theory and the local density approximation, we investigate YBCO/metal interfaces. As the lattice mismatch between YBCO and Pd is rather small (0.7%), we choose Pd as the metallic constituent. It is generally accepted that the carrier density is modified at grain boundaries. Since this band bending should take place on the length scale of the lattice constant it can be reproduced by LDA supercell calculations. In particular, we use a supercell consisting of two YBCO unit cells alternating with five Pd layers along the orthorhombic c-axis. Following experimental results, the YBCO layers entering our calculations terminate by CuO chains.

Our results show that the electronic density of states at the interface depends crucially on the details of the local atomic structure. Therefore we have relaxed the atomic positions to minimize the forces on the ions. We compare two possible interface geometries, where the Pd atoms are placed on the Cu or O atoms of the CuO chains, respectively. For these configurations we determine the charge distribution across the interface.

TT 7.17 Mon 14:00 P1

Characterization of Top-Seeded Melt-Grown Bulk Superconductors by Hall Probe Mapping Techniques — •S. Haindl[1], H.W. Weber[1], N. Hari Babu[2], D. A. Cardwell[2], S. Meslin[3], J. Noudem[3], L. Shlyk[4], and G. Krabbes[4] — [1]Atomic Institute of the Austrian Universities, TU Vienna, Austria — [2]IRC in Superconductivity, University of Cambridge, UK — [3]CRISMAT-ENSICAEN, CNRS/UMR, France — [4]IFW Dresden, Germany

We report on the characterization of top-seeded melt-grown (TSMG) single grain bulk superconductors by two Hall probe mapping techniques. Scanning the trapped field distribution following magnetization of the sample in an external field is an established method of characterizing these materials. This technique enables both determination of the maximum trapped field after complete field penetration of the bulk sample, and identification of growth-induced inhomogeneities within the sample microstructure. A new mapping technique known as Magnetoscan has been developed over the past two years and recently improved to yield more useful information about the quality of bulk superconductors. This technique involves scanning simultaneously a small permanent magnet and a Hall probe over the unmagnetized superconducting surface of the bulk sample. Interesting results have been obtained using the magnetoscan technique, including direct imaging of different growth sectors in bulk samples and the identification of inhomogeneities such as cracks and grain-boundaries and the mapping of artificial holes in the single grain microstructure.

TT 7.18 Mon 14:00 P1

Nanometer-scale superconducting domains observed on $NdBa_2Cu_3O_{7-\delta}$ — •Pintu Das[1], Dirk Mautes[1], Michael R. Koblischka[1], Thomas Wolf[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, University of Saarbruecken, D-66041 Saarbruecken, Germany — [2]Forschungzentrum Karlsruhe GmbH, Instiitute of Solid State Physics, D-76021 Karlsruhe, Germany

In understanding high temperature superconductivity, the recent focus is at the local-scale electronic modulation and its influence towards superconductivity in general. The granular structure and atomic-scale

modulation of the density of states in $Bi_2Sr_2CaCu_2O_{8+\delta}$ have been observed [1,2]. Here we report Scanning Tunneling Spectroscopic (STS) results obtained on the (ab) plane of a slightly underdoped $NdBa_2Cu_3O_{7-\delta}$ (T_c= 93.5 K) twinned single crystals at 4.2 K. Recent results proved that the NdBCO surface is highly clean and stable in air, showing atomic resolution at room temperature [3]. We used the STS imaging technique to study the electronic inhomogeneity and we observe that there are superconducting domains of $\sim$ 3 nm length scale separated by nonsuperconducting regions, similar to that observed in $Bi_2Sr_2CaCu_2O_{8+\delta}$. In the superconducting domains, the size of the energy gap spatially varies from $\sim$ 16 meV to $\sim$ 44 meV. The average gap size is found to be $\sim$ 22 meV. We discuss these data and the possible origin of the inhomogeneous electronic structure of the respective materials.

[1] Lang et al., Nature 415, 412 (2002)
[2] McElroy et al., Nature 422, 592 (2003)
[3] Ting et al., Appl. Phys. Lett. 72, 2035 (1998)

TT 7.19 Mon 14:00 P1

Nanoscale stripe structures in $SmBa_2Cu_3O_x$ superconductors — •M. Winter[1], M. R. Koblischka[1], Th. Wolf[2], X. Yao[3], A. Hu[4], and U. Hartmann[1] — [1]Institute of Experimental Physics, University of Saarbrücken, P.O.Box 151150, 66041 Saarbrücken, Germany — [2]Forschungzentrum Karlsruhe GmbH, Institute of Solid State Physics, D-76021, Karlsruhe, Germany — [3]Department of Physics, Shanghai Jiao Tong University, 1954 Huashan Road, Shanghai 200030, P. R. China — [4]Department of Physics, University of Waterloo, 200 Univ. Ave. West, Waterloo, ON N2L 3P7, Canada

AFM and STM scans on $SmBa_2Cu_3O_x$ (SmBCO) melt-processed samples prepared using different techniques revealed the presence of nanoscale stripe-like structures, sometimes parallel over several micrometers, sometimes wavy. These structures consist of chemical compositional fluctuations and act as effective δT_c pinning centers due to their wavelength of typically 10-60 nm which is comparable to the ideal pinning-center size of 2 ξ (10 nm for $YBa_2Cu_3O_x$ in the ab-plane). Compared to similar structures in ternary (Sm,Eu,Gd)$Ba_2Cu_3O_x$ (SEG) and (Nd,Eu,Gd)$Ba_2Cu_3O_x$ (NEG)) systems, where the stripes appear either as plateau-like stripes or as chains of aligned clusters, the stripes in SmBCO always appear as plateau-like stripes with a height of 1 Å- 8Å. These pinning structures throughout the whole sample volume may be a key to improve critical current densities especially at high external magnetic fields.

TT 7.20 Mon 14:00 P1

How superstructure free is superstructure free Pb-BSCCO ? — •L. Dudy, B. Müller, B. Ziegler, A. Krapf, H. Dwelk, R.-P. Blum, C. Janowitz, and R. Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Pb- substituted BSCCO single crystals have been investigated by LEED and variable temperature VT- STM. While LEED pictures showed no superstructure spots in the range $30eV \leq E_{kin} \leq 320eV$, a closer look by VT- STM revealed that an ordered, alternating topographical formation of nano- domains with and without superstructure occurred. Independent of these geometrical nano- domains a long range ordering in the local density of states detected by corrugation analysis was also observed.

TT 7.21 Mon 14:00 P1

Unusual Nernst effect in various superconductors — •C. Hess[1], E. Ahmed[1], C. Falkenberg[1], D. Souptel[1], G. Behr[1], B. Büchner[1], U. Ammerahl[2], and A. Revcolevschi[2] — [1]IFW Dresden, Germany — [2]Laboratoire de Physico-Chimie des Solides, Université Paris-Sud, France

We present experimental results of the Nernst-effect in the normal state of various superconductors. In particular, we investigated the high temperature superconductor $La_2Sr_xCuO_4$ with and without Eu-doping. The Eu-ions suppress superconductivity and stabilize a stripe phase in the CuO_2-planes of the materials. We find that the relatively large Nernst-coefficient which has previously been reported for the normal state in pure $La_2Sr_xCuO_4$ is also present in the Eu-doped materials extending deep into the stripe ordered phase. We compare these results with the Nernst-effect of the superconductor YNi_2B_2C.

TT 7.22 Mon 14:00 P1

Rare earth substitutions and phase diagram studies in the ruthenocuprate system — •Eugenio Casini[1], Thomas P. Papageorgiou[2], Antonio Vecchione[3], Consiglia Tedesco[4], and Hans F. Braun[1] — [1]Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]HochFeld-Magnetlabor Dresden, Forschungszentrum Rossendorf, D-01314 Dresden, Germany — [3]INFM and Dipartimento di Fisica "ER Caianiello", Universitá di Salerno — [4]Dipartimento di Chimica, Università di Salerno, I-84081 Baronissi (Salerno), Italy

Coexistence of superconductivity and magnetism in the ruthenocuprate compounds has been the object of many investigations. $RuSr_2GdCu_2O_{8-\delta}$ is the most studied member of this class of materials and is the first and single known oxide in the quinary Sr-Gd-Ru-Cu-O system. Discording studies about the effect of the rare earth elements on the crystal structure and physical properties of these materials are reported. The formation of the $RuSr_2NdCu_2O_{8-\delta}$ compound is investigated following different preparation paths. Under standard conditions with the reported nominal composition a three-phase mixture is obtained. The concurring phases are indentified as: $(Sr_{1-x}Nd_x)(Ru_{1-x}Cu_x)O_y$, $Sr_2NdRuCuO_7$ and $(Sr_{14-x}Nd_x)Cu_{24}O_{41}$. A characterization of these compounds is carried out by XRD, DTA and EDX analysis whereas superconducting and magnetic properties are determined with ac and dc susceptibility measurements. Magnetic transitions in the temperature range 10-20K and 20-30K are detected for the $Sr_2NdRuCuO_7$ and $(Sr_{14-x}Nd_x)Cu_{24}O_{41}$ compounds, respectively. The $Sr_2NdRuCuO_7$ compound has not been previously reported.

TT 7.23 Mon 14:00 P1

Theory of magnetic excitations in bilayer cuprates — •Hiroyuki Yamase and Walter Metzner — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569, Stuttgart, Germany

We calculate the dynamical magnetic susceptibility $\mathrm{Im}\chi(\mathbf{q},\omega)$ in the bilayer t-J model in slave-boson mean-field approximation. At low temperature, where the d-wave superconducting state is realized, a pronounced peak in $\mathrm{Im}\chi(\mathbf{q},\omega)$ appears at $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$ and $\omega=\omega_{\mathbf{Q}}^{\mathrm{res}}$. For $\omega<\omega_{\mathbf{Q}}^{\mathrm{res}}$ strong spectral weight spreads around $\mathbf{Q}$, forming a diamond shaped pattern in $\mathbf{q}$-space. This spectral weight is due to a collective mode, known as "resonance mode" in the cuprates. The ω versus $\mathbf{q}$ dispersion of the mode is bent downwards around $\mathbf{Q}$. For $\omega>\omega_{\mathbf{Q}}^{\mathrm{res}}$, strong signals of $\mathrm{Im}\chi(\mathbf{q},\omega)$ tracing an upward dispersion are found. In the normal state, $\mathrm{Im}\chi(\mathbf{q},\omega)$ exhibits only a broad maximum at $\mathbf{q}=\mathbf{Q}$, that is incommensurate signals appear only in the d-wave pairing state. The above results hold in both odd ($q_z=\pi$) and even ($q_z=0$) channels. The most relevant experimentally observed features of magnetic excitations in bilayer cuprates are well captured by slave-boson mean-field theory.

TT 7.24 Mon 14:00 P1

Theory of the in-plane anisotropy of magnetic excitations in YBCO — •Hiroyuki Yamase and Walter Metzner — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569, Stuttgart, Germany

A pronounced xy-anisotropy was observed in recent neutron scattering experiments for magnetic excitations in untwinned YBCO.[1] The relatively small anisotropy of the bare band structure due to the orthorhombic crystal symmetry seems to be enhanced by correlation effects. A natural possibility is that the system is close to a Pomeranchuk instability associated with a d-wave Fermi surface deformation (dFSD).[2,3] We investigate this possibility in the bilayer t-J model within a self-consistent slave-boson mean-field theory. We show that the dFSD correlations drive a pronounced xy-anisotropy of magnetic excitations at low doping and at relatively high temperatures, providing a scenario for the observed xy-anisotropy also in $YBCO_{6.6}$ and $YBCO_{6.5}$, and in the pseudogap phase. [1] V. Hinkov *et al.*, Nature **430**, 650 (2004). [2] H. Yamase and H. Kohno, J. Phys. Soc. Jpn. **69**, 332 (2000); **69** 2151 (2000). [3] C. J. Halboth and W. Metzner, Phys. Rev. Lett. **85**, 5162 (2000).

TT 7.25 Mon 14:00 P1

Theory of ultrafast nonequilibrium dynamics in superconductors — •Julia Unterhinninghofen[1], Andreas Knorr[1], and Dirk Manske[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70596 Stuttgart

A theory of the dynamical ultrafast optical excitation of model superconductors is presented. We consider excitation of a nonequilibrium

quasiparticle distribution via a femtosecond optical pulse and the subsequent scattering with optical phonons. The scattering processes lead to a recombination of the excited quasiparticles to equilibrated cooper pairs. Using the density matrix formalism, relaxation processes on a picosecond timescale and time-resolved pump-probe spectra are calculated.

TT 7.26 Mon 14:00 P1

Spin and Charge Josephson effects between non-uniform superconductors with coexisting helimagnetic order — •Ilya Eremin[1,2], Flavio S. Nogueira[3], and Rene-Jean Tarento[4] — [1]Max-Planck Institut für Physik komplexer Systeme, Nöthnitzerstr 38, D-01187 Dresden, Germany — [2]Institut für Mathematische/Theoretische Physik, Technische Universität Carolo-Wilhelmina zu Braunschweig, D-38106 Braunschweig, Germany — [3]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [4]Laboratoire de Physique des Solides, UMR 8502 - Université Paris-Sud, Bât. 510, F-91405 Orsay Cedex, France

We consider the spin and charge Josephson current between two non-uniform superconductors with helimagnetic order. We demonstrate that the presence of the helimagnetic phase generates a spin Josephson effect and leads to additional contributions to both single-particle and Josephson charge current. It is shown that for such systems the AC effect differs more radically from the DC effect than in the case of a BCS superconductor. The most interesting effect occurs in the presence of an external magnetic field and in absence of voltage, where we show that the charge Josephson current can be tuned to zero while the spin Josephson current is non-vanishing. This provides a well controlled mechanism to generate a spin supercurrent in absence of charge currents.

TT 7.27 Mon 14:00 P1

Enhancement of pairing due to the presence of resonant cavities — •K. Morawetz[1,2], B. Schmidt[1], M. Schreiber[1], and P. Lipavsky[3] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2

A correlated fermion system is considered surrounding a finite cavity with virtual levels. The pairing properties are calculated and the influence of the cavity is demonstrated. To this end the Gell-Mann and Goldberger formula is generalized to many-body systems. We find a possible enhancement of pairing temperature if the Fermi momentum times the cavity radius fulfills a certain resonance condition which suggests an experimental realization.

[1] K. Morawetz, M. Schreiber, B. Schmidt, P. Lipavský, Enhancement of pairing due to the presence of resonant cavities, Phys. Rev. B 72 (2005) 174504-1-5

[2] K. Morawetz, M. Schreiber, B. Schmidt, A. Ficker, P. Lipavský, Correlated two-particle scattering on finite cavities, Phys. Rev. B 72 (2004) 014301-1-15

TT 7.28 Mon 14:00 P1

Bernoulli potential in type-I and weak type-II superconductors: Electrostatic potential above the vortex lattice — •K. Morawetz[1,2], P. Lipavsky[3], J. Kolacek[4], E.H. Brandt[5], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2 — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [5]Max-Planck-Institute for Metal Research, 70506 Stuttgart, Germany

The electrostatic potential above the Abrikosov vortex lattice, is evaluated within the Ginzburg-Landau theory. Unlike previous studies we include the surface dipole. Close to the critical temperature, the surface dipole reduces the electrostatic potential to values below sensitivity of recent sensors. At low temperatures the surface dipole is less effective and the electrostatic potential remains observable as predicted earlier. We propose an experimental measurement by NMR to access this field which can yield informations about material parameters.

[1] P. Lipavský, K. Morawetz, J. Kolacek, J. J. Mares, E. H. Brandt, M. Schreiber, Bernoulli potential in type-I and weak type-II supercoductors: III. Electrostatic potential above the vortex lattice Phys. Rev. B 71 (2005) 024526-1-7, II. Surface dipole, Phys. Rev. B 70 (2004) 104518-1-7, I. Surface charge, Phys. Rev. B 69 (2004) 024524-1-7

TT 7.29 Mon 14:00 P1

Theory of Ultrafast Pump-Probe-Spectra of BCS-type Superconductors — •Sabine Körbel, Tilmann Kuhn, and Vollrath Martin Axt — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster

Ultrafast optical excitation yields information about the microscopic interaction mechanisms in different materials. The theoretical description and modelling has been successfully carried out for semiconductors within the density-matrix-formalism. We applied the same formalism to the BCS-type superconductor. In particular we study the dynamical electrical conductivity after exciting the system by a picosecond pump pulse with an energy slightly above the superconducting gap. Our results show that the nonequilibrium dynamics of the gap is strongly correlated to the dynamics of the quasiparticles which are generated by the pump pulse, and their coherences. We show the influence of particle number and energy distribution on pump probe spectra.

TT 7.30 Mon 14:00 P1

Qualitative Modeling of the Quasiparticle Green's Function in Cuprates Based on ARPES Data — •Dmytro Inosov[1], Sergey Borisenko[1], Alexander Kordyuk[1,2], Volodymir Zabolotnyy[1], Jochen Geck[1], Andreas Koitzsch[1], Jeorg Fink[1], Martin Knupfer[1], and Bernd Büchner[1] — [1]Leibnitz-Institut für Festkörper- und Werkstofforschung, IFW-Dresden, P.O.Box 270116, D-01171 Dresden, Germany — [2]Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

ARPES data provides a detailed view of the renormalized band structure in cuprates and, consequently, is a key to the self-energy and the quasiparticle Green's function. However, due to the matrix elements and experimental specifics, comparison with the results provided by different experimental techniques is not straightforward. A model which would allow such a comparison with STM, INS, and RS data is proposed.

TT 7.31 Mon 14:00 P1

Effect of Zn and Ni impurities on the quasiparticle renormalization in Bi-2212 — •V. B Zabolotnyy[1], S. V. Borisenko[1], A. A. Kordyuk[1,2], J. Fink[1], J. Geck[1], A. Koitzsch[1], M. Knupfer[1], B. Büchner[1], H. Berger[3], A. Erb[4], C. T. Lin[5], and B. Keimer[5] — [1]Institute for Solid State Research, IFW-Dresden, Germany — [2]Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine — [3]Institute of Physics of Complex Matter, EPFL, CH-1015 Lausanne, Switzerland — [4]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften,Walther-Meißner Strasse 8, 85748 Garching, Germany — [5]Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The Cu substitution by Zn and Ni impurities and its influence on the mass renormalization effects in angle resolved photoelectron spectra (ARPES) of $Bi_2Sr_2CaCu_2O_{8-\delta}$ is addressed. We show that the nonmagnetic Zn atoms have much stronger effect both in nodal and antinodal parts of the Brillouin zone than magnetic Ni. The observed changes are consistent with the behaviour of the spin resonance mode as seen by inelastic neutron scattering in YBCO. This strongly suggests that the "peak-dip-hump" and the "kink"in ARPES on the one side and neutron resonance on the other are closely related features.

TT 7.32 Mon 14:00 P1

Azimuthal polarization dependence of x-ray absorption of Bi-2201 single crystals — •B. Müller, R. Mitdank, L. Dudy, J. Rasch, B. Ziegler, L. Lasogga, H. Dwelk, A. Krapf, C. Janowitz, and R. Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

The hole concentration in the CuO_2-planes is one of the most important parameters of high-Tc superconductors and x-ray absorption spectroscopy (XAS) is well known to be an excellent experimental tool for its determination. For polycrystalline ceramic materials this has been demonstrated by analysing the so-called pre-peak at the $O1s - 2p$ absorption line [1] and a satellite line at the $Cu2p - 3d$ transition [2]. Also the single-CuO_2 layer superconductor Bi-2201 has been studied recently [3].

For single crystalline superconductors, on the other hand, likewise analyses gave completely non-systematic results. The reason for such an unexpected behavior is a distinct dependence of the absorption on the azimuthal polarization of the synchrotron radiation. A strong dependence on the polarization vector parallel and perpendicular to the surface is

well known [1], but a dependence on orientation within the CuO_2-plane has not been considered so far.

[1] J. Fink et. al., Springer Series in Solid-State Sciences Vol. 91, 406 (1989)
[2] A.Q. Pham et. al., Phys. Rev. B 48, 1249 (1993)
[3] M. Schneider et. al., Phys. Rev. B 72, 014504 (2005)

TT 7.33 Mon 14:00 P1

Spin-Orbit Coupling Effects In The 3-Kelvin Phase Of Sr_2RuO_4 — •Florian Loder — Experimentalphysik VI, Universität Augsburg, D-86135 Augsburg

The inhomogeneous superconducting phase in the Sr_2RuO_4, called 3-Kelvin phase, has been shown to occur at interfaces between the bulk material and μm-size Ru-inclusions. It has been proposed that the interface region would be characterized by the strain-induced RuO_6 octahedra rotation around the c-axis. Here we show that this gives rise to a staggered antisymmetric spin-orbit coupling which in a homogeneous magnetic field induces both a uniform and a staggered spin component. This spin-orbit coupling influences the superconducting spin-triplet phase nucleating at the interface. A particularly interesting aspect is the possibility to induce a quasi particle gap in $\vec{Q} = (\pi, \pi, 0)$-nested Fermi surface by an applied magnetic field. This gives rise to an intriguing novel form of paramagnetic limiting and would explain the puzzling observation of the suppression of the upper critical field of the inhomogeneous 3-Kelvin phase.

TT 7.34 Mon 14:00 P1

Spectroscopic investigations on Na_xCoO_2 — •T. Kroll[1], A.A. Aligia [2], J. Geck[1], D. Hawthorn [3], C. Hess[1], T. Schwieger[1], G. Krabbes[1], C. Sekar[1], D. Batchlor[4], M. Knupfer[1], J. Berger[5], J. Fink[1], G.A. Sawatzky[3], and B. Büchner[1] — [1]IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany — [2]Centro Atomico Bariloche (CAB), Av. Bustillo 9500, 8400 S.C. de Bariloche, Argentina — [3]Advanced Materials and Process Engineering Laboratory (AMPEL), 2355 East Mall, Vancouver, BC, V6T 1Z4, Canada — [4]Universität Würzburg, Am Hubland, D-97074 Würzburg — [5]Institute of Physics of Complex Matter, EPFL, CH-1015 Lausanne, Switzerland

Since the discovery of superconductivity in 2003 in $Na_{0.3}CoO_2 1.3H_2O$ many investigations have been performed on these materials. In order to understand the physics behind the rich phase diagram of Na_xCoO_2 in more detail a good knowledge of its electronic structure is crucial. In this poster we present the results of different spectroscopic methods such as NEXAFS and XPS on a wide doping range for different temperatures and polarisation as well as cluster calculations which helps to understand the electronic structure of Na_xCoO_2.

TT 7.35 Mon 14:00 P1

Pressure-induced changes in the quasi-one-dimensional superconductor β-$Na_{0.33}V_2O_5$ studied by Raman spectroscopy — •S. Frank[1], C. A. Kuntscher[1], I. Gregora[2], T. Yamauchi[3], and Y. Ueda[3] — [1]1.Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany — [2]Institute of Physics ASCR, Praha, Czech Republic — [3]Institute for Solid State Physics, University of Tokyo, Tokyo

β-$Na_{0.33}V_2O_5$ is one of the first known inorganic quasi-one-dimensional superconductors. The pressure - temperature phase diagram is remarkable, showing a superconducting phase for pressures higher than 7 GPa in direct vicinity to a charge-ordered phase. The mechanism of the superconductivity and its relation to the charge ordering is not clear.

In a recent infrared study under pressure major changes in the reflectivity spectra were observed above 12 GPa, in particular the appearance of additional, relatively broad excitations [1]. A redistribution of charge with a possible relation to structural changes was suggested as a possible explanation. To obtain a deeper understanding of the changes occurring at 12 GPa we carried out polarization-dependent Raman spectroscopy under pressure at room temperature. The results are discussed in terms of a possible structural phase transition at 12 GPa.

Supported by the DFG, Emmy Noether-program.

[1] C.A. Kuntscher et al., Phys. Rev. B **71**, 220502(R) (2005)

TT 7.36 Mon 14:00 P1

Interaction corrections in Andreev reflection processes — •Markus Müller and Wolfgang Belzig — Universität Konstanz, Fachbereich Physik, D-78457 Konstanz, Germany

Understanding the conductance properties is of elementary interest when investigating electronic transport in nanostructures. We focus on the junction between a conventional superconductor and a normal metal. We consider a system of a one-dimensional weakly interacting electron gas on one and a superconductor on the other side, separated by a single potential localized in the interface region. Due to electron-electron interaction the Andreev reflection amplitudes are modified. A Poor Man's renormalization group procedure is used to handle logarithmic divergencies appearing in a perturbative treatment. Our approach is similar to the studies of conduction of a weakly interacting one-dimensional electron gas through a single barrier, realized by Matveev, Yue, and Glazman [Phys. Rev. Lett. **71**, 3351 (1993)]. The renormalized Andreev reflection amplitudes are calculated for any energy, and interface potentials of arbitrary strength. We discuss the temperature and voltage dependence of the Andreev conductance and compare with experimental results found by Morpurgo et al. [Science **286**, 263 (1999)]

TT 7.37 Mon 14:00 P1

Impact of the transport supercurrent on the zero-bias conductance peak — •Sergei Shevchenko and Alexander Omelyanchouk — Institute for Low Temp. Phys. and Eng., Lenin Ave. 47, 61108 Kharkov, Ukraine.

The impact of the supercurrent on the density of states in superconducting structures is investigated. Namely two situations were studied: (i) of a film containing a weak link and (ii) a film of a d-wave superconductor. In Ref. [1] we have shown that in the situation when the transport supercurrent flows in the region of suppressed order parameter (in the vicinity of the weak link as in the case (i) or at the boundary of a d-wave superconductor, case (ii)) the quasiparticles create the countercurrent. In this work we show that these quasiparticles are responsible for the appearance of the zero-bias conductance peak. Particularly we investigate the impact of the transport supercurrent flowing in parallel to the boundary on the conductance of the SIN-structure and discuss its observability with the scanning tunneling spectroscopy, as in Ref. [2]. We also discuss the relation of our results to the experiment, presenting alternative explanation of the experimental results of Ref. [2].

[1] Yu.A. Kolesnichenko, A.N. Omelyanchouk, and S.N. Shevchenko, Phys. Rev. B 67, 172504 (2003); Low Temp. Phys. 30, 213 (2004). [2] J. Ngai, P. Morales, and J.Y.T. Wei, Phys. Rev. B 72, 054513 (2005).

TT 7.38 Mon 14:00 P1

Proximity effect in superconducting MgB_2/Fe/MgB_2 trilayer — •B. Sahoo[1], W. Keune[1], V. Kuncser[2], A. I. Chumakov[3], and R. Rueffer[3] — [1]Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]National Institute for Physics of Materials, Bucharest-Magurele, Romania — [3]European Synchrotron Radiation Facility, Grenoble, France

By Mössbauer spectroscopy (CEMS) we have observed, at about Tc, an anomaly in a annealed superconducting MgB_2(500 Å)/ ^{57}Fe(40 Å)/MgB_2(500 Å) trilayer (Tc = 25 K) in the T-dependence of the spectral center-line shift, which does not follow the usual Debye behavior. This anomaly is absent in a nonsuperconducting multilayer. We have not observed anomalies in the T-dependence of the magnetic hyperfine field, and also not in the ^{57}Fe phonon density of states (PDOS) measured by nuclear resonant inelastic X-ray scattering with 3 meV resolution. Hence the observed anomaly at Tc may be either due to the modification of the low-energy part (< 3 meV) of the PDOS (at present not accessible experimentally), or due to the change of the s-electron density at the ^{57}Fe nucleus, because of Cooper pair formation in the superconducting state.
Sponsored by DFG (GRK277)

TT 7.39 Mon 14:00 P1

Proximity effect and multiple Andreev reflections in diffusive superconductor-normal-metal-superconductor junctions — •Jan C. Hammer[1], Juan Carlos Cuevas[1,2,3], Juha Kopu[1,4], Janne K. Viljas[1], and Matthias Eschrig[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049-Madrid, Spain — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe — [4]Low Temperature Laboratory, Helsinki University of Technology, P.O.Box 2200, FIN-02015 HUT, Finland

We present a theory of the current-voltage characteristics in diffusive superconductor-normal-metal-superconductor junctions. By solving the time dependent Usadel equation we are able to describe the phase-coherent transport for arbitrary length of the normal wire and arbitrary temperature. We show how the interplay between proximity effect and

multiple Andreev reflections gives rise to a rich subgap structure in the conductance and how it is revealed in the non-equilibrium distribution function.

TT 7.40 Mon 14:00 P1

Diamagnetic screening properties of Nb/Ag and Nb/Ag/Fe layered structures — •C. Sürgers[1], H. Stalzer[1], A. Cosceev[1], and H. v. Löhneysen[1,2] — [1]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

The diamagnetic properties of Nb/Ag and Nb/Ag/Fe layered structures of various thicknesses are investigated by means of SQUID and vibrating sample magnetometry. Data were taken for different temperatures in magnetic fields slightly tilted from the orientation parallel to the surface. For Nb/Ag double layers, below the diamagnetic transition of the Nb layer a second transition caused by the proximity-induced screening currents in the Ag layer is observed. Furthermore, a peculiar position dependence of the Ag magnetization signal is likely to be due to the missing formation of Andreev bound states along the lateral extensions of the film. While for Ag layers thicker than the coherence length or penetration depth of Nb an additional Fe layer on top of Ag destroys the coherence of Andreev pairs, the diamagnetic signal of Ag is recovered if the Ag layer thickness is strongly reduced. This is interpreted as being due to the competition of proximity-induced superconductivity by Nb and pair breaking by Fe.

TT 7.41 Mon 14:00 P1

Superconducting Proximity Effect in Co_2MnGe/V/Co_2MnGe Trilayers — •Dirk Sprungmann, Kurt Westerholt, and Hartmut Zabel — Institut für Experimentalphysik/Festkörperphysik,Ruhr-Universität Bochum, 44780 Bochum, Germany

We have studied the superconducting proximity effect in the trilayer system Co_2MnGe/V/Co_2MnGe. The motivation of this work was, whether the exchange field of the ferromagnetic Heusler alloy affects the critical temperature T_c in the same way as simple elementary ferromagnets do. For this purpose we measured the critical temperature T_c at different thicknesses of the V and the Co_2MnGe layers and determined the critical fields $H_{c\parallel}(T)$ and $H_{c\perp}(T)$ as a function of temperature. We applied the theory of Z. Radovic et al. and L.R. Tagirov to the data and obtained the coherence lengths of the pair wave function in the superconducting Vanadium ξ_s and in the ferromagnetic Heusler compound ξ_F. Additionally the theoretical fits provide the characteristic transparency parameters of the V/Co_2MnGe interface. The comparison of the experimental results and the theory reveals quantitative agreements with the classical proximity effect. However, quantitatively we also find inconsistencies in the parameters we have derived. This is due to the spin glass type of magnetic order for small thicknesses of the Co_2MnGe-phase, which is a complication compared to the classical proximity effect.
We acknowledge financial support through SFB 491.

TT 7.42 Mon 14:00 P1

Superconducting Spin Valve Effect of a V Layer Coupled to an Antiferromagnetic [Fe/V] Superlattice — •Dirk Sprungmann, Kurt Westerholt, Hartmut Zabel, R. Brucas, B. Hjörvarsson, D.A. Tikhonov, and I.A. Garifullin — Institut für Experimentalphysik/Festkörperphysik,Ruhr-Universität Bochum, 44780 Bochum, Germany

We have studied the superconducting properties of V-layers deposited on an antiferromagnetically coupled $[Fe_2V_{11}]_{20}$ superlattice (20 periods, 2 monolayers of Fe, 11 monolayers of V). The upper critical magnetic field $H_{c2\parallel}(T)$ for the direction parallel to the film plane exhibits an anomalous T-dependence for magnetic fields up to the ferromagnetic saturation field of the superlattice, indicating that the superconducting transition temperature T_S unambiguously depends on the relative magnetization orientation of the Fe_2 layers. This so called superconducting spin valve effect reaches up to 6% for the relative difference in T_S between the superlattice in ferromagnetic saturation and in the antiferromagnetic state and is more than one order of magnitude larger than observed in similar systems before. The shift proves, that the pair breaking effect of a ferromagnetic layer is reduced, if within the range of the superconducting correlation length another ferromagnetic layer with antiparallel spin orientation exists.
We acknowledge financial support through SFB 491.

TT 7.43 Mon 14:00 P1

Adiabatic pumping in a Superconductor-Normal-Superconductor weak link — •Michele Governale[1,2], Fabio Taddei[2], Rosario Fazio[2], and Frank Hekking[3] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]NEST-CNR-INFM & Scuola Normale Superiore, I-56126 Pisa, Italy — [3]LPMMC, CNRS & Université Joseph Fourier, BP 166, 38042 Grenoble CEDEX 9, France

Pumping consists in the transport of particles obtained by varying periodically in time some properties of a mesoscopic conductor[1].

We present a formalism to study adiabatic pumping between two superconducting terminals connected through a normal region, where charging effects are negligible (superconductor - normal -superconductor weak link). In this system, at low enough temperature, pumping is due to the adiabatic transport of Cooper pairs, and the pumped charge is related to the Berry phase accumulated, in a pumping cycle, by the Andreev bound states. We analyze in detail the case when the normal region is short compared to the superconducting coherence length. In this regime, the pumped charge turns out to be an even function of the superconducting phase difference. Hence, it can be distinguished from the charge transferred due to the standard Josephson effect.

[1] P.W. Brouwer, Phys. Rev. B **58**, R10135 (1998).

TT 7.44 Mon 14:00 P1

Magnetotransport in Lateral S/F/S Junctions — •Wilfried Meindl[1], Marco Aprili[2,3], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]CSNSM-CNRS, Université Paris Sud, Orsay, France — [3]LPQ-ESPCI, 75005 Paris, France

The antagonism of superconductivity and magnetism is investigated by fabricating lateral superconductor/ferromagnet/superconductor junctions. Niobium strips connected by a bridge of the dilute ferromagnet PdFe were produced using shadow evaporation techniques. The length of the bridge varied between 200 and 600 nm and the Fe-concentration was 5 %. Measurements of the resistance as a function of an in-plane magnetic field show periodic oscillations, whose amplitude can reach up to 10% of the base resistance, and a hysteretic dip around zero. The oscillations appear close to the superconducting transition and vanish again at lower temperatures. The dip is associated with the magnetization reversal in PdFe.

TT 7.45 Mon 14:00 P1

Magnetotransport and Josephson Effect in Periodic Superconductor/2DEG Structures — •Franziska Rohlfing[1], Gustaaf Borghs[2], Dieter Weiss[1], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]IMEC, Leuven, Belgium

We report on differential resistance measurements of arrays of multiple Josephson junctions as a function of out-of-plane and in-plane magnetic field. The junction array is made of 80 400 nm wide niobium stripes in 600 nm distance in good metallic contact with the two-dimensional electron gas in an InAs quantum well. The differential resistance shows oscillations in the out-of-plane magnetic field with an oscillation period determined by the area of a single junction. A trapezoidal modulation of the stripe width results in additional minima in the resistance at higher fields, indicative of a two-dimensional network of Josephson junctions. The supercurrent at 0.4 K is suppressed down to 10% by a parallel magnetic field on a scale of 20 mT, while a small fraction of the supercurrent survives up to 300 mT.

TT 7.46 Mon 14:00 P1

Fabrication of high stability shadow masks for complex hybrid structures — •Markus Gaass[1], Marco Aprili[2,3], Peter Tranitz[1], Werner Wegscheider[1], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg — [2]CSNSM-CNRS, Université Paris Sud, Orsay, France — [3]LPQ-ESPCI, 75005 Paris, France

We have developed and optimized a new thermostable mask system for shadow evaporation of refractory metals like Nb. The mask system consists of a PES sacrificial layer on which a 50nm thick Si_3N_4 film is deposited by PECVD at 275°C. The SiN is then covered with PMMA resist and patterned using conventional electron beam lithography and reactive ion etching with CHF_3. A free standing SiN-mask is created by removal of the PES with an isotropic etch in an oxygen plasma. The resulting masks are thermally and mechanically extraordinarily stable and

show only minor deformations after deposition of 100nm Nb. This allows the fabrication of shadow masks for complex hybrid structures using angle evaporation techniques. We present first experiments on the magnetic response of superconducting loops with embedded ferromagnetic Josephson junctions using this technique.

TT 7.47 Mon 14:00 P1

Morphology of epitaxial Al/AlO_x/Al trilayers — •Jonathan Eroms[1], H.W. Zandbergen[1], R. Delhez[2], A.H. Verbruggen[1], C.J.P.M. Harmans[1], and J.E. Mooij[1] — [1]Kavli Institute of Nanoscience Delft, TU Delft, The Netherlands — [2]Department of Materials Science and Engineering, TU Delft, The Netherlands

For increasing the Josephson junction quality in our superconducting qubit circuits we investigate growth of epitaxial aluminum films in a molecular beam epitaxy system. Here we present results on the crystalline structure of the bottom and top Al electrode in an Al/AlO_x/Al layer stack. We monitor the growth in situ by RHEED and ex situ with x-ray diffraction and high-resolution TEM. The bottom Al layer can be grown epitaxially in (111) orientation on Si(111) surfaces. The Al surface is oxidized by introducing a low pressure of oxygen into the growth chamber, and an amorphous AlOx film is formed. Growing aluminum onto this layer still gives a (111) oriented film, but in different rotational orientations. Depending on the oxygen exposure, the top Al layer either follows the orientation of the lower Al film, but with strong incorporation of twin crystals, or forms a random (111) texture.

TT 7.48 Mon 14:00 P1

Fabrication and characterization of Al/AlO_x based superconducting flux-qubits — •Martin Goeppl, Sonia Dandl, Tobias Heimbeck, Karl Madek, Matteo Mariantoni, Georg Wild, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, D-85748 Garching

Superconducting qubits based on superconducting loops containing an odd number of Josephson junctions with a coupling energy larger than the charging energy are called flux qubits. The qubit states are given by a symmetric superposition of currents flowing clockwise and counterclockwise when it is frustrated by applying a magnetic field corresponding to half a flux quantum in the loop. The system can be read out by a *dc* SQUID comprising the qubit.

We are fabricating flux qubits based on Al/AlO_x/Al tunnel junctions, using electron beam lithography and shadow evaporation technique. A crucial point was to establish and optimize the oxidation process for the lower electrode in order to fabricate Josephson junctions with well defined critical currents. Furthermore, the design of the electromagnetic environment is an important issue, which is required to isolate the qubit environmental sources of decoherence. Measurements on various test structures (Josephson junctions, SQUIDs, qubits) were used to analyze and further optimise the fabrication parameters.

This work is supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft

TT 7.49 Mon 14:00 P1

Fractional Josephson vortices as candidates for the observation of macroscopic quantum effects — •T. Gaber[1], E. Goldobin[1], K. Buckenmeier[1], K. Vogel[2], O. Crasser[2], R. Walser[2], W. P. Schleich[2], D. Koelle[1], and R. Kleiner[1] — [1]Physikalisches Institut, Experimentalphysik II,Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen — [2]Universität Ulm, Abteilung Quantenphysik, D-89069 Ulm

It is established experimentally that in long Josephson junctions (LJJ), where the phase dynamics can be mapped to the sine-Gordon equation with phase discontinuities, fractional vortices can appear spontaneously. In contrast to fluxons which are solitons and can move freely along LJJs, fractional vortices are pinned at the discontinuities and may have positive or negative polarity. They are useful for information encoding and are similar to spin-$\frac{1}{2}$ systems. In contrast to fluxon based devices, a fractional vortex can represent the ground state of the system which makes it more robust.

Fractional vortices, fractional vortex molecules and vortex crystals are interesting systems to study macroscopic quantum effects. We discuss the quantum properties of a single fractional vortex in a 0-π LJJ and a two-fractional-vortex molecule in a 0-π-0 LJJ and give an estimation of the crossover temperature in typical experiments. Several possibilities to construct and manipulate the quantum states of one or more vortices are presented. Possible readout schemes using integer fluxons and/or RSFQ logic are discussed.

TT 7.50 Mon 14:00 P1

Current and phase distribution in Josephson junctions with ferromagnetic interlayer — •Martin Weides[1], Dietmar Doenitz[2], Hermann Kohlstedt[1,3], Dieter Koelle[2], and Reinhold Kleiner[2] — [1]Institute for Solid State Research, Research Centre Juelich, Germany — [2]Physikalisches Institut - Experimentalphysik II, Universität Tübingen — [3]Department of Material Science and Department of Physics, University of Berkeley, USA

We use Low Temperature Scanning Electron Microscopy (LTSEM) to image current and phase distribution in low-T_C SINFS Josephson junctions (JJ) with diluted ferromagnetic $Ni_{60}Cu_{40}$ used as F-interlayer. Our technology [1] enables us to fabricate high quality junctions with low parameter spread. The configuration of magnetic domains in the F-interlayer is, amongst others, determined by the shape-anisotropy. The in-plane magnetization forms magnetic domains, which influence Cooper pair and quasiparticle transport trough the F-interlayer. We use annular and elliptical junction geometries for this work.
The imaging is based on the electron-beam-induced local heating of a resistively biased junction [2]. The beam-induced voltage-change is detected by Lock-In technique and is proportional to the Josephson current. The interaction between the local magnetic configuration of the JJ and external magnetic fields with respect to the transport current is studied.
[1] Weides et al., to appear in Physica C
[2] R. Gross and D. Koelle, Reports on Progress in Physics 57 (1994)

TT 7.51 Mon 14:00 P1

Internal Dissipation of Silicon at Cryogenic Temperatures — •Ronny Nawrodt[1], Anja Zimmer[1], Sandor Nietzsche[1], Wolfgang Vodel[1], Tina Clausnitzer[2], Ernst-Berhard Kley[2], Andreas Tünnermann[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena — [2]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Strasse 15, D-07745 Jena

Internal dissipation at a certain temperature is the origin of thermal noise. Optical interferometric gravitational wave detectors are sensitivity limited by the thermal noise of their optical components (e.g. end mirrors, cavity couplers, beam splitters). The main contributions to this noise are due to the substrate, the optical coating, and the suspension. The thermal noise can be reduced by cooling to cryogenic temperatures. In addition the overall mechanical quality factor as a measure of dissipation should preferable increase at low temperatures. The experimental details of a new cryogenic apparatus for investigations of the temperature dependency of the dissipation of different substrate materials in the range of 5 to 300 K are presented. The main focus is on silicon as a well suited material for cryogenic optics due to its special low temperature properties. Results on Si[100] and Si[111] are presented and discussed.

This work is supported by the German DFG under contract SFB TR7.

TT 7.52 Mon 14:00 P1

Characterization and Noise-Measurements on HTSC-Flip-Chip-Gradiometers with Different Antennas — •Tobias Foerster[1], Henrik Schneidewind[2], Christoph Becker[1], Veit Grosse[1], Ralf Bechstein[1], Frank Schmidl [1], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D 07743 Jena — [2]Institut für Physikalische Hochtechnologie e.V.(IPHT), Bereich Magnetik-Quantenelektronik, Albert-Einstein-Straße 9, D 07745 Jena

To optimize our HTSC-dc-SQUID gradiometric sensors with galvanically coupled antennas we investigated the performance of antennas on a separate substrate. These antennas are connected to a dc-SQUID-gradiometer in a Flip-Chip-Configuration.

Different combinations of thin-film and substrate materials, like TBCCO on Al_2O_3 or $LaAlO_3$ and YBCO on $SrTiO_3$, were used to produce antennas with variable layouts. The antennas were characterized concerning their critical current densities, critical temperature and noise properties to demonstrate their suitability for high resolution magnetic measurements in a Flip-Chip-Configuration.

Field-Gradient-Resolution and noise properties of multiple Flip-Chip-Sensors where then determined and compared.

TT 7.53 Mon 14:00 P1

Microwave power distribution in the near-field regime of a 98 GHz source — •Felix Stewing, Andre Kaestner, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, TU Braunschweig, Hans-Sommer-Straße 66, 38106 Braunschweig

A new method for measuring microwave near-field radiation is presented. We use a scanning microscope equipped with a high-T_C Josephson-cantilever of $LaAlO_3$ to measure near-field power distributions in three dimensions with 100 nm spatial resolution. The height approach is piezo-controlled with a resolution of a few micrometers in z-direction (perpendicular to the surface).

First results are presented for high-frequency properties and possible spatial resolution of the Josephson cantilevers. The influence of the dielectric material $LaAlO_3$ on the measured microwave radiation pattern from a source of 98 GHz is investigated. The calculated and measured electromagnetic power distributions are compared.

TT 7.54 Mon 14:00 P1

Magnetic calorimeters for a direct neutrino mass measurement using ^{187}Re β decay — •Loredana Gastaldo[1], Daniel Haug[1], Markus Linck[1], Andreas Burck[1], Hannes Rotzinger[1], Andreas Fleischmann[1], Christian Enss[1], Viatcheslav Zakosarenko[2], Ronny Stolz[2], Jürgen Kunert[2], and Hans-Georg Meyer[2] — [1]Kirchhoff Institute for Physics, Im Neuenheimer Feld 227, D-69120 Heidelberg, Germany — [2]Institute for Physical High Technology, Albert-Einstein-Str. 9, D-07745 Jena, Germany

Metallic magnetic calorimeters (MMC) with Au:Er sensors are used as particle detectors in several research fields like absolute activity measurements of radioactive isotopes, high resolution x-ray spectroscopy and material analysis. The typical energy resolution of MMCs is in the range of few eV at 6 keV, which makes them promising candidates to detect the electrons emitted by ^{187}Re, whose end point energy of the continuous spectrum is about 2.5 keV. The analysis of the ^{187}Re spectrum is nowadays the only competitive technique for direct neutrino mass search besides KATRIN (KArlsruhe TRItium Neutrino experiment) investigating tritium β decay. The work presented describes the development of a MMC configuration that is suitable to detect the β decays occurring in a superconducting rhenium absorber. The detector is based on a gradiometric SQUID with integrated meander-shaped pickup coil. We discuss the general performance of the detector, the thermalization times, the noise contributions and the observed energy resolution.

TT 7.55 Mon 14:00 P1

Large area metallic magnetic calorimeters for ^{36}Cl absolute activity measurement — •M. Linck[1], A. Burck[1], E. Leblanc[2], M. Loidl[2], H. Rotzinger[1], T. Scarbrough[1], A. Fleischmann[1], and C. Enss[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Laboratoire National Henri Becquerel, CEA Saclay, France

The measurement of the activity and the energy spetrum of α and β emitting radioactive sources is of great importance in a large number of field ranging from medicine to the characterization of nuclear waste. At the same time the limitations of conventional detector techniques make this effort a highly non-trivial problem in radion metrology. Usually a number of techniques has to be combined including liquid scintilation detectors which are known for their poor energy resolution and energy dependent quantum efficiency. We have developed a detector based on a metallic magnetic calorimenter (MMC), with a metallic absorber that covers the full solid angle of 4-π around the source. Because of the calorimetric principle it has equal sensitivity for α, β and γ radiation and a quantum efficiency of nearly 100%. The MMC is based on a planar Au:Er Sensor and a meander-shaped pickup coil. We will show the data of a first experiment measuring the decay of ^{36}Cl and compare the result to the theoretically expected spectrum for this second order forbidden β^--decay. We discuss the observed contributions to the noise, the quantum efficiency and the achieved energy resolution.

TT 7.56 Mon 14:00 P1

Study of superconducting and magnetic microcalorimeters for a high sensitivity neutrino mass measurement experiment — •Loredana Gastaldo[1,2] and Daniel Haug[1] — [1]Kirchhoff Institute for Physics, Im Neuenheimer Feld 227, D-69120 Heidelberg, Germany — [2]University and INFN Genoa, Via Dodecaneso 33, I-16146 Genoa, Italy

Since the neutrino oscillation experiments have proved that neutrinos are massive particles, the question if it is possible to determine its absolute value can be addressed with a very high precision β decay experiment. An international collaboration is growing around the project of Microcalorimeter Arrays for a Rhenium Experiment (MARE) for measuring the neutrino mass with a sensitivity of about $0.2eV/c^2$. Here we present the status of the development of superconducting and magnetic low temperature microcalorimeters for the detection of ^{187}Re beta decay.

TT 7.57 Mon 14:00 P1

Commensurability and ratchet effects in Nb thin films with artificial pinning site — •M. Kemmler[1], C. Gürlich[1], H. Pöhler[1], M. Siegel[2], M. Neuhaus[2], R. Kleiner[1], and D. Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen — [2]IMS, Universität Karlsruhe, Hertzstr. 16, D-76187 Karlsruhe

We investigate artificial pinning arrays - formed by (sub-) micron-sized holes (antidots) of various shape in Nb thin films. For measurements of electric transport and low-frequency noise we use a highly sensitive liquid Helium-cooled dc SQUID amplifier. The sample temperature is controlled and stabilized close to the Nb transition temperature T_c via an optical, essentially noiseless heating system. Measurements of critical current I_c vs. magnetic flux density B close to T_c reveal pronounced matching effects, i.e. an enhancement of I_c when the flux line lattice is commensurate with the antidot lattice. We also find such matching effects in the low-frequency flux noise, i.e. a suppression of the flux noise at the matching fields. By reshaping the artificial pinning sites it is possible to construct Abrikosov-vortex-ratchets [1,2]. For our measurements of ratchet effects triangular antidots are used. Measurements of the vortex response to an ac current drive reveal pronounced voltage rectification. We find a strong dependence of the voltage output on temperature, ac current amplitude and the magnetic field.

[1] J. Van de Vondel et al., Phys. Rev. Lett. **94**, 057003 (2005) .
[2] J. E. Villegas, et al., Science **302**, 1188 (2003).

TT 7.58 Mon 14:00 P1

Polarised neutron scattering on the flux line lattice (FLL) in Niobium — •Sebastian Mühlbauer[1], Robert Georgii[2], and Peter Böni[1] — [1]Physikdepartment E21, TU-München, 85747 Garching — [2]ZWE FRM-II, 85747 Garching

Recent polarised small angle neutron scattering (SANS) measurements of the flux line lattice (FLL) of superconducting niobium, performed on the SANS-2 at GKSS and on MIRA at the FRM-II showed clear polarisation dependent scattering, similarly measured by [1,2], that cannot be explained by means of the ideal model of the FLL. In ideal isotropic superconductors no spin dependent scattering occurs, because the flux lines are orientated parallel to the applied magnetic field B as well as the polarization of the neutrons is parallel to B [3]. Spin dependent scattering only occurs either i) assuming a non zero nuclear scattering length distribution with the same periodicity as the FLL (interference term) corresponding to the pinning centres or ii) assuming an individual bending of the flux lines, ruling out the geometrical constraint $B \parallel FLL$. We present new results, obtained by means of polarised neutron scattering on several niobium samples of a different residual resistivity ratio (RRR) and hence different pinning properties. These measurements were conducted on the cold spectrometer MIRA at the FRM-II in Garching.

[1] K. Neumann, et al, Eur. Phys. J. B **1**, 5-9, (1998)
[2] Experimental Report 5-51-229
[3] E. M. Forgan, et al., Physica B **267-268**, 115 (1999)

TT 7.59 Mon 14:00 P1

Vortex Matching in Niobium Films with Periodic Pinning Arrays produced by Micellar Technique — •M. Oettinger[1], J. Eisenmenger[1], C. Steiner[1], C. Pfahler[1], S. Brieger[1], A. Plettl[1], A. Dietrich[1], B. Koslowski[1], H.-G. Boyen[1], A. Ethirajan[1], P. Walther[2], and P. Ziemann[1] — [1]Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Zentrale Einheit Elektronenmikroskopie, Universität Ulm, D-89069 Ulm, Germany

An enhanced stability of a vortex lattice is expected whenever it matches a regular array of pinning centers without disturbing its preferred triangular order. The observation of such matching effects is challenging at temperatures much smaller than the critical temperature since artificial pinning centers should have sizes of a few nanometers, i.e. comparable to the coherence length, and should be periodically arranged. For the preparation of a triangular lattice of artificial pinning centers we

first prepare a closed packed monolayer of $HAuCl_4$ loaded inverse micelles of diblock-copolymers onto a substrate. By applying a H-plasma the micelles are transformed into a triangular lattice of Au particles with diameters ≈ 10 nm. The particles serve as an etching masks for patterning arrays of pillars into the surface of a Si substrate. In a Nb thin film grown on top, pinning centers are formed at the pillars. Clear matching effects are observed even at temperatures much lower than the critical temperatures. Moreover an unusual "second"critical current is observed, indication two very different types of pinning mechanisms: Strong pinning on artificial pinning centers and weaker pinning by natural, randomly positioned pinning centers and "caging"in interstitial regions.

TT 7.60 Mon 14:00 P1

Enhancement of the vortex pinning in superconducting MgB_2 films — •Anatolie Sidorenko[1,2,3], Vladimir Zdravkov[1,2], Christian Leierer[2], Andreas Heinrich[2], Siegfried Horn[2], Reinhard Tidecks[2], Achim Wixforth[2], Thomas Koch[3,4], and Thomas Schimmel[3,4] — [1]IAP, LISES, ASM, Kishinev, Moldova — [2]IP, Universität Augsburg, Germany — [3]AP, Universität Karlsruhe, Germany — [4]INT, Forschungszentrum Karlsruhe, Germany

Superconducting MgB_2 films have extremely high critical current density, up to $j_c \sim 10^7/cm^2$ at 15 K in zero magnetic field what makes this novel superconductor very attractive for technical applications. But magnesium diboride exhibits a rapid loss of the current carrying capabilities in strong magnetic fields, caused by thermomagnetic instabilities leading to a rapid decrease of the activation energy for magnetic flux motion for $U_0(B)$ in fields of $B > 1$ Tesla. There are two possible ways to solve the problem of the too low pinning force for high magnetic fields: a) by covering the MgB_2 film with an electronicly isolated highly thermoconducting metallic layer to prevent thermomagnetic instabilities; b) by embedding artificial pinning centers within the film to increase the pinning force and thus the activation barrier for thermally activated flux flow. In the present work we report about the results of our experiments where we used both ways: a) coating of the MgB_2 film with Cu-layers ($0.3\mu m - 1.0\mu m$ thick) for thermo stabilization; b) the adsorption of ferromagnet nanoparticles (10nm - 50nm Fe and Ni particles) on the surface of the MgB_2 film.

TT 7.61 Mon 14:00 P1

Granularity and Spontaneous Vortex State for the Weakly Ferromagnetic Superconductor $RuSr_2GdCu_2O_8$ — •Thomas P. Papageorgiou[1], Ennio Casini[2], Hans F. Braun[2], Thomas Herrmannsdörfer[1], Andrea D. Bianchi[1], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Rossendorf, D-01314 Dresden, Germany — [2]Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

In the high-T_c cuprate $RuSr_2GdCu_2O_8$ (Ru1212) weak ferromagnetism ($T_N^{Ru} \simeq 130$ K) coexists with superconductivity ($T_{c,onset} \simeq 50$ K). This rises the interesting question concerning the formation of a spontaneous vortex state (SVS) in the case that the internal magnetic field is greater than the first critical field H_{c1}. Recently, the formation of a SVS has been proposed for Ru1212 after the phase diagram for this compound was constructed from dc-magnetization and resistance measurements [1]. We show, by a comparison of resistance with ac-susceptibility and dc-magnetization measurements, where both the intra- and inter-granular superconducting transition are obvious, that the granular nature of the investigated samples has to be carefully considered in the investigations of possible SVS formation. A particular SVS with vortices pinned in the intergrain area is much more likely. Single crystals would be required to unambiguously demonstrate the formation or non-formation of a spontaneous vortex state in bulk Ru1212.

[1] C. Y. Yang, B. C. Chang, H. C. Ku, Y. Y. Hsu, cond-mat/0507014

TT 7.62 Mon 14:00 P1

Evidences for Flux Line Termination Inside of a Highly Anisotropic Superconductor: A Magnetic Force Microscopy Study — •Ung Hwan Pi[1], Alexander Schwarz[1], Marcus Liebmann[2], Zheong Gu Khim[3], Dong Ho Kim[4], and Roland Wiesendanger[1] — [1]University of Hamburg, IAP, Jungiusstr. 11, 20355 Hamburg — [2]Present Address: RWTH Aachen, Department of Physics, 52056 Aachen — [3]School of Physics, SNU, Seoul 151-742, South Korea — [4]Dept. of Physics, Yeungnam University, Kyungsan, South Korea

In highly anisotropic layered superconductors like $Bi_2Sr_2CaCu_2O_{8+\delta}$, the Josephson coupling between each layer is so weak that the phase coherence in c-direction is negligible and the termination of the flux line inside the sample is not forbidden by topology of the phase. Mints *et al.*[1] have reported in a theoretical study that the termination of the flux line inside the sample is energetically favorable for small enough samples. Our magnetic force microscopy study performed on the $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal showed some evidences supporting this prediction. Since all flux lines have single flux quantum, they should exhibit the same contrast. However, we could observe a somewhat weaker contrast at several flux lines near an antiphase boundary. Two weak-contrast flux lines sometimes merged into one flux line with a stronger contrast. These weak magnetic contrasts are possible candidates for flux lines terminating beneath the sample surface.

[1] G. Mints *et al.* Phys. Rev. B **61**, 1623 (2000).

TT 7.63 Mon 14:00 P1

The transverse sound propagation in the superfluid helium inside carbon nanotube — •Vilchynskyi Stanislav and Tkachenko Olena — Kiev national Taras Shevchenko university

In the present work it was shown that it is possible of the propagation of the transverse quantized sound in superfluid helium inside carbon nanotube. This sound are caused of the geometrical parameters of the helium system and dynamical characteristic of the vortex thread in superfluid helium

TT 7.64 Mon 14:00 P1

Study the dependence between the pair interaction potential in the Bose liquid ^{4}He and and quasiparticle spectrum of superfluid ^{4}He at $T = 0$ — •Vitaliy Bardic and Stanislav Vilchynskyi — Kiev national Taras Shevchenko university

As well known the multiparticle collective effects in the Bose liquid lead to an essential renormalization of the pair interaction between atoms of superfluid helium. Self-consistent numerical calculations of the boson self-energy, polarization operator, pair order parameter, and quasiparticle spectrum of superfluid ^{4}He at $T = 0$, involving an iteration scheme with the single fitting parameter—the value of the repulsion potential at $r = 0$, have allowed us to find conditions for the theoretical spectrum $E(p)$ to coincide with the experimentally observed elementary excitation spectrum in ^{4}He. It is shown that the roton minimum in the quasiparticle spectrum $E(p)$, which corresponds to a maximum in the structural formfactor $S(q)$ of a Bose liquid, is directly associated with the first negative minimum of the Fourier component of the renormalized potential $\tilde{V(p)}$ of the pair interaction between bosons.

TT 7.65 Mon 14:00 P1

The Kinetics Asymmetry of the BCC-HCP Phase Transition in Solid Helium-4 — •Yegor Vekhov, Nikolay Mikhin, Andrey Polev, Eduard Rudavskii, and Alexandr Birchenko — B.Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov 61103 , UKRAINE

The subject of research is a solid helium-4. Samples were made by blocking capillary technique. The kinetics of the BCC-HCP structure phase transition was investigated by precise pressure measurement under constant value. The precision of pressure measurement is about 3 mbar and of temperature one is about 5 mK. During step wise temperature changes, within one phase (BCC or HCP), pressure change is described by one-exponential time dependence. During step wise cooling of the sample from the BCC region to the HCP it was found the pressure, at first, is decreasing to the extent of thermal compression of the overcooling BCC phase then, after some delay (5-500 s), the pressure is relaxing once again that is accompanied by a heat generation. The second stage of the pressure relaxation is described by superposition of two exponential dependences with short time constant (1-3 s - directly the BCC-HCP transition) and with long time constant (5-10 s - the relaxation process of defects which were formed during lattice rebuilding). During the inverse HCP-BCC phase transition the delay is practically not observed that can be explained by less BCC nucleation energy [1,2].

[1] T.A.Johnson and C.Elbaum, J. Low Temp.Phys., 107, 317 (1997). [2] Y.Okuda, H.Fujii, Y.Okumura, and H.Mackana, J. Low Temp.Phys., 121, 725 (2000).

TT 7.66 Mon 14:00 P1

Light scattering on an N-component Bose-Einstein condensate in an optical lattice — •Oleksandr Fialko, Christopher Moseley, and Klaus Ziegler — Universität Augsburg, Universitätsstr. 1,D-86135 Augsburg, Germany

We consider an N-component system of strongly interacting bosons in an optical lattice. On each lattice site a boson can occupy one of N different states. Tunneling is possible between neighboring lattice sites and different states. For this model we calculate the static structure factor and the density-density correlation function, both for zero and finite temperatures,in the limit $N \to \infty$ and in a $1/N$ expansion to study the properties of the BEC and the Mott-insulating phase.

TT 7.67 Mon 14:00 P1

Low-temperature investigation on thermal properties of glasses — •Astrid Netsch[1], Sabine Wolf[1], Hsin-Yi Hao[2], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg, Germany — [2]Jet Propulsion Laboratory, California Institute of Technology. Pasadena, California 91103, USA

The thermal conductivity of glasses at temperatures below 1 K is generally described by phononic thermal transport. The mean free path of the phonons is limited by scattering processes between heat-carrying phonons and tunneling systems. It seems plausible that mutually interacting tunneling systems can also contribute to thermal transport in glasses. This additional transport channel is supposed to be extremely small compared to the phononic contribution. We have performed experiments on the thermal conductivity of a glass capillary array which contains holes on a triangular lattice that serve as extra scatterers for thermal phonons. For measuring thermal conductivity of such diminutive magnitude, our contact-free technique has proven to be a suitable choice because of its extremly small parasitic heating. Our results show a thermal conductivity which varies roughly with T^3 down to about 50 mK as expected for boundary scattering of phonons. Below this temperature, the thermal conductivity deviates from this dependence and follows a weaker power law. So far it is not clear whether this deviation is caused by a non-phonon contribution to the thermal transport in glasses, or if a cross-over regime occurs in which the wave length of the thermal phonons becomes comparable with the lattice constant of the array of holes.

TT 7.68 Mon 14:00 P1

Dielectric polarisation echos on partially deuterated organic glassformers — •Marek Bartkowiak[1], Masoomeh Bazrafshan[1], Herbert Zimmermann[2], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kichhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Max-Planck-Institut für medizinische Forschung, Heidelberg, Germany

The properties of amorphous solids are governed by tunnelling systems, at temperatures below a few Kelvin. Ever since tunnelling processes were considered to describe the anomalous low temperature behaviour of glasses the question about their microscopic origin is posed. Newly discovered magnetic field effects in the dielectric properties of glasses containing atoms with nuclear quadrupole moments have opened a path to a possible microscopic theory of tunnelling processes in amorphous materials. Recent studies of the magnetic field dependence of polarisation echos generated in partially deuterated glycerol have provided first insights regarding the tunnelling motion of glycerol molecules. We have now extended our investigations towards other organic glassformers. We present first data and discuss possible conclusion about the microscopic nature of tunnelling systems in these materials.

TT 7.69 Mon 14:00 P1

Quantum oscillations of thermoelectric force in quasi-two-dimensional conductors — •Danica Krstovska and Olga Galbova — Faculty of Natural Sciences, Department of Physics, P. O.Box 162, Skopje, Macedonia

The dependence of the thermoelectric force transverse to the layers in a layered conductor with a quasi-two-dimensional electron energy spectrum on the magnitude and orientation of the strong magnetic field in relation to the layers is theoretically analyzed. Giant quantum oscillation of the thermoelectric field versus 1/H, have been predicted, which will facilitates the experimental study of quantum oscillatory effects. It is shown that when the temperature gradient is directed along the normal n to the layers, the amplitude of the quantum oscillations substantially exceeds the smoothly varying part of the thermoelectric force transverse to the layers. This quantum oscillation effect can be used to a high degree of accuracy as a good spectroscopic method for experimental study of the characteristics of the Fermi surface of layered conductors.

TT 7.70 Mon 14:00 P1

Effect of H_2 and D_2 impurities on the structure and properties of solid Ne. Phase diagram of binary system Ne-nD_2 — •Nikolay Galtsov, Prokhvatilov Anatolii, and Strzhemechny Mikhail — Verkin Institute for Low Temperature Physics and Engineering of NAN Ukraine, 47 Lenin ave., Kharkov, 61103, Ukraine

Solid solutions of normal hydrogen and deuterium with neon, quench deposited from gas mixtures, were studied by powder x-ray diffraction for hydrogens contents from 2 to 70 mol.-% at temperatures from 5 K to melting temperatures. The structure of Ne-nH_2 and Ne-nD_2 condensates was investigation immediately after preparation. The boundary of homogeneous cubic hydrogen-in-neon solutions has been established to be about 2 mol-%, deuterium-in-neon - to be about 5 mol-%, under the specific sample preparation conditions. At higher nominal H_2 (D_2) concentrations, a hexagonal hcp_2 phase in addition to the cubic *fcc* phase forms. The volumes of the elementary cells of both phases are close to that of pure neon. The phase hcp_2 seems to be a perfect storage of hydrogen and deuterium: it can contain up to 85 mol.-% H_2 and up to 60 mol-% D_2. The hcp_2 disappeared as the condensates were warmed up to the melting temperatures. The metastable hexagonal phase observed in neon-rich mixtures studied here is apparently identical in nature to that found previously in hydrogen-rich mixtures: both hexagonal phases have roughly the same lattice parameters. The phase boundaries have been established for the entire entration range and proposed a full of phase diagram Ne-nD_2.

TT 7.71 Mon 14:00 P1

Thermal Conductivity of Solid Ethanol in the Three Polymorphous Phases — •Alexey Yushchenko, Alexander Krivchikov, Korolyuk Oksana, Gorodilov Boris, and Manzhelii Vadim — B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine

Solid ethyl alcohol can be obtained in three metastable long-living phases - position glass, an orientationally-disordered (static disorder) crystal (orientational glass) and a crystal with dynamic orientational disorder. The orientationally - ordered monoclinic - system crystal is the only thermodynamically equilibrium solid phase of the alcohol.
In this work the temperature dependence of the thermal conductivity of solid ethanol was measured in all solid phases under equilibrium vapor pressure at 2-159 K by the steady-state potentiometric method. The glass phase was obtained by cooling the container with liquid nitrogen at an extremely high rate (over 50 K/min). The orientationally - disordered bcc crystal phase was formed on hardening the slowly overcooled liquid at T = 125 K. An orientationally - ordered crystal evolved in the process of rapid crystallization provoked by heating the bcc phase to over 116 K. The recrystallized sample was then annealed for several days at a temperature close to the melting point.
Obtained data have been analyzed in the borders of the soft potential model.

TT 7.72 Mon 14:00 P1

Thermal conductivity of gas clathrate hydrates at low temperatures — •Olesya Romantsova, Alexander Krivchikov, Gorodilov Boris, Korolyuk Oksana, and Manzhelii Vadim — B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine

Clathrate hydrates are open polymorphous crystal structures related to ordinary ice. However, $\kappa(T)$ of gas hydrates is similar to glass. The understanding of the causes responsible for the glass-like behavior in gas hydrates will be helpful in finding a microscopic mechanism of the thermal transport in disordered solids.
The thermal conductivity of the THF and xenon hydrates has been measured using the steady-state technique in the intervals 2-220 K and 2-170 K, respectively. Two samples of THF hydrate were grown in the measuring cell during 7 min (fast cooling) and 70 min (slow cooling). For the sample of THF hydrate (slow cooling) in the interval 15-97 K and for xenon hydrate in the interval 56-97 K the behavior of $\kappa(T)$ shows an anomaly: the thermal conductivity decreases by almost over 50 per cent as the temperature increases. This observation is attributed to the consequence of resonant scattering where the coupling of the lattice with "rattling" motions of Xe dominates the thermal resistivity at high temperature. The thermal conductivity in the low temperature regime is found to follow the prediction of the soft-potential model. The comparative analysis of the thermal conductivities of two hydrates with different guest molecules can provide new information about the mechanisms of phonon scattering in crystal hydrates.

TT 7.73 Mon 14:00 P1

Electron diffraction study of clusters formed in a supersonic jet of Ar-Kr gas mixture — •Oleksandr Danylchenko, Spartak Kovalenko, and Vladimir Samovarov — B. Verkin Institute for Low Temperature Physics and Engineering of the NASU, 47, Lenin Ave., 61103 Kharkiv, Ukraine

Rare-gas clusters, characterized by a relatively simple character of the atomic interaction forces, are convenient model objects for testing various theoretical scenarios that describe mechanisms and velocities of formation of various physical properties in macrosystems. Rare-gas clusters also can serve as a model system for the metallic clusters, which are important from the viewpoint of their application. A large amount of papers are dedicated to the study of the structure of pure rare gases. At the same time, multicomponent clusters are much less studied so far. Here we study the structure and nucleation of clusters formed in an adiabatically expanding gas mixture Ar-Kr by electron diffraction. We found that small admixtures of Kr (1000 and 5000 ppm) cause an essential increase in Ar cluster size. This effect is due to the substitution of the heterogeneous clusterization for the homogeneous one. In this case, core aggregations are composed mainly of Kr atoms. This result correlates well with the data of optical measurements. It is also shown that at great concentrations of Kr (200000 ppm) only Kr clusters are formed. Argon is a carrying gas and favors temperature lowering in the Kr aggregations. We demonstrate that in large crystalline clusters (10^4-10^5 atoms per cluster) an hcp structure is realized. We discuss possible processes responsible for the formation of the hcp structure.

TT 8 Correlated Electrons: Heavy Fermions

Time: Monday 14:30–17:45 Room: HSZ 301

TT 8.1 Mon 14:30 HSZ 301

Tunneling spectroscopy experiments on epitaxial UNi_2Al_3 thin films — •Andrey Zakharov, Martin Jourdan, and Hermann Adrian — Johannes Gutenberg-University, Institute of Physics, Staudinger Weg 7, 55128 Mainz, Germany

We are presenting the results of tunneling spectroscopy experiments performed on the heavy fermion superconductor UNi_2Al_3. Planar junctions consisting of an a*-axis oriented UNi_2Al_3 thin film as a base electrode, AlOx insulating layer and a metal counter electrode were prepared employing an in vacuo process. The MESA structures made by photolitography were investigated as well as simple cross-junctions. The observation of the well-known superconducting density of states of the counter electrode (Pb) allows the evaluation of the junction quality. The tunneling conductivity will be discussed in the framework of density of states and barrier effects.

TT 8.2 Mon 14:45 HSZ 301

Electronic properties of a*-oriented thin films of the Heavy-Fermion superconductor UPd_2Al_3 — •Michael Foerster, Martin Jourdan, and Hermann Adrian — J.-Gutenberg-Universität Mainz

By combining epitaxial thin films in a*-orientation of the hexagonal unit cell with optical lithography, we were able to perform precision measurements of temperature dependent resistivity and Hall effect. In contrast to the isostructural, isoelectronical UNi_2Al_3, no dependence of the superconducting transition on the current direction was observed. Also the Hall measurements show only a small anisotropy, and the low temperature behaviour can be understood using Fermi liquid theory.

Additionally, resonant magnetic x-ray scattering confirmed the existence of complete long range magnetic order in the samples, proving the high quality of our thin films. Tunneling experiments in a*-direction are of high interest to further investigate the symmetry of the unconventional sc-order parameter in this model system for Heavy-Fermion superconductivity. First results of such experiments will be presented.

TT 8.3 Mon 15:00 HSZ 301

High pressure study of $YbIr_2Si_2$ — •M. Nicklas, H. Q. Yuan, Z. Hossain, C. Geibel, and F. Steglich — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany.

We present a high pressure study of the electrical transport properties of the heavy fermion compound $YbIr_2Si_2$ in the temperature range down to 60 mK and for pressures up to 10 GPa. On basis of the resistivity data we establish a pressure-temperature phase diagram. At atmospheric pressure $YbIr_2Si_2$ exhibits a Landau Fermi-liquid state below 200 mK which persists upon applying pressure. For $P \geq 7$ GPa a drop in resistivity indicates the development of antiferromagnetic order at low temperatures. The Neél temperature is increasing with further increasing pressure. We compare our results on $YbIr_2Si_2$ to $YbRh_2Si_2$.

TT 8.4 Mon 15:15 HSZ 301

The role of geometrical frustration in $YbInCu_4$, where In is substituted with Cd or Rh — •Veronika Fritsch[1,2], Joe D. Thompson[1], and John L. Sarrao[1] — [1]Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

$YbInCu_4$, which is well-known for its unique first-order valence transition, crystallizes in the cubic $AuBe_5$-structure, as do all compounds RInCu$_4$ with R = Gd - Lu. In this structure the magnetic rare-earth ions are located on a fcc-lattice and therefore form networks of tetrahedra. Geometrical frustration of magnetism was discovered in the compounds RInCu$_4$ (R = Gd - Tm)[1]. Substitution of In in RInCu$_4$ with Cd increases the electrical conductivity significantly and therefore destroys the frustration. The high-temperature phase of $YbInCu_4$ is equivalent to the frustrated RInCu$_4$ compounds: the localized magnetic moments of the Yb form a fcc-lattice. However, the frustration found in the other RInCu$_4$ compounds can not be found in $YbInCu_4$ at low temperatures due to the valence transition destroying the localized magnetic moment. Substituting In with Cd or Rh initially raises the temperature of the valence transition and subsequently suppresses it. While Cd-substitution not only suppresses the valence transition but also the frustration due to enhancement of conductivity, Rh-substitution preserves the low electrical conductivity. Here we present measurements of the magnetic and transport properties of the two series $YbIn_{1-x}Cd_xCu_4$ and $YbIn_{1-x}Rh_xCu_4$ and discuss the role of geometrical frustration in both systems.
[1] V. Fritsch *et al.*, Phys. Rev. B **71**, 132402, (2005)

TT 8.5 Mon 15:30 HSZ 301

Quasi quartet CEF ground state with possible quadrupolar ordering in the tetragonal compound $YbRu_2Ge_2$ — •H. S Jeevan[1], Z Hossain[2], and C Geibel[1] — [1]MPI-CPfS Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Physics, I.I.T-Kanpur, 208016. India

In search for new Yb-base stoichiometric systems which are close to quantum critical point at ambient pressure, we have synthesized and investigated single crystals of $YbRu_2Ge_2$, an homologue of $YbRh_2Si_2$. From the systematic of the known YbM_2X_2 (M = d elements, X = Si, Ge) we had hoped that this compound will be nonmagnetic and located close to a QCP. But surprisingly we found that in YbRu2Ge2, Yb is in a stable trivalent state and present some kind of ordering at a much higher temperature Tm =10K then in presently known Yb-compounds. High temperature magnetic susceptibility follows Curie-Weiss behavior with effective moment very close to that expected for trivalent Yb ions. Low temperature susceptibility exhibits a peak at ~6 K presumably due to antiferromagnetic type of order. Resistivity linearly decreases with temperature down to about 50 K, then increases with further decreasing temperature due to Kondo interaction, passes though a maximum at 10 K below which the resistivity undergoes a rapid decrease due to freezing out of spin disorder scattering. The Specific heat of $YbRu_2Ge_2$ shows two large peaks, one at 10K and another at 6K, the low temperature anomaly corresponding to the antiferromagnetic transition as detected by chi(T). The nature of the high temperature anomaly in specific heat is under investigation.

TT 8.6 Mon 15:45 HSZ 301

Field-induced enhancement of the linear static susceptibility in heavy-fermion YbAgGe — •P. G. Niklowitz[1,2], C. Paulsen[3], S. L. Budko[4], P. C. Canfield[4], and J. Flouquet[1] — [1]DRFMC/SPSMS/CEA-Grenoble, F-38054 Grenoble Cedex 9, France — [2]Physik Department, E21, Technische Universität München, James-Franck-Str., D-85748 Garching — [3]CRTBT/CNRS, BP 166, F-38042 Grenoble Cedex 9 — [4]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Hexagonal YbAgGe is a recently discovered heavy-fermion (HF) system with $T_K \approx 25$ K, γ of a few hundred mJ/molK^2 and planar magnetic anisotropy $\chi_{ab}/\chi_c \approx 3$ at low temperatures. Two antiferromagnetic phases AF1 and AF2, become fully suppressed with fields $H_{c1} = 1.9$ T and $H_{c2} = 3.0$ T, when the field is applied in the *ab*-plane. Furthermore, there are indications for a transition or crossover at a field $H_{c3} = 4.9$ T and low-T resistivity measurements suggest a strong enhancement of thermally excited fluctuations close to H_{c3}. The resistivity is non-Fermi-liquid (NFL) like close to H_{c3}. We have now measured the magnetisation of single crystals of YbAgGe up to 8 T and down to 50 mK with the field applied along the a-axis. The results confirm the first-order character of the transition between the AF1 and AF2 phase. No clear signature of the suppression of the AF2 phase is found. However, the static linear susceptibility becomes enhanced when approaching H_{c3}, especially at the lowest temperatures. This enhancement suggests that magnetic fluctuations are at the origin of field-induced NFL behaviour in YbAgGe, but that ferromagnetic fluctuations are not the only ingredient.

— 15 min. break —

TT 8.7 Mon 16:15 HSZ 301

$CeCu_{6-x}Au_x$ NMR studies Part I - crystal field analysis and the assignment of Cu sites — •Bernd Pilawa, Max Winkelmann, Gerda Fischer, and Elmar Dormann — Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

In $CeCu_{6-x}Au_x$ the Ce^{3+} $4f^1$ $^2F_{5/2}$ groundstate is split into three doublets. The crystal field splitting is known from neutron scattering forx=0.5 and 0. A calculation of the magnetic susceptibility using one antiferromagnetic molecular field constant λ as approximation for the Kondo like shielding and the influence of orbit and spin scattering on the interaction of the Ce moments describes the experimental data quite well.

We managed to calculate the electric field gradients at the 5 inequivalent Cu sites of $CeCu_6$ with the WIEN2k-Software-Package. Spectra generated with these parameters fit to NMR-spectra measured for oriented single crystal powder samples at various temperatures between 5k and 100k at a magnetic field of 7T. Therefore the information in various NMR- and NQR-studies can now be compared to the crystallographic information.

TT 8.8 Mon 16:30 HSZ 301

$CeCu_{6-x}Au_x$ NMR studies Part II - Analysis of NMR line shift — •Max Winkelmann[1], Bernd Pilawa[1], M.S.S. Brooks[2], and Elmar Dormann[1] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Commission of the European Communities, Joint Research Center, Institut of Transuranium Elements, D-76021 Karlsruhe, Germany

We have carried out various NMR-measurements on the well-known heavy-fermion system $CeCu_{6-x}Au_x$. As a result we present Cu-site specific bare Knight shift data and transferred hyperfine interaction coupling constants α in thetemperature range from 100K down to 5K, derived from NMR-spectra in a magnetic field of 7T. The interaction coupling constants are showing alternating signs which can be understood by the variing contribution of s,p and d electrons which are calculated by ab initio self-consistent band structure calculations.

While substituting the Cu(2)-site with Au the transferred hyperfine interactioncoupling constants decrease, whereas the absolut line-shift is increasing. Thiscould be explained by a larger susceptibility of $CeCu_5Au_1$. For one of the Cu sites evidence for the anisotropy of the transferred field coupling constant is obtained.

TT 8.9 Mon 16:45 HSZ 301

Probing the Electronic Properties of the Heavy-Fermion Superconductor $CeCoIn_5$ — •G. Goll[1], T. Brugger[1], M. Marz[1], T. Sayles[2], and M. B. Maple[2] — [1]Phys. Inst., Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Inst. for Pure and Applied Phys. Sciences, University of California, San Diego, La Jolla, CA 92093, USA

In many U- and Ce-based heavy-fermion superconductors, as well as in the oxide superconductors, the superconducting (sc) properties differ from those of a classical superconductor due to the presence of strong electron-electron correlations [1]. A recent example is $CeCoIn_5$, a heavy-fermion superconductor with $T_c = 2.3$ K, where among other exotic properties a power-law behavior of the thermodynamic and transport properties in the sc state gives evidence that the order parameter (op) has line nodes and probably $d_{x^2-y^2}$ symmetry. Several groups performed point-contact (pc) experiments on $CeCoIn_5$ in order to elucidate the gap structure. However, there is still some controversy on the interpretation of the structures in the differential conductance dI/dV vs. V which has mainly to do with the determination of the regime of current flow through the pc. We report on measurements of dI/dV vs. V on Pt-$CeCoIn_5$ pc's in the normal and sc states down to 30mK in zero and applied magnetic fields and we discuss the pc regime in detail. In the normal state the spectra exhibit a pronounced asymmetry which is not affected by an applied field up to $B = 6$ T. The spectra in the sc state support a *d*-wave op scenario for $CeCoIn_5$, in line with the pc data obtained by other groups. [1] G. Goll: *Unconventional Superconductors*, STMP, Vol. 214, Springer-Verlag 2005.

TT 8.10 Mon 17:00 HSZ 301

Fermi surface and renormalization effects in heavy fermion superconductors — •Andreas Koitzsch[1], Sergey Borisenko[1], Jochen Geck[1], Volodymyr Zabolotnyy[1], Dmytro Inosov[1], Martin Knupfer[1], Jörg Fink[1], Bernd Büchner[1], and Eric Bauer[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Los Alamos National Laboratory, Los alamos, Mew Mexico 87545, USA

The heavy fermion compounds of the type $CeTIn_5$ (T = Co, Ir, Rh) show a rich variety of interesting solid-state phenomena which have shifted them under the focus of current research. Firstly, the compound $CeCoIn_5$ shows superconductivity below T = 2,3 K at ambient pressure. This is the record value for heavy fermion superconductors. The interplay between the Kondo effect and the RKKY interaction, the close neighborhood between magnetism and superconductivity and the vicinity to a quantum critical point decisively influence the low-energy physics of these systems.

We investigated the electronic structure of this materials by angle-resolved photoemission spectroscopy. We measured the Fermi surface and the band structure along the high-symmetry directions. We compare our results to de-Haas-van-Alphen experiments and to band structure calculations and discuss the signatures of the low-energy mass renormalization.

TT 8.11 Mon 17:15 HSZ 301

Low-energy interactions in the heavy-fermion state of $Ce_3Rh_4Sn_{13}$ — •Ulrike Köhler[1], André Strydom[2], Adam Pikul[1], Silke Paschen[3], Niels Oeschler[1], and Frank Steglich[1] — [1]MPI CPfS, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Physics Dept., University of Johannesburg, South Africa — [3]Institut für Festkörperphysik, TU Wien, Austria

Previous magnetization measurements on $Ce_3Rh_4Sn_{13}$ were reported with a Curie-Weiss behaviour and a small Weiss temperature of -14 K. No magnetic ordering was observed down to 2 K. The resistivity displayed a negative temperature coefficient from room temperature down to 4.2 K apart from a minimum near 30 K, which was attributed to Kondo interactions. These intriguing properties, together with the lack of any thermodynamic data on $Ce_3Rh_4Sn_{13}$ prompted us to study this compound by magnetization, resistivity, Hall effect, specific heat and thermal transport between 40 mK and 300 K and in applied magnetic fields. The results point to the relevance of a particularly small crystal-electric field splitting together with a low-temperature Kondo interaction, both of which become evanescent in the ground state of strongly correlated electrons in $Ce_3Rh_4Sn_{13}$.

TT 8.12 Mon 17:30 HSZ 301

Crossover from divalent to valence fluctuating state of Eu in $EuCu_2(Ge_{1-x}Si_x)_2$ probed by ^{63,65}Cu-NMR — •M. Baenitz[1], Eva Brüning[1], Andrei Gippius[2], Anakan Rajarajan[1], Elena Morozova[2], Zakir Hossain[3], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Moscow State University, Moscow, Russia — [3]Department of Physics, Indian Institute of Technology, Kanpur, India

Temperature dependent ^{63,65}Cu field sweep NMR investigations on a series of $EuCu_2(Ge_{1-x}Si_x)_2$ powder samples (x = 0, 0.3, 0.65, 0.7, 1) are presented. $EuCu_2$ (Ge, Si)$_2$ is unique among Eu-intermetallics because, upon tuning from a divalent antiferromagnetically ordered state for x = 0 to a valence fluctuating state for x = 1, Heavy Fermion behaviour was found around $x \approx 0.7$. The Knight shift ^{63,65}K is negative for all stoichiometries. Hyperfine fields are largest for the antiferromagnetically ordered Ge-rich compounds, and smallest for the valence fluctuating pure silicon compound (x = 1). For the $x = 0.3$ compound, above $T_N \approx 19$K,$^{63}K(T)$ exhibits a Curie-Weiss like behaviour ($\approx -10\%$ at 20 K) whereas for $EuCu_2Si_2$ a temperature independent shift of $^{63}K(T) \approx -1.5\%$ is found. Our results are discussed in terms of formation of heavy quasiparticles and/or presence of valence fluctuations of Eu.

TT 9 Transport: Nanoelectronics III - Molecular Electronics

Time: Monday 14:00–17:45 Room: HSZ 304

TT 9.1 Mon 14:00 HSZ 304

Franck-Condon blockade beyond sequential tunneling — •Jens Koch[1], Felix von Oppen[1], and A. V. Andreev[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Department of Physics, University of Washington, Box 351560, Seattle, WA 98195, U.S.A.

Recent studies of electronic transport through single-molecule devices have revealed that the coupling of electronic degrees of freedom to a well-defined mode of molecular vibrations may result in a significant current suppression (Franck-Condon blockade). This effect also has characteristic consequences for Fano factors and noise spectra. However, similar to the case of Coulomb blockade, higher-order processes beyond sequential tunneling may become relevant in the blockade regime. Here, we discuss the effects of such corrections on the current-voltage characteristics and noise properties of the system.

TT 9.2 Mon 14:15 HSZ 304

Electromechanical properties of a biphenyl transistor — •Andrea Donarini, Utpal Sarkar, Milena Grifoni, and Klaus Richter — Theoretische Physik, Universitätsstraße 31, D-93053 Regensburg

Electrical transport through gated single molecules (also called molecular transistors) has become since a few years an active research field both theoretically and experimentally [1]. We investigate the interplay between electrical and mechanical degrees of freedom in transport across a biphenyl molecule in the Coulomb blockade regime. In particular, we analyze the role played in the electrical transport by the twisting mode between the phenyl rings. At low biases we can restrict our analysis to the neutral and anionic (one extra electron) state of the molecule only. The neutral molecule has two stable configurations at finite dihedral angles ($\theta \approx \pm\pi/4$) while the anion state is planar. Charge transitions between the electrical states are thus modulated by Franck Condon amplitudes that account for the torsional degree of freedom yielding big phonon blockade effects [2]. We study the system using a generalized master equation for the reduced density matrix. We find that, due to the mechanically degenerate neutral state, the coherencies and not only the populations of the reduced density matrix determine the transport characteristics [3].

[1] A. Yacoby *et al.* Nature **436**, 677 (2005)
[2] J. Koch, F. von Oppen, Phys. Rev. Lett. **94**, 206804 (2005)
[3] A. Donarini, U. Sarkar, M. Grifoni and K. Richter in preparation

TT 9.3 Mon 14:30 HSZ 304

Controlled Nanogap Manufacturing for Single Molecule Contacts by Electromigration — •Veit Wagner, Arne Hoppe, and Jörg Seekamp — International University Bremen

Electrical measurements of single molecules require a pair of electrodes separated by a nanogap of only a few nanometers. Many preparation methods lack the possibility to form an additional gate electrode. We report on nanogap formation by electromigration using the substrate as additional gate electrode. A small metal wire of typically 100 nm width is broken by imposing a high current density at l-He temperature. At room temperature (RT) this approach usually leads to gaps much larger than molecular sizes. Recently Strachan et al. reported on successful nanogap production at RT by using an active control scheme for the applied voltage in dependence of the measured conductivity of the wire. Following this approach we present an alternative control scheme, which includes in addition the time derivative of the conductivity and the average noise level. Gold nanowires of 100 nm width and 20nm height with a Ti adhesion layer on a SiO2-surface were prepared by e-beam lithography. A current level of about 5 mA is usually sufficient to start the electromigration process at room temperature. We test different wire shapes, e.g. a long thin wire of constant thickness or a thick wire with a lithographically defined short narrowing. We find the long thin wire to be more demanding for our control loop than a wire with a short narrowing. The regulation behavior of our control loop for various regions of the process is discussed. With our approach we can reproducibly manufacture gaps at RT with gap sizes smaller than 10 nm.

TT 9.4 Mon 14:45 HSZ 304

Atomic-Scale Quantum Switches: An Approach towards Quantum Electronics at Room Temperature — •Thomas Schimmel[1,2], Fangqing Xie[1], and Christian Obermair[1] — [1]Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — [2]Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

Using a novel electrochemical approach, we demonstrate the fabrication of bistable atomic-scale metallic point contacts, which can be reproducibly opened and closed by means of a voltage applied to an independent third electrode used as a gate electrode [1]. In this way, an electrical circuit can be opened and closed by the controlled and reproducible reconfiguration of the contacting atoms. After the fabrication of the atomic-scale contact by electrochemical deposition of silver within a nanoscale gap, the bistable configuration of the contact is achieved by an electrochemical cycling process. When the contact is closed, is shows conductance quantization, the conductance being $G_0 = 2e^2/h$ or predefined multiples of this value, the on-state conductance being controlled by the cycling parameters. The device reproducibly operates at room temperature. It represents a first demonstration of an atomic relay or transistor, opening intriguing perspectives for the emerging fields of quantum electronics and logics on the atomic scale.

[1] F.-Q. Xie, L. Nittler, Ch. Obermair and Th. Schimmel, Phys. Rev. Lett. 93, 128303 (2004).

TT 9.5 Mon 15:00 HSZ 304

Spin-dependent transport through individual carbon nanotubes — •Emiliano Pallecchi[1], Dominik Preusche[1], Elsa Thune[1], Benoit Witkamp[2], Alberto Morpurgo[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Kavli Institute of Nanoscience, TU Delft, Netherlands

We report on experiments on carbon nanotubes (CNTs) with ferromagnetic contacts made from $Pd_{0.6}Fe_{0.4}$ alloys. The nanotubes and the micromagnetic properties of the contacts have been characterized by high resolution TEM and Lorentz-microscopy. We have performed low temperature magnetoconductance measurements on individually contacted CNTs as a function of gate voltage and magnetic field. From the weak localization effect in multiwall CNTs we get a signature of the band structure. The low field magnetoconductance shows a hysteretic switching behavior that we attribute to the magnetization reversal of the contacts. The amplitude of the low-field magnetoconductance varies strongly with gate voltage.

TT 9.6 Mon 15:15 HSZ 304

Electron transport in bundles of metallic single-walled carbon nanotubes — •Christoph Wolfgang Marquardt[1], Frank Hennrich[1], Hilbert v. Löhneysen[2,3], and Ralph Krupke[1] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — [2]Universität Karlsruhe, Physikalisches Institut, 76128 Karlsruhe, Germany — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

Concerning the electronic transport properties, an individual metallic single-walled carbon nanotube (SWNT) has been described as a Luttinger liquid system (LL). This regime can describe the power law behaviour found in the temperature dependent conductance, as well as in the voltage dependent differential conductance [1]. In heterogeneous bundles of SWNTs, that are composite bundles of metallic and semiconducting tubes, similar power law behaviour has been observed [2], which implies, that the metallic tubes in a heterogeneous bundle are well decoupled from each other by the semiconducting nanotube matrix. During the fabrication of carbon nanotubes both metallic and semiconducting ones are produced. Using dielectrophoresis as method to separate these types [3], we are able to prepare samples of bundles of exclusively metallic SWNTs, i.e. without the semiconducting nanotube matrix. Here we present measurements of the transport characteristics of such samples, that show obvious deviation from the LL behaviour.

[1] M. Bockrath et al., Nature 397 (1999) 598 [2] R. Krupke et al., Nano Lett. 3 (2003) 1019 [3] R. Krupke et al., Science 301 (2003) 344

TT 9.7 Mon 15:30 HSZ 304

Contact dependence of carrier injection in carbon nanotubes: An *ab initio* study — •Norbert Nemec[1], David Tománek[2], and Gianaurelio Cuniberti[1] — [1]Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824-2320

We combine *ab initio* density functional theory with transport calculations to provide a microscopic basis for distinguishing between 'good' and 'poor' metal contacts to nanotubes. Comparing Ti and Pd as examples of different contact metals, we trace back the observed superiority of Pd to the nature of the metal-nanotube hybridization. Based on large scale Landauer transport calculations, we suggest that the 'optimum' metal-nanotube contact combines a weak hybridization with a large contact length between the metal and the nanotube.

TT 9.8 Mon 15:45 HSZ 304

Scaling law for the conductance of gold nanotubes — •Miriam del Valle[1,2], Carlos Tejedor[1], and Gianaurelio Cuniberti[2] — [1]Dpto. Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]Institute of Theoretical Physics, Universität Regensburg, Germany

A new form of gold nanobridges has been recently observed in ultrahigh-vacuum experiments, where the gold atoms rearrange to build helical nanotubes, akin in some respects to carbon nanotubes. The good reproducibility of these wires and their unexpected stability will allow for conductance measurements and make them promising candidates for future applications . We present here a study of the transport properties of these nanotubes in order to understand the role of chirality and of the different orbitals in conductance. The conductance per atomic row shows a light decreasing trend as the diameter grows, which can be also seen through an analytical formula based on a one-orbital model.

— 15 min. break —

TT 9.9 Mon 16:15 HSZ 304

Electron-vibration interactions in transport through atomic gold wires — •Janne Viljas[1], Juan-Carlos Cuevas[1,2,3], Fabian Pauly[1], and Michael Häfner[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie

The effect of electron-vibration coupling on the conduction through molecular-scale conductors has recently gained considerable attention. Atomic wires formed in metallic point contacts are very simple examples of "molecular"conductors, and are ideal test systems for understanding inelastic transport at the molecular scale. Making use of tight-binding models, we describe the influence of electron-vibration processes on the conductance-voltage characteristic of atomic gold wires [1]. The signature of the excitation of vibrations is usually a series of downward steps. We study systematically how the step heights and voltage positions vary under stretching of wires with varying numbers of atoms, and find a good overall agreement with recent experiments [2].

[1] J. K. Viljas *et al.*, cond-mat/0508470.
[2] N. Agraït *et al.*, Phys. Rev. Lett. **88**, 216803 (2002).

TT 9.10 Mon 16:30 HSZ 304

Nonequilibrium excitations of molecular vibrons — •Dmitry Ryndyk, Michael Hartung, and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, Germany

We consider the nonequilibrium quantum vibrations of a molecule clamped between two macroscopic leads in a current-carrying state at finite voltages. Our approach is based on the nonequilibrium Green function technique and the self-consistent Born approximation. Kinetic equations for the average populations of electrons and vibrons are formulated in the weak electron-vibron coupling case and self-consistent solutions are obtained. The effects of vibron emission and vibronic instability are demonstrated using few-orbital models. The importance of the electron-vibron resonance is shown.

[1] D.A. Ryndyk, M. Hartung, and G. Cuniberti, Phys. Rev. B, to appear; cond-mat/0508143

TT 9.11 Mon 16:45 HSZ 304

Conjugation effects in transport through single-molecule junctions - a theoretical study — •Fabian Pauly[1], J. K. Viljas[1], J. C. Cuevas[1,2,3], and Gerd Schön[1,3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie

Electrical conduction through molecules depends critically on the delocalization of the molecular electronic orbitals and their connection to the leads. Thiolated conjugated molecules are therefore considered good candidates for molecular conductors [1]. Inspired by the recent synthesis of molecules [2] we investigate theoretically the electronic transport through a series of organic molecules, in which the conjugated π-system has either been stabilized or broken by the use of side groups. For the analysis, we use our newly developed transport program based on the DFT quantum chemistry software TURBOMOLE [3].

[1] C. Joachim, J.K. Gimzewski, A. Aviram, Nature 408, 541-548 (2000)
[2] M. Elbing, PhD Thesis, FZ Karlsruhe (2005)
[3] K. Eichkorn, O. Treutler, H. Öhm, M. Häser, and R. Ahlrichs, Chem. Phys. Letters 242, 652 (1995)

TT 9.12 Mon 17:00 HSZ 304

Electronic Transport through C_{60} — •Tobias Böhler, Jochen Grebing, and Elke Scheer — Universität Konstanz

The electronic transport through a single or a few C_{60} molecules is studied experimentally with the help of the mechanically controllable break-junction (MCB) technique [1]. The tip electrodes of the MCB are fabricated of aluminum or gold. The molecule is evaporated onto an opened break-junction under UHV conditions and at low temperatures. At room and low temperature the experiment shows evidence that the conductance of a single C_{60} molecule between gold contacts is in the order of 0,1 G_0. This can be seen in opening and closing curves as well as in time-dependent fluctuations of the conductance. First results of C_{60} between Al electrodes are presented.

[1] T. Böhler et al. Nanotechnology 15 (2004) 465

TT 9.13 Mon 17:15 HSZ 304

Kondo effect in molecular magnets — •Christian Romeike, Maarten R. Wegewijs, Walter Hofstetter, and Herbert Schoeller — ITP A, RWTH Aachen

Motivated by recent experiments by Heersche et al. [1] we investigate linear transport through a single molecular magnet (SMM) in the regime of strong coupling to the electrodes. The molecule is modeled by a spin Hamiltonian incorporating the generic properties of a SMM: an easy-axis anisotropy, an easy-plane anisotropy perturbation leading to the quantum tunneling of magnetic moment (QTM) and a large spin ($S > 1/2$). Using a scaling analyses and the numerical renormalization group we find that for half-integer spin S the molecule acts as an anisotropic, effective pseudo-spin 1/2 Kondo-impurity of which electrons can resonantly scatter. Electron- and spin-tunneling processes *cooperate*

to produce a quantum tunneling of the magnetization (QTM) (which is forbidden by time-reversal symmetry for isolated SMMs with half-integer S) and a zero-bias anomaly in conductance. The Kondo temperature is found to depend sensitively on the ratio of the easy-plane and easy-axis anisotropies in a non-monotonic way. We discuss criteria for candidate SMMs for transport experiments.

[1] H. Heersche et al., cond-mat/0510732

TT 9.14 Mon 17:30 HSZ 304

Multifractal energy spectra and anomalous diffusion properties of wave packets in incommensurate double-walled carbon nanotubes — •Shidong Wang and Milena Grifoni — Theoretische Physik, Universität Regensburg, 93053 Regensburg

We calculate the energy spectra of incommensurate doubled-walled carbon nanotubes (DWNTs) by approximating the structures with closely related commensurate ones. The energy spectra show multifractal properties. By using the relation between the moments of wave packets and the multifractal dimensions of the energy spectra (F. Piéchon PRL 76, 4372 (1996)), we obtain the diffusive exponent σ_2, where $\langle x^2 \rangle \sim t^{2\sigma_2}$. The exponent σ_2 strongly depends on the coupling between shells varying from $\sigma \to 1/2$ (diffusive limit) for very strong coupling to $\sigma \to 1$ (ballistic limit) for weak coupling. We compare our results with numerical estimates of σ_2 of wave packets in incommensurate DWNTs (S. Roche et al. PRB 64, 121041 (2001); PLA 285, 94 (2001)), and we obtain very good quantitative agreement.

TT 10 Symposium Solid State Meets Quantum Optics

Time: Monday 14:30–17:30 Room: HSZ 02

Invited Talk

TT 10.1 Mon 14:30 HSZ 02

Circuit QED: Quantum Optics With Superconducting Electrical Circuits — •Steven Girvin — Sloane Physics Lab, Yale University, New Haven, CT 06520-8120 USA

Recent experimental breakthroughs have led to the construction of artificial superconducting 'atoms': electrical circuit elements whose state variables (voltages and currents) are intrinsically quantum mechanical. When placed inside a high Q resonator, these 'atoms' can strongly interact with single microwave photons. Tests of this new realization of strong-coupling cavity QED are now underway in the labs of Rob Schoelkopf and Michel Devoret at Yale. Recent experimental and theoretical results on quantum control, measurement and back action will be presented. Practical possibilities for generation of photon Fock states and squeezed vacuum states will be discussed. In addition to being a new test bed for quantum optics, this architecture has many promising features for quantum computation.

Invited Talk

TT 10.2 Mon 15:00 HSZ 02

Cooper-Pair Molasses: Cooling a Nanomechanical Resonator with Quantum Noise — •Keith Schwab[1], Akshay Naik[1], Olivier Buu[1], Matthew LaHaye[1], Aashish Clerk[2], Andrew Armour[3], and Miles Blencowe[4] — [1]Laboratory for Physical Sciences and University of Maryland, College Park — [2]McGill University — [3]University of Nottingham — [4]Dartmouth College

We are performing ultra-low temperature experiments with a radio-frequency, nanomechanical resonator coupled to a superconducting single electron transistor, a system which has demonstrated the closest approach to the uncertainty principle for continuous position detection, and the closest approach to the quantum ground state of a mechanical system [1]. Recently, we have used the resonator to detect the asymmetric, quantum noise of the SET, which produces the back-action close to what is required by the uncertainty principle. In addition, have discovered an unexpected cooling mechanism, analogous to optical molasses, which is a result of resonant Josephson effects in the transistor. Using these techniques and devices, we are anticipating the observation of squeezed, superposition, and entangled states of a mechanical device. One future application for this technology could be in quantum information devices.

[1] LaHaye, Buu, Camarota, Schwab, "Approaching the Quantum Limit of a Nanomechanical Resonator," Science 304, 74 (2004).

Keynote Talk

TT 10.3 Mon 15:30 HSZ 02

Fermionic atoms in a crystal structure of light — •Tilman Esslinger — ETH Zürich, Quantum Optics, HPF D4, Hönggerberg, CH-8093-Zürich

A general introduction to the physics of ultracold atoms in optical lattices will be given. These systems provide a new avenue for designing and studying many-body quantum systems. Exposed to the crystal structure of interfering laser waves the fermionic atoms behave much like electrons in a solid. However, the properties of this synthetic material can be changed at will. The collisional interaction between fermionic atoms in different spin states can be tuned using a Feshbach resonance and the dimensionality is controlled almost like a parameter. In the experiment we have been able to directly image the Fermi surface of the atoms in the optical lattice and to study the transition of the system from a conducting state to a band insulator. Using a Feshbach resonance we have dynamically induced a coupling between the lowest energy bands and formed molecules in the optical lattice. The unique versatility of atoms in optical lattices may allow the study of a whole catalogue of phenomena linked to solid-state physics or even to mimic the physics underlying high-temperature superconductivity.

— 15 min. break —

Keynote Talk

TT 10.4 Mon 16:30 HSZ 02

Nonclassical States, Tomography, and Quantum Information in Circuit QED — •E. Solano[1,2], M. Mariantoni[3], M.J. Storcz[4], F.K. Wilhelm[4], W.D. Oliver[5], A. Emmert[3], A. Marx[3], R. Gross[3], and H. Christ[1] — [1]Max-Planck Institute for Quantum Optics, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany — [2]Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado 1761, Lima, Peru — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, D-85748 Garching, Germany — [4]Department Physik, CeNS and ASC, LMU, Theresienstrasse 37, D-80333 München, Germany — [5]MIT Lincoln Laboratory, 244 Wood Street, Lexington, Massachussets 02420, USA

We show that flux-based qubits can be coupled to superconductive resonators by means of a quantum-optical Raman excitation scheme and utilized for the deterministic generation of propagating microwave single photons. We introduce also a microwave quantum homodyne technique that enables the measurement of single photons and other weak signals, and full state reconstruction via quantum tomography, realizing linear optics on a chip [1]. These generation and measurement protocols are building blocks for the generation of nonclassical states [2] and the advent of quantum information [3] in the field of circuit QED.

[1] M. Mariantoni *et al.*, cond-mat/0509737.
[2] M.J. Storcz, M. Mariantoni, A. Emmert, R. Gross, F.K. Wilhelm, H. Christ, and E. Solano, in preparation.
[3] H. Christ, M. Mariantoni, and E. Solano, in preparation.

This work was supported by the SFB 631 of the DFG.

Keynote Talk

TT 10.5 Mon 17:00 HSZ 02

Integrated Atom Optics on a Bose-Einstein-Chip — •Claus Zimmermann — Physikalisches Institut, Universität Tübingen

Bose-Einstein condensates trapped in miniaturized magnetic traps offer interesting perspectives for integrated matter wave optics on a micro chip. In recent experiments the basic properties of such Bose-Einstein chips have been investigated including effects caused by the interaction of the atoms with chip surface. Now, first matter wave interferences have been observed on a chip. This opens the door for the construction of on chip atom interferometers for sensitive detection of forces and accelerations. For the future, superconducting micro traps may allow for tailoring novel quantum systems with condensates coupled to Cooper pair wave functions.

TT 11 Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

Time: Tuesday 09:30–13:00 Room: HSZ 301

TT 11.1 Tue 09:30 HSZ 301

Observation of Andreev bound states in YBCO/Au/Nb ramp-type Josephson junctions — •B. Chesca[1], D. Doenitz[1], T. Dahm[2], R. P. Huebener[1], D. Koelle[1], R. Kleiner[1], A. Ariando[3], H.J.H. Smilde[3], and H. Hilgenkamp[3] — [1]Physikalisches Institut - Experimentalphysik II, Universität Tübingen — [2]Institut für Theoretische Physik, Universität Tübingen — [3]Faculty of Science and Technology and Mesa+ Research, Institute, University of Twente

We present [1] temperature, magnetic field, and crystallographic orientation dependencies of the quasiparticle tunneling spectra of YBCO/Au/Nb junctions. With Nb superconducting, the proximity gap induced in the Au layer appears in the spectra as well defined coherence peaks and a dip at the center of a broadened zero-bias conductance peak (ZBCP).The data are consistent with the formation of Andreev bound states (ABS) at the junction interfaces supporting a d-wave symmetry of the order parameter in YBCO. We tested both proposed models of ABS assisted quasiparticle tunneling between two superconductors: the convolution model and the series connection of two decoupled interfaces model, and proved the first one applies to our case. In high contrast to Josephson tunneling, the quasiparticle spectra are crystallographic orientation insensitive: a ZBCP is observed no matter whether the tunneling occurs in the (100) or (110) directions consistent with microscopic roughness at the junction interface. The formation of ABS is insensitive to the twinned or untwinned character of the YBCO film. [1] B. Chesca et al., submitted to Phys. Rev. B(cond-mat/0506734, 2005)

TT 11.2 Tue 09:45 HSZ 301

Multiple 0 - π - transitions of Josephson - junctions with Ni_3Al as weak ferromagnetic interlayer — •Frank Born[1], M. Siegel[1], E. Hollmann[2], H. Braak[3], C.M. Schneider[3], and M.Yu. Kupriyanov[4] — [1]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH) — [2]ISG2, Forschungszentrum Jülich GmbH — [3]IFF, Forschungszentrum Jülich GmbH — [4]Institute of Nuclear Physics, Moscow State University

Andreev - reflection is the central mechanism for the superconducting proximity effect. In a NS bi-layer the correlation of electron-like and hole-like quasi-particles decays exponentially with distance from the interface due to the de-phasing of its wave functions. In the case of a ferromagnetic material the Andreev - reflection picture is strongly modified: the spins of electron-like and hole-like quasi-particles are opposite orientated. This results under the influence of the exchange field in an energy shift and the creation of a nonzero momentum, leading to an additional spatially oscillation of the superconducting correlation amplitude. We report on experimental studies about superconducting coupling through a thin Ni3Al film. Depending on the deposition process the alloy is either only paramagnetic or it is magnetically ordered. In the paramagnetic regime the critical supercurrent, IC, decays exponentially over several nm, thus showing the pure proximity effect. In the ferromagnetic regime up to six damped oscillations of critical current on F-layer thickness was observed, revealing 0 - π - shifts in the ground state of Josephson junctions.

TT 11.3 Tue 10:00 HSZ 301

Triplet supercurrent through a half-metallic ferromagnet — •S. T. B. Goennenwein[1,2], R. S. Keizer[2], T. M. Klapwijk[2], G. Miao[3,4], G. Xiao[4], and A. Gupta[3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Kavli Insitute of NanoScience, Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands — [3]MINT Center, University of Alabama, Tuscaloosa, USA — [4]Physics Department, Brown University, Providence, USA

Superconductivity and ferromagnetism usually do not coexist, as the Cooper pairs in conventional superconductors are spin singlets (pairs of electrons with antiparallel spin), while the ferromagnetic exchange interaction requires parallel spins. However, the existence of long-range superconducting *triplet* correlations in a ferromagnet in proximity to a conventional superconductor has been suggested.

Using electron-beam lithography, sputtering, and lift-off, we have patterned two NbTiN electrodes on top of a thin CrO_2 film. We find that a Josephson supercurrent flows through this weak link for electrode separations of up to 1 μm at $T = 1.7$ K. The magnitude of the supercurrent oscillates as a function of the strength of an externally applied magnetic field (Fraunhofer pattern), and characteristically depends on the magnetization orientation in the CrO_2 layer. We interpret these findings as evidence for a spin triplet supercurrent in the half-metallic ferromagnet CrO_2, and discuss possible mechanisms for the singlet to triplet conversion at the superconductor-ferromagnet interface.

TT 11.4 Tue 10:15 HSZ 301

Interplay of magnetic and superconducting proximity effects in FSF trilayers — •Tomas Lofwander, Thierry Champel, Johannes Durst, and Matthias Eschrig — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

We present theoretical results on the interplay of magnetic and superconducting orders in diffusive ferromagnet-superconductor-ferromagnet trilayers. The induced triplet superconducting correlations throughout the trilayer lead to an induced spin magnetization. We include self-consistency of the order parameter in the superconducting layer at arbitrary temperatures, arbitrary interface transparency, and any relative orientation of the exchange fields in the two ferromagnets. We propose to use the torque on the trilayer in an external magnetic field as a probe of the presence of triplet correlations in the superconducting phase.

TT 11.5 Tue 10:30 HSZ 301

Influence of an inhomogeneous exchange field on the proximity effect in disordered superconductor-ferromagnet hybrid structures — •Thierry Champel, Tomas Lofwander, and Matthias Eschrig — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

We investigate the effect of an inhomogeneous exchange field on the proximity effect in superconductor-ferromagnet (S/F) hybrid structures within the quasiclassical theory of superconductivity. The superconducting proximity effect induces triplet correlations in the structure that are sensitive to the local quantization axis of the exchange field in the ferromagnet. As an example, we consider an in-plane spiral order in the ferromagnet. The coexistence of pair correlations results into a sensitivity of the superconducting transition temperature on the spatial variation of the exchange field in S/F bilayers. We show that the inhomogeneity also tends to suppress the oscillating behavior of the pair amplitudes in F. Finally we investigate the influence of the exchange field inhomogeneity on the π-state in SFS junctions.

TT 11.6 Tue 10:45 HSZ 301

Odd Triplet Superconductivity in Superconductor/Ferromagnet Structure with a Spiral Magnetic Structure. — •Alexandra Anishchanka — Ruhr-Universität Bochum, Theoretische Physik III, NB 6/23, Universitätsstr. 150, 44801, Bochum

We analyze a superconductor-ferromagnet (S/F) system with a spiral magnetic structure in the ferromagnet F for a weak and strong exchange field. The long-range triplet component (LRTC) penetrating into the ferromagnet over a long distance is calculated for both cases. In the dirty limit (or weak ferromagnetism) we study the LTRC for conical ferromagnets. Its spatial dependence undergoes a qualitative change as function of the cone angle. At angles close to pi/2 the LTRC decays in the ferromagnet exponentially in a monotonic way. If the cone angle exceeds a certain value, the exponential decay of the LTRC is accompanied by oscillations with a period that depends on the cone angle. This oscillatory behavior leads to a similar dependence of the Josephson critical current in SFS junctions on the thickness of the F layer. In the case of a strong ferromagnet the LTRC decays over the length which is determined by the wave vector of the magnetic spiral and the exchange field.

TT 11.7 Tue 11:00 HSZ 301

Spin-dependent Transport Through Nanostructured S/F Point Contacts — •M. Stokmaier[1], G. Goll[1], C. Sürgers[1,2], D. Weissenberger[3], F. Pérez-Willard[2,3], and H. v. Löhneysen[1,2,4] — [1]Physikalisches Institut, Universität Karlsruhe — [2]DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe — [3]Laboratorium für Elektronenmikroskopie, Universität Karlsruhe — [4]Forschungszentrum Karlsruhe, Institut für Festkörperphysik

Andreev reflection at the superconductor/ferromagnet (S/F) interface in a ballistic point contact strongly depends on the degree of spin polarization of the ferromagnetic electrode. The spin polarization of the current can be determined by analysis of point-contact spectra using a theoretical model which takes into account two spin-dependent transmission coefficients for the majority and minority charge carriers of the ferromagnet [1]. Here we study the spin-dependent transport through nanostructured Al/Fe point contacts. The samples have been fabricated by deposition of Al and Fe on either side of a thin Si_3N_4 membrane with a nanostructured hole in it. Differential conductance measurements $G(V)$ have been performed in a dilution refrigerator at temperatures $T \geq 20\,\mathrm{mK}$ and various magnetic fields. These results are compared with previous data taken on Al/Co and Al/Ni point contacts in order to determine how the current spin-polarization is related to the spin polarization of the bulk magnetic material.
[1] F. Pérez-Willard *et al.*, Phys. Rev. B **69**, 140502(R) (2004).

— 15 min. break —

TT 11.8 Tue 11:30 HSZ 301

Imaging of Domain Superconductivity in a Ferromagnet-Superconductor-Bilayer by Low Temperature Scanning Laser Microscopy — •H. Eitel[1], J. Fritzsche[2], R. Szymczak[3], V.V. Moshchalkov[2], R. Kleiner[1], and D. Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Nanoscale Superconductivity and Magnetism Group, K.U. Leuven, Belgium — [3]Polish Academy of Science, Institute of Physics, Warsaw, Poland

We present a spatially resolved analysis of the electric transport properties of a superconductor-ferromagnet hybrid system. This hybrid consists of a Nb thin film micro bridge on top of a $PbFe_{12}O_{19}$ single crystal whose easy axis is perpendicular to the plane of the Nb film. We used low-temperature scanning laser microscopy (LTSLM) to image regions of Nb at the transition temperature T_c as a function of temperature T and applied magnetic field H_{app}, up to the saturation field H_s of $PbFe_{12}O_{19}$. The LTSLM images give direct evidence that so called "domain superconductivity" in Nb is induced due to the magnetic domain structure of the ferromagnet. I.e., T_c of the Nb film is larger in areas above a magnetic domain with magnetization direction opposite to H_{app}, because in those areas the Nb experiences a reduced total magnetic field. By changing H_{app} from zero up to H_s, the evolution of the magnetic domain structure can be traced by LTSLM. The correlation of the LTSLM images with integral $R(T, H)$ data obtained during LTSLM imaging and with room temperature AFM-images of the $PbFe_{12}O_{19}$ domain structure and its dependence on H_{ext} will be discussed.

TT 11.9 Tue 11:45 HSZ 301

Re-entrant superconductivity in Nb/Cu_xNi_{1-x} bilayers — •V. Zdravkov[1,2], A. Sidorenko[1,2], G. Obermeier[1], S. Gsell[1], M. Schreck[1], C. Müller[1], S. Horn[1], R. Tidecks[1], and L. Tagirov[3] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]Institute of Applied Physics, LISES ASM, Kishinev 2028 Moldova — [3]Laboratory of Theoretical Physics, Kazan State University, Kazan, Russia

The first pronounced experimental observation of the re-entrant phenomenon in superconductor/ferromagnet $Nb/Cu_{0.4}Ni_{0.6}$ bilayers is reported. A non-monotonous dependence of the superconducting critical temperature T_c is observed, strongly depending on the ferromagnet layer thickness, with a complete disappearance of superconductivity for a narrow range of F-layer thicknesses.

The observation is a manifestation of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) - like state and can be described by a theoretical model, based on the modified SF-boundary conditions [1].
[1] Sidorenko, A.S., Zdravkov, V.I., Prepelitsa, A.A., Helbig, C., Luo, Y., Gsell, S., Schreck, M., Klimm, S., Horn, S., Tagirov, L.R., and Tidecks, R. (2003) Oscillations of the critical temperature in superconducting Nb/Ni bilayers, Ann.Phys.(Leipzig) 12, 37-50.

TT 11.10 Tue 12:00 HSZ 301

Effect of Microwaves on the Current-Phase-Relation of diffusive SNS Junctions — •Martin Füchsle, Johannes Bentner, Peter Tranitz, Werner Wegscheider, and Christoph Strunk — Institut für experimentelle und angewandte Physik, Universität Regensburg

We investigate the current-phase-relation (CPR) of long diffusive superconductor - normal metal - superconductor (SNS) Josephson junctions under microwave irradiation. In contrast to earlier experiments that focused on the I-V characteristics of current-biased junctions, we directly measure the full CPR by means of Micro-Hall-Magnetometry. The measurements are done in the high-temperature regime $E_{Th} < k_BT \ll \Delta$, where E_{Th} is the Thouless energy and $\hbar\omega \approx E_{Th}$.
We find that the occupation of the Andreev states in the N region can be strongly affected by microwave radiation. A strong deviation of the CPR from the well-known sinusoidal $I(\Phi)$ relation is observed: depending on the applied frequency and amplitude, the supercurrent can be strongly suppressed and the maximum current can appear at phase differences smaller than $\pi/2$. At some frequencies, the $\sin(\Phi)$ term in the CPR can be completely suppressed, resulting in a dominant second harmonic. The results may be qualitatively interpreted in terms of a simple model for the spectrum of low-lying Andreev bound states.

TT 11.11 Tue 12:15 HSZ 301

Impedance and field profiles of thin ohmic or superconducting strips with applied ac current — •Ernst Helmut Brandt — Max-Planck-Institut für Metallforschung, Stuttgart

A long wire carrying an applied ac current is a standard problem in electrodynamics when the wire is cylindric. The circular symmetric solutions far away from the current contacts are easily obtained for an ohmic wire with resistivity ρ and for a superconducting wire with London depth λ. When the wire has a non-circular cross section the problem becomes much more complex. Apparently, no analytic or transparent numerical solutions are available, not even for the complex impedance of thin strips that is needed, e.g., in the theory of SQUID systems. This contribution presents the inductance, resistance, and magnetic field and current distributions of thin long ohmic or superconducting strips and their dependences on λ, ρ, ac frequency, and strip length l. Approximate analytic expressions are given for the inductance and resistance. Interestingly, the inductance per unit length of the strip depends on its length while the field and current distributions and the susceptibility and resistance are independent of l. As compared to cylindrical wires, the skin effect in thin ohmic strips is much weaker (logarithmic).

TT 11.12 Tue 12:30 HSZ 301

Superconducting surfaces under electric fields — •K. Morawetz[1,2], P. Lipavský[3], J. Koláček[4], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2 — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic

A boundary condition for the Ginzburg-Landau wave function at surfaces biased by a strong electric field is derived within the de Gennes approach. This condition provides a simple theory of the field effect on the critical temperature of superconducting layers [1,2]. The electric-field dependent surface energy is calculated which provides an alternative explanation of the Tao effect where one observes a formation of a macroscopic sphere out of superconducting grains due to the electric field. The electrostatic potential above the Abrikosov vortex lattice is calculated as well where we include the surface dipole. We propose an experimental measurement by NMR to access this field which can yield informations about material parameters [3].
[1] P. Lipavský, K. Morawetz, J. Kolacek, Ginzburg-Landau theory of superconducting surfaces under electric fields, PRB in press
[2] K. Morawetz, Electric field dependence of pairing temperature and tunneling, Phys. Rev. B 66, 172508
[3] P. Lipavský, K. Morawetz, J. Kolacek, J. J. Mares, E. H. Brandt, M. Schreiber, Bernoulli potential in type-I and weak type-II supercoductors: III. Electrostatic potential above the vortex lattice Phys. Rev. B 71 (2005) 024526-1-7, II. Surface dipole Phys. Rev. B 70 (2004) 104518-1-7, I. Surface charge Phys. Rev. B 69 (2004) 024524-1-7

TT 11.13 Tue 12:45 HSZ 301

Nonequilibrium magnetism with superconductors — •Fabio Taddei[1], Francesco Giazotto[1], Rosario Fazio[1,2], and Fabio Beltram[1] — [1]NEST-CNR-INFM & Scuola Normale Superiore, Pisa — [2]International School for Advanced Studies (SISSA), Trieste, Italy

Electrostatic control of the magnetization of a normal mesoscopic conductor is analyzed in a hybrid superconductor-normal-superconductor system. This effect stems from the interplay between the non-equilibrium condition in the normal region and the Zeeman splitting of the quasiparti-

cle density of states of the superconductor subjected to a static in-plane magnetic field. Unexpected spin-dependent effects such as magnetization suppression, *diamagnetic-like* response of the susceptibility as well as spin-polarized current generation are the most remarkable features presented. The impact of scattering events is evaluated and let us show that this effect is compatible with realistic material properties and fabrication techniques.

TT 12 Correlated Electrons: Low-dimensional Systems - Models

Time: Tuesday 09:30–12:30 Room: HSZ 304

TT 12.1 Tue 09:30 HSZ 304

Entropy of fermionic models on highly frustrated lattices — •Andreas Honecker[1] and Johannes Richter[2] — [1]Technische Universität Braunschweig, Mendelssohnstrasse 3, 38106 Braunschweig, Germany — [2]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg, 39016 Magdeburg, Germany

Fermionic models and quantum antiferromagnets at high magnetic fields on highly frustrated lattices are characterized by a lowest single-particle band which is completely flat. On the one hand, this is known to give rise to *flat-band ferromagnetism* for the repulsive Hubbard model on such lattices. On the other hand, exact ground states consisting of *localized magnons* have recently been constructed and studied for the quantum Heisenberg antiferromagnet on the same lattices. Here we combine both aspects and discuss the entropy and ground state degeneracy on such lattices. Spinless fermions not only provide a simple soluble example, but also give rise to a class of ground states of the repulsive Hubbard model. The sawtooth chain is discussed in particular detail.

TT 12.2 Tue 09:45 HSZ 304

Magnetic properties of 2D frustrated spin systems at finite temperatures — •Burkhard Schmidt, Nic Shannon, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We present an analysis of the magnetic properties of two-dimensional frustrated spin systems at finite temperatures. Our numerical results are determined using the finite-temperature Lanczos method for small clusters of spins [1].

In particular, the magnetisation of the two-dimensional frustrated J_1-J_2 Heisenberg model on a square lattice will be discussed as a function of temperature, applied magnetic field, and frustration angle $\phi = \tan^{-1}(J_2/J_1)$. We will cover the full phase diagram of the model with $\phi = -\pi \ldots \pi$, with a focus on the two spin-liquid regions at the edges of the collinear antiferromagnetic phase (ordering vector $(\pi, 0)$ or $(0, \pi)$) for both ferro- and antiferromagnetic nearest-neighbour coupling J_1.

Experimental realisations of the model discussed are two-dimensional layered Vanadate compounds. A comparison to the available experimental data will be given.

[1] N. Shannon et al., Eur. Phys. J. B **38** (2004) 599

TT 12.3 Tue 10:00 HSZ 304

Effective model for the band insulator - Mott insulator transition — •Leonildo Tincani[1], Reinhard Noack[1], and Dionys Baeriswyl[2] — [1]Fachbereich Physik, Philipps Universität Marburg, D-35032 Marburg, Germany — [2]Département de Physique, Université de Friburg, CH-1700 Fribourg, Switzerland

Starting from the ionic Hubbard model, we derive an effective spin-one model which contains the relevant physics for the band insulator-Mott insulator transition found at half filling and study it numerically using the density-matrix renormalization group. We find that the effective model yields the same sequence of two transitions and critical behavior as the ionic Hubbard model. We then perform scaling studies of the charge, spin and mass gaps in order to clarify the nature of the two quantum phase transitions. We present numerical evidence that there is an Ising-like transition between the band insulator and a spontaneously dimerized insulating phase and a Berezinskii-Kosterlitz-Thouless-like transition between the dimerized and the Mott phase. We then discuss the application of similar methods to more general models such as one with three ions of two types in the unit cell.

TT 12.4 Tue 10:15 HSZ 304

Charge and Spin Dynamics of Strongly Correlated Quasi One-Dimensional Insulators — •Holger Benthien[1] and Eric Jeckelmann[2] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Institut für Theoretische Physik, Universität Hannover

We calculate the momentum- and frequency-resolved dynamical spin and charge structure factors as well as the the one-particle spectral function of the extended Hubbard model. The method we apply is the dynamical density-matrix renormalisation group algorithm (DDMRG), which allows for an exact calculation of dynamical correlation functions for any range of energies and parameters. We present strong evidence that this simple model with a single set of parameters can qualitatively and quantitatively explain data from recent neutron scattering, photoemission (ARPES) and resonant inelastic X-ray scattering (RIXS) [1] experiments in the prototypical quasi one-dimensional insulator $SrCuO_2$.

[1] Y.-J. Kim, J.P. Hill, H. Benthien, F.H.L. Essler, E. Jeckelmann, H.S. Choi, T.W. Noh, N. Motoyama, K.M. Kojima, S. Uchida, D. Casa, and T. Gog, Phys. Rev. Lett. **92**, 137402 (2004).

TT 12.5 Tue 10:30 HSZ 304

Finite temperature ac conductivity of disordered Luttinger liquids — •Bernd Rosenow[1,2], Andreas Glatz[3,2], and Thomas Nattermann[2] — [1]Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA — [2]Institut f"ur Theoretische Physik, Universeit"at zu K"oln, D-50937 K"oln — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

Due to the strong effect of interactions in one spatial dimension, elementary charge excitations of a Luttinger liquid are plasmons. Backscattering of electrons from a random impurity potential creates single particle excitations, which strongly interact with these plasmons. In this way, backscattering from the impurity potential is modified by interactions and acquires a strong energy dependence first described in [1]. Based on a finite temperature renormalization group (RG) calculation [2], we determine the ac conductivity and include both the renormalization of the impurity strength and of the charge dynamics. The latter was neglected in [1], where the conductivity was calculated using the effective impurity strength obtained from the RG. We discuss the full frequency and temperature dependence of the conductivity and compare our results with those of [1].

[1] T. Giamarchi and H.J. Schulz, Phys. Rev. B 37, 325 (1988). [2] A. Glatz and T. Nattermann, Phys. Rev. Lett. 88, 256401 (2002).

TT 12.6 Tue 10:45 HSZ 304

Quantum Monte Carlo studies of the one-dimensional t-J-model at finite temperature — •Stefan Harrer, Catia Lavalle, and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart, D-70550 Stuttgart, Germany

We developed a quantum Monte Carlo algorithm to simulate the one dimensional t-J-model at finite temperature. It is an extension of the previously developed zero-temperature hybrid-loop-algorithm [1]. As in the zero temperature case, the algorithm is a combination of the determinantal and the loop algorithm, however, simulations are performed in the grand canonical ensemble. Both equal-time as well as time displaced correlation functions can be obtained.

[1] C. Lavalle, M. Arikawa, S. Capponi, F.F. Assaad, and A. Muramatsu, Phys. Rev. Lett. **90**, 216401 (2003).

— 15 min. break —

TT 12.7 Tue 11:15 HSZ 304

Hybridized mechanism of pairing of fermions in single-walled carbon nanotubes — •Igor Karnaukhov — Institute of Metal Physics, Vernadsky Street 36, 03142 Kiev, Ukraine

The discovery of high-temperature superconductivity in new exotic and perspective materials such as carbon nanotubes has greatly stimulated the investigation of new mechanisms of the superconductivity, the formulation of adequate low-dimensional models of strongly correlated electron systems. The remarkable electronic properties of single-walled carbon nanotubes (SWNT) are due to the special band structure, the most important peculiarity of the band structure is the crossing of two subbands near the Fermi level. The two-band fermion model with boundary fields describing the band structure of SWNT is proposed and

solved exactly by means of the nested Bethe ansatz. The fermions in two subbands shifted one another interact via inner- and inter-band on-site Coulomb interactions, one-particle and correlated on-site hybridizations. It is shown that two component electron liquid state, one of which is defined by an attractive effective electron-electron interaction, is realized in the case of a strong hybridized interaction. The attractive interaction leads to the formation of spinless bound state of Cooper-type pairs and 'superconducting' component of electron liquid. The strong boundary interaction leads to the formation of local spin-singlet boundary states, that induce the Mott-Hubbard metal-insulator phase transition (MIPT) in the chain. MIPT is realized at increasing of the magnetic field, fixing a gigantic magneto resistivity in the region of fields of the phase transition, and a gapless dielectric state - at critical boundary field.

TT 12.8 Tue 11:30 HSZ 304

Charge Response in Quasi-1D Wigner Lattice Systems — •Anup Mishra[1], Matthias Mayr[2], and Peter Horsch[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany. — [2]Dept. of Physics, Univ. of Tennesse, Knoxville, USA

Doped edge-sharing Cu-O chain compounds are ideal realizations of 1D Wigner lattices(WL). Such chains are found in the recently synthesized $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ systems [1] and are also structural elements in the composite compound $Sr_{14-x}Ca_xCu_{24}O_{41}$. As a result of the structure the hopping matrix elements t_l and hence the kinetic energy are small compared to the Coulomb energy. At low temperature the charge order resulting from Coulomb interaction $V_l \sim V/l$ generates modulated Heisenberg chains with varying distance between spins. We discuss the charge dynamics of WL starting from a model of spinless fermions. We give a detailed discussion of domain-wall excitation spectra and excitonic states at doping $x = 1/2$. In the model with t_1 only the resulting periodicity of WL charge modulation may also be explained by a $4k_F$ charge-density wave(CDW) arising from a Fermi surface instability. However due to the $\approx 90°$ Cu-O-Cu bond angle in edge-sharing chains $|t_2| > |t_1|$. Presence of t_2 does not affect the classical WL order, but it changes the Fermi surface topology. This allows to distinguish the WL from the CDW on the basis of the modulation period. We present a detailed phase diagram taking into account t_1, t_2 and V_l. [1] P. Horsch, M. Sofin, M. Mayr, and M. Jansen, Phys. Rev. Lett. **94**, 076403 (2005).

TT 12.9 Tue 11:45 HSZ 304

Finite quantum wires with long-range interactions — •Imke Schneider and Sebastian Eggert — FB Physik, Univ. Kaiserslautern, 67663 Kaiserslautern

We consider the local density of states of a finite quantum wire with more realistic long range interactions and a high energy cutoff. In order to use the Luttinger liquid formalism it is necessary to introduce a changing effective interaction parameter as a function of momentum. We show that it is possible to modify the formalism so that the electron distribution in individual states can be analyzed with help of a recursive formula. In limiting cases the well-known powerlaws can be recovered. Our results allow quantitative comparisons with numerical simulations of lattice models.

TT 12.10 Tue 12:00 HSZ 304

Fermi edge singularities at finite temperature — •Carsten von Zobeltitz and Holger Frahm — Institut für Theoretische Physik, Universität Hannover, 30167 Hannover

Fermi edge singularities (FES) as observed e.g. in X-ray absorption or tunneling experiments for non-interacting electrons can be described analytically by means of bosonization [1]. Within this approach we compute the thermal broadening of these singularities. This allows to collapse data from different temperatures onto a single curve. The same approach is used to describe edge singularities appearing in 1d correlated systems described by a Luttinger liquid. Applications to tunneling through semiconductor quantum dots are discussed.
[1] K.D. Schotte and U. Schotte, Phys. Rev. **182** (1969) 479

TT 12.11 Tue 12:15 HSZ 304

Integrable spin-boson models including counter-rotating terms — •Andreas Osterloh[1], Holger Frahm[1], and Luigi Amico[2] — [1]Institut für theoretische Physik, Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany. — [2]MATIS-INFM & Dipartimento di Metodologie Fisiche e Chimiche (DMFCI), Universita' di Catania, viale A. Doria 6, I-95125 Catania, Italy

We study interacting spin-boson models related to integrable XXX spin-chains with generic open boundary conditions. We particularly focus on spin-boson interactions which contain rotating as well as counter-rotating terms. Models with either rotating or counter-rotating terms are termed (generalized) Jaynes-Cummings and Tavis-Cummings models, respectively, and they are known to be integrable. Those cases where the algebraic Bethe ansatz can be done after a static gauge transformation are demonstrated to have a conserved particle number and hence belong to the former class of models. In order to overcome this restriction, dynamic gauge transformations are taken into account. The resulting Hamiltonian is obtained and diagonalized by means of the algebraic Bethe ansatz. The Bethe equations are presented and discussed.

TT 13 Correlated Electrons: Metal Insulator Transition - Part 1

Time: Tuesday 11:45–13:00 Room: HSZ 105

TT 13.1 Tue 11:45 HSZ 105

Multiple ordering processes and the insulator-metal transition in epitaxial PrCaMnO films — •Christian Jooss[1], Peter Moschkau[1], Sebastian Schramm[1], Christine Borchers[1], and Yimei Zhu[2] — [1]Institute of Materials Physics, University of Goettingen, Germany — [2]Brookhaven National Laboratory, Upton NY, USA

$Pr_{1-x}Ca_xMnO_3$ films in the doping range between $0.3 < x < 0.5$ represent an extremely interesting manganite system for the study of the interplay of different kinds of ordering (charge, orbital, lattice and spin) and the related drastic changes of the transport properties. Recently, it was suggested [1] that a possible specific kind of bond-centered charge ordered state could give rice to ferroelectric properties of this material. We have investigated epitaxial PrCaMnO films on (001) $SrTiO_3$ substrates grown by pulsed laser deposition. The films exhibit an insulator metal (IM) transition in applied magnetic and electric fields below the charge ordering temperature $T_c \approx$230 K with resistivity changes of up to seven orders of magnitudes. Furthermore, an electric field induced remanet resistivity change is observed at temperature above T_c. High-resolution transmission electron microscopy reveals the presence of orbital and charge ordering. In the x=0.3 samples the correlation lengths of the charge and orbital ordering domains differs and we observe an inhomogeneous charge ordered ground state. We discuss the relation between structure, different types of ordering and electronic transport properties of this material.
[1] D. V. Efremov, J. van den Brink and D. I. Khomskii, Nature Materials 3 (2004) 853.

TT 13.2 Tue 12:00 HSZ 105

Resonant soft x-ray diffraction from magnetite thin films — •J. Schlappa[1], C. F. Chang[1], C. Schüssler-Langeheine[1], H. Ott[1], Z. Hu[1], E. Schierle[2], E. Weschke[2], G. Kaindl[2], A. Tanaka[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Experimentalphysik, Freie Universität Berlin — [3]Department of Quantum Matter, ADSM, Hiroshima University

Magnetite (Fe_3O_4) undergoes a first-order transition at the Verwey temperature, T_V, which is for bulk samples around 120 K. This transition is accompanied by a change of the crystal structure from the cubic to monoclinic. The electronic origin of this transition is still a matter of considerable controversy. Using resonant soft x-ray diffraction at the Fe $L_{2,3}$ resonance from magnetite thin films, we studied spectroscopically the electronic origin of the (001/2) and (001) superstructure peaks, which both occur below T_V. The resonances of the two superstructure peaks differ significantly and indicate that the (001) peak is caused by charge order on the octahedral B sites, while the (001/2) peak, which describes a doubling of the unit cell below T_V, is caused by an order involving only Fe^{2+} ions on B sites.

TT 13.3 Tue 12:15 HSZ 105

Disorder effects in manganites: Griffiths phase regime in $La_{1-x}Sr_xMnO_3$ — •J. Deisenhofer[1], D. Braak[2], H.-A. Krug von Nidda[1], J. Hemberger[1], R.M. Eremina[3], V.A. Ivanshin[4], A.M. Balbashov[5], G. Jug[6], A. Loidl[1], T. Kimura[7], and Y. Tokura[7] — [1]EP V, Center for Electronic Correlation and Magnetism, University of Augsburg, Germany — [2]TP II, Institute for Physics, University of Augsburg, Germany — [3]E.K. Zavoisky Physical-Technical Institute, Kazan, Russia — [4]Kazan State University, Kazan, Russia — [5]Moscow Power Engineering Institute, Moscow, Russia — [6]Dipartimento di Fisica e Matematica, Universita' dell'Insubria, Como, Italy — [7]Department of Applied Physics, University of Tokyo, Japan

By means of electron spin resonance and magnetic susceptibility measurements a novel triangular phase regime has been discoverd in the system $La_{1-x}Sr_xMnO_3$. This phase is characterized by the coexistence of ferromagnetic entities within the globally paramagnetic phase far above the magnetic ordering temperature. The nature of this phase can be understood in terms of Griffiths singularities arising due to the presence of correlated quenched disorder in the orthorhombic phase.

TT 13.4 Tue 12:30 HSZ 105

On the nature of the pressure-induced insulator-to-metal transition in $LaMnO_3$ — •A. Yamasaki, M. Feldbacher, O. K. Andersen, and K. Held — Max-Planck Institut für Festkörperphysik, Stuttgart

Since the discovery of colossal magnetoresistance (CMR), manganites have been intensively studied. In this talk, we focus on the pressure-induced insulator-to-metal (IM) transition which was found experimentally by Loa *et al.* [1] in the undoped parent compound $LaMnO_3$ with configuration $t_{2g}^3e_g$. This transition occurs at room temperature, well above the magnetic ordering (T_N=140 K) and well below the cooperative Jahn-Teller temperature (T_{oo}=740 K at 0 GPa), and at a hydrostatic pressure of 32 GPa where the JT distortion appears to be completely suppressed [1]. The IM transition thus seems to be a bandwidth-driven Mott-Hubbard transition of the e_g electrons and points to the dominating importance of the Coulomb repulsion between two e_g electrons on the same site. We employ the local density approximation combined with static and dynamical mean-field theories (LDA+U and LDA+DMFT) and conclude that the insulator-to-metal transition observed at 32 GPa in paramagnetic $LaMnO_3$ at room temperature is *not* a Mott transition, but is caused by the overlap of the majority-spin e_g bands, orbitally polarized by the Coulomb repulsion.

[1] I. Loa *et al.*, Phys. Rev. Lett. **87**, 125501 (2001).

TT 13.5 Tue 12:45 HSZ 105

DMFT calculations for manganites with electron-phonon Interaction — •Yi-feng Yang and Karsten Held — Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

The metal-insulator transition in manganites such as $La_{1-x}Ca_xMnO_3$ has attracted much interest in recent years, but the mechanism is still not fully understood. There has been a debate whether the local Coulomb interaction or the electron-phonon interaction is more important. We present here the first dynamical mean field theory calculation for two e_g bands, taking into account both interactions, as well as the Hund coupling to the local t_{2g} electrons. For undoped system, our results show that both Coulomb and electron-phonon interaction are necessary to describe $LaMnO_3$. We also show spectra for doped manganites.

TT 14 Symposium Molecular Electronics

Time: Tuesday 09:30–12:15 Room: HSZ 02

Invited Talk

TT 14.1 Tue 09:30 HSZ 02

Single-Molecule Transistor — •Hongkun Park — Department of Chemistry and Department of Physics, Harvard University, 12 Oxford Street, Cambridge, MA 02138, USA

In this presentation, I will describe the fabrication of three-terminal devices (transistors) incorporating individual molecules and discuss their utility in probing the coupling between the electronic motion and other molecular degrees of freedom. Examples that will be discussed include (1) the excitation of the internal vibrational motion of a molecule induced by single-electron hopping, (2) the Kondo resonance in single-molecule transistor caused by correlated spin screening, (3) the spin-level structures in the Mn12O12 cluster, a prototypical single-molecule magnet, and (4) electroluminescence from individual CdSe nanorods caused by inelastic electron scattering.

Invited Talk

TT 14.2 Tue 10:00 HSZ 02

Three-terminal transport through molecular junctions — •Herre van der Zant — Kavli Institute of Nanoscience, Lorentzweg 1, 2628 CJ Delft, The Netherlands

With electrochemical etching and electromigration, nanogaps on an aluminum gate have been made and small organic molecules of different lengths have been trapped between the electrode pairs. Temperature-dependent transport measurements as a function of gate voltage show that the molecules are weakly coupled to the leads. Samples with the same molecule share common features. For some molecular systems, we find that at low temperatures smaller molecules are worse conductors than longer ones. Asymmetric junctions with a sulphur-gold bonding only on one side, exhibit current-voltage characteristics with steps that are absent for symmetric ones. Coulomb blockade measurements on OPV-3 and OPV-5 show excited states and Kondo behavior. The excitations are associated with vibrational modes and a very good correspondence with Raman spectra is found. Excitations in the single-molecule magnet Mn-12 (S = 10 ground state) are related to non-degenerate spin states. Negative differential resistance and complete current suppression at low bias are explained by a new kind of spin blockade.

Keynote Talk

TT 14.3 Tue 10:30 HSZ 02

Transport through single molecules: vibrational and magnetic excitations — •Maarten Wegewijs, Christian Romeike, Herbert Schoeller, and Walter Hofstetter — Institut fuer theoretische Physik A RWTH-Aachen

We discuss the effects of vibrational and magnetic excitations localized on a molecule on the electron tunneling transport.

In the limit of weak tunnel coupling, we show that a distortion of the vibrational potential shape induced by the charging leads to marked transport signatures. Quantum interference of the mechanical motion of the molecule shows up as a suppression of the transport current. Secondly, we show that quantum-tunneling of the magnetic moment in a single molecular magnet leads to oscillations of the transport current and shot-noise. These molecules exhibit a large ground state spin S and a magnetic anisotropy barrier. The weak quantum tunneling effects do not affect the electron addition spectrum but nevertheless lead to visible non-equilibrium shifts of current and noise resonances.

In the limit of strong tunnel coupling we investigate Kondo-tunneling through single-molecular magnets. We show that the quantum-tunneling of the magnetic moment induces a Kondo effect in the electron transport.

— 15 min. break —

Keynote Talk

TT 14.4 Tue 11:15 HSZ 02

Novel quantum transport effects in single-molecule junctions — •Felix von Oppen — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Single-molecule junctions differ from more conventional nanstructures such as quantum dots due to the coupling between the electrons and few, well-defined vibrational modes. In this talk, I show that this coupling can lead to transport in the form of a self-similar hierarchy of avalanches of many electrons as well as to tunneling of electron pairs. Self-similar avalanche transport occurs in the regime of strong electron-phonon coupling when the current drives the molecular vibrations out of thermal equilibrium. Tunneling of electron pairs dominates transport when the polaronic renormalization leads to a negative effective charging energy of the molecule.

This work was done in collaboration with Jens Koch (Berlin) and M.E. Raikh (Utah)

Keynote Talk

TT 14.5 Tue 11:45 HSZ 02

Electron Transport through Single Molecules — •Heiko B. Weber[1], Daniel Secker[1], Rolf Ochs[2], Mark Elbing[2], Ferdinand Evers[2], Max Köntopp[2], and Marcel Mayor[2,3] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Angewandte Physik, D-91058 Erlangen — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — [3]Universität Basel, Dep. of Chemistry, St. Johanns-Ring 19, CH-4056 Basel

We will report on experiments with single molecule junctions, performed with the mechanically controlled break-junction technique. A review is given on the capabilities of the technique and the results obtained so far. The importance of the molecular structure, the local environment, the contacts, and the electronic polarizability will be elucidated.

As a particular example, we will present a redesigned Aviram-Ratner experiment [1] with a molecule that was designed to form a single-molecule diode when contacted from two sides. Indeed, the IVs show a pronounced asymmetry, whereas a blind experiment with symmetric molecules resulted in symmetric IVs. A closer analysis of the data, involving theoretical models, suggests that the bias-dependent charge reconfiguration of the electronic structure is responsible for the diode-like characteristics.

[1] M. Elbing, R. Ochs, M. Köntopp, M. Fischer, C. von Hänisch, F. Weigend, F. Evers, H. B. Weber, M. Mayor: *A single-molecular diode.* In: Proc. Natl. Acad. Sci. USA (2005), Nr. 102, S. 8815 - 8820.

TT 15 Transport: Nanoelectronics II - Spintronics and Magnetotransport - Part 1

Time: Tuesday 12:30–13:00 Room: HSZ 02

Invited Talk

TT 15.1 Tue 12:30 HSZ 02

Electric field control of spin transport in carbon nanotubes — •Takis Kontos[1,2], Sangeeta Sahoo[1], Juerg Furer[1], Christian Hoffmann[1,3], Matthias Gräber[1], Audrey Cottet[1,4], and Christian Schönenberger[1] — [1]Institute of Physics, University of Basel, Klingelbergstrasse 82, CH-4056, Basel, Switzerland — [2]LPA, ENS, 24, rue Lhomond, 75231 Paris Cedex 05, France — [3]CRTBT, Grenoble, France — [4]LPS, Université Paris-Sud, 91405, Orsay, France

Spintronics is an approach to electronics in which the spin of the electron is exploited to control the electric resistance R of devices. One basic building block is the spin-valve, which is formed if two ferromagnetic electrodes are separated by a thin tunnelling barrier. In such devices, R depends on the orientation of the magnetization of the electrodes. It is usually larger in the antiparallel than in the parallel configuration. The relative difference of R, the so-called magneto-resistance (MR), is then positive.

The MR may become anomalous (negative), if the transmission probability of electrons through the device is spin or energy dependent. This offers a route to the realization of gate-tunable MR devices. Using carbon nanotubes with a new type of ferromagnetic contacts [1] (based on the $Pd_{1-x}Ni_x$ alloy), we demonstrate a spin field-effect transistor (Spin-FET), in which the amplitude and the sign of the MR are tunable with the gate voltage in a predictable manner [2].

[1] S. Sahoo, T.Kontos, C. Schönenberger and C. Sürgers , Appl. Phys. Lett. 86, 112109 (2005)

[2] S. Sahoo, T. Kontos, J. Furer, C. Hoffmann, M. Gräber, A. Cottet and C. Schönenberger Nature Phys. 2, 99 (2005)

TT 16 Solids At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ...

Time: Tuesday 09:30–11:30 Room: HSZ 105

TT 16.1 Tue 09:30 HSZ 105

Slave-boson approach for Bose-Einstein condensate in optical lattices — •Christopher Moseley and Klaus Ziegler — Institut für Physik, Universität Augsburg, 86135 Augsburg

A strongly interacting Bose-Einstein condensate in an optical lattice is treated by applying a slave-boson approach to hard-core bosons. A mean-field calculation for the condensate wave function leads to a renormalized Gross-Pitaevskii theory that describes both the dilute regime (like the conventional Gross-Pitaevskii equation) and the dense regime. Finite temperature effects as well as the phase transition to the Mott insulating state are found within this approach. Moreover, we calculate the quasiparticle excitation spectrum that in the dilute regime agrees with Bogoliubov theory.

TT 16.2 Tue 09:45 HSZ 105

Supersolid Bosons on the Triangular Lattice — •Stefan Wessel[1] and Matthias Troyer[2] — [1]Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland

The zero temperature phase diagram of hardcore bosons on the triangular lattice with nearest neighbor repulsion is determined using quantum Monte Carlo simulations. The system exhibits an extended supersolid phase emerging from an order-by-disorder effect as a novel way of a quantum system to avoid classical frustration. We analyze the nature of the supersolid phase and its stability in competition with phase-separation, which we find to occurs in other regions of parameter space.

TT 16.3 Tue 10:00 HSZ 105

Josephson tunneling between two Bose-Einstein condensates, coupled via an atmoic quantum dot. — •Ingrid Bausmerth[1], Uwe R. Fischer[2], and Anna Posazhennikova[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Wolfgang-Gaede-Str. 1, 76128 Karlsruhe — [2]Institut für Theoretische Physik, Eberhard-Karls-Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen

We study the Josephson tunneling effect in the system of weakly coupled BECs. This setup is known to exhibit a novel quantum phenomenon - macroscopic self-trapping (MST). We consider the way MST is affected by an atomic quantum dot embedded between the two condensates.

TT 16.4 Tue 10:15 HSZ 105

Temperature in One-Dimensional Bosonic Mott Insulators — •Kai P. Schmidt[1], Alexander Reischl[2], and Götz S. Uhrig[3] — [1]Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne, CH 1015 Lausanne, Switzerland — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Theoretische Physik, Geb. 38, FR 7.1, Universität des Saarlandes, D-66123 Saarbrücken, Germany

The Mott insulating phase of a one-dimensional bosonic gas trapped in optical lattices is described by a Bose-Hubbard model. A continuous unitary transformation is used to map this model onto an effective model conserving the number of elementary excitations. We obtain quantitative results for the kinetics and for the spectral properties of the low-energy excitations for a broad range of parameters in the insulating phase. By these results, recent Bragg spectroscopy experiments are explained. Evidence for a significant temperature of the order of the microscopic energy scales is found. The temperature scale deduced from the spectroscopy is embedded in a consistent picture of the thermodynamic properties of bosons in the Mott insulating phase when loaded adiabatically into one-dimensional optical lattices. We find a crucial dependence of the temperature in the optical lattice on the doping level of the Mott insulator. In the undoped case, the temperature is of the order of the large onsite Hubbard interaction. In contrast, at a finite doping level the temperature jumps almost immediately to the order of the small hopping parameter.

TT 16.5 Tue 10:30 HSZ 105

Generation of coherent matter waves from correlated insulators — •Karen Rodriguez[1], Salvatore Manmana[1,2], Marcos Rigol[3], Reinhard Noack[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57 / V, 70550 Stuttgart — [2]AG Vielteilchennumerik, Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — [3]Physics Department, University of California, Davis, CA 95616, USA

We study the evolution of matter waves resulting from the free expansion of an initially confined Mott-insulator, using a variant of the time-dependent density matrix renormalization group method (DMRG) that approximates the time-evolution operator within a Krylov subspace. A carefull comparison with the exact solution in the case of hard-core bosons [1] is performed, in order to determine the limitations of the algorithm. Finally, we discuss the expansion of soft-core bosons.

[1] M. Rigol and A. Muramatsu, Phys. Rev. Lett. **93**, 230404 (2004); *ibid.* **94**, 240403 (2005).

TT 16.6 Tue 10:45 HSZ 105

About the dependence of distribution for the superfluid density of He^4 absorbed in a narrow single walled carbon nanotube in the vicinity of the λ-transition. — •Vilchynskyi Stanislav and Tkachenko Olena — Kiev Taras Shevchenko National University

We report the results of an iteration calculations of the temperature dependence of λ-transition and distribution for the superfluid density of He^4 absorbed in a narrow single walled carbon nanotube in the vicinity of λ-transition. The calculations were made for different values of the carbon nanotube diameter and a value of an inoculating interaction V_0 (the depth of a potential well). We demonstrate the decrease of the temperature of the λ -transition and superfluid density in He^4 absorbed in the nanotube and find an appropriate "temperature shift". It was shown that that if the nanotube's diameter is invariable, the increment of the interaction between a superfluid helium and carbon atoms will reduce to the decreasing of superfluid density (but to the increasing of the "temperature shift"). In this case the appearance of of superfluid component decelerates.

TT 16.7 Tue 11:00 HSZ 105

Thermodynamics of strongly anisotropic roton system in superfluid ^{4}He — •Valeriy Slipko[1], Igor Adamenko[1], Konstantin Nemchenko[1], and Adrian Wyatt[2] — [1]Karazin Kharkov National University, Svobody Sq. 4, Kharkov 61077, Ukraine — [2]School of Physics, University of Exeter, Exeter EX4 4QL, United Kingdom

Recently strongly anisotropic quasiparticle systems have been created in liquid ^{4}He [1, 2]. The strong anisotropy means that the drift velocity can be close to the Landau critical velocity. By using the phonon-roton model, we have obtained analytical expressions for all thermodynamical functions up to the Landau critical velocity. It turns out that for strongly anisotropic quasiparticle systems of superfluid ^{4}He, the temperature at which the contributions of phonons and rotons are comparable, decreases with increasing drift velocity. This creates a rather unusual situation; rotons can dominate in the whole temperature range. This is in contrast to isotropic quasiparticle systems, where the roton contribution to the thermodynamical functions, is negligible for temperatures less than 0.5 K. The reason for this unusual behavior of the roton thermodynamics is that, for velocities close to critical value, we cannot consider rotons as a classical gas which obeys Boltzmann statistics. Instead it must be considered by Bose statistics. The effective roton energy gap decreases when the drift velocity increases. This results in a large roton number density compared to the phonon number density, even at very low temperatures.

[1] Vovk R.V., Williams D.H. and Wyatt A.F.G. Phys. Rev. B68, 134508 (2003).

[2] Wyatt A.F.G. and Brown M. Physica B, 165&166, (1990).

TT 16.8 Tue 11:15 HSZ 105

Bilayer helium-3: a new two dimensional heavy fermion system with quantum criticality — •Michael Neumann, Jan Nyéki, Brian Cowan, and John Saunders — Dept. of Physics, Royal Holloway, Univ. of London, United Kingdom

Previous work [1] has shown how monolayer ^{3}He adsorbed on graphite behaves as a two dimensional Mott-Hubbard system, complete with a "metal-insulator" transition. We report new results on bilayer ^{3}He, which behaves as a two-dimensional two-band heavy fermion fluid. Evidence for this behaviour derives from extensive heat capacity and magnetisation measurements of ^{3}He adsorbed on graphite pre-plated by a solid bilayer of ^{4}He. The first ^{3}He layer adsorbed on this composite substrate remains fluid up to and beyond layer promotion. However, it is observed to solidify significantly before the second ^{3}He layer is completed. Remarkably, at fluid coverages on the verge of solidification, we observe a distinctive heat capacity and magnetisation maximum, which occurs at progressively lower temperatures as the coverage is increased. The magnetic instabilities in the fluid and the close analogies with quantum critical heavy fermion systems will be discussed in detail.

[1] Evidence for a Mott-Hubbard Transition in a Two-Dimensional ^{3}He Fluid Monolayer, A. Casey, H. Patel, J. Nyéki, B. P. Cowan, and J. Saunders. Phys. Rev. Lett. 90, 115301 (2003)

TT 17 Superconductivity: Thin Film Preparation

Time: Tuesday 14:00–14:45 Room: HSZ 02

TT 17.1 Tue 14:00 HSZ 02

Growth of superconducting $Na_{0.3}CoO_2{\cdot}1.3D_2O$ thin films — •Y. Krockenberger[1,2], I. Fritsch[1], G. Cristiani[1], C. Bernhard[3], L. Alff[2], and H-U. Habermeier[1] — [1]Max Planck Institut for Solid State Research, 70569 Stuttgart, Germany — [2]Technische Universitaet Darmstadt, 64287 Darmstadt, Germany — [3]Universite de Fribourg, Ch. du Musée 3, CH-1700 Fribourg

Layered cobaltates attracted much interest since superconductivity was found in hydrated samples [1]. The electronic and structural analogies between $Na_{0.3}CoO_2{\cdot}1.3H_2O$ and high T_c copper oxides suggests that their superconductivity may have a similar origin based on strong electron correlation. Furthermore, Terasaki et al. [2] reported large thermoelectric power values for Na_xCoO_2 with metallic resistivity behavior suggesting a promising material for thermoelectrical applications. Here, we report, that Na_xCoO_2 can be stabilized as a thin film by pulsed laser deposition technique in the doping range from $x = 0.25$ up to $x = 1.0$. In order to achieve superconducting thin films (with $T_c \approx 4.4$ K) a new process involving slow waterizing in a constant humidity is required. The sodium content has been decreased after depositing a $Na_{0.6}CoO_2$ thin film by soft chemical methods. These thin films have been characterized by x-ray diffraction, and resisitivity measurements. Additionally, the surface quality enabled us to perform far infrared spectroscopy in the range of λ =100 to 1000 cm^{-1} for various doping levels. (1) K. Takada *et al.*, Nature 422, 53 (2003). (2) I. Terasaki *et al.*, Phys. Rev. B 56, R12685 (1997). (3) Y. Krockenberger *et al.*, APL 86, 191913 (2005).

TT 17.2 Tue 14:15 HSZ 02

New method to obtain superconducting $Sr_{1-x}La_xCuO_2$ thin films by PLD — •V. Leca[1], G. Visanescu[1], G. Rijnders[2], D. H. A. Blank[2], S. Bals[3], R. Kleiner[1], and D. Koelle[1] — [1]Physikalisches Institut–Experimentalphysik II, Univ. Tübingen, Germany — [2]Univ. Twente, Faculty of Science and Technology, Enschede, The Netherlands — [3]EMAT, Univ. Antwerp (RUCA), Antwerp,Belgium

Difficulties in fabricating single-phase infinite-layer (IL) type $Sr_{1-x}La_xCuO_2$ thin films with good superconducting characteristics hampered the investigation of basic properties such as the pairing symmetry of this class of electron-doped superconducting cuprates. A new synthesis approach to obtain single-phase $Sr_{1-x}La_xCuO_2$ ($x = 0.10 - 0.175$) thin films grown by pulsed laser deposition (PLD) on $KTaO_3$ and $SrTiO_3$ substrates will be presented. The IL phase is obtained after oxidation of the as-deposited oxygen-deficient $Sr_{1-x}La_xCuO_{2-\delta}$ films having a $2\sqrt{2}a_p \times 2\sqrt{2}a_p \times c$ structure (a_p, c represent the perovskite subcell parameters). An increased stability of the IL phase for the entire studied La doping range (x=0.10-0.175) was achieved by applying this synthesis approach. Superconductivity was obtained for the $x = 0.15 - 0.175$ films, with the highest transition temperature $T_{c,zero} = 17$ K for $x = 0.15$. This result indicates a shift of the superconducting region towards a higher La doping level as compared to previous studies. For the $Sr_{1-x}La_xCuO_2$ films grown on $BaTiO_3/SrTiO_3$, superconductivity was observed for x=0.15 only when the $BaTiO_3$ buffer layer is relaxed, following an *in-situ* annealing step, confirming that tensile strain is required in order to induce superconductivity in the $Sr_{1-x}La_xCuO_2$ films.

TT 17.3 Tue 14:30 HSZ 02

$YBa_2Cu_3O_{7-\delta}$ Thin Films Prepared by Polymer-Assisted Deposition (PAD) — •Claudia Apetrii[1], Heike Schlörb[1], Irene von Lampe[2], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Berlin, Englische Str. 20, 10587 Berlin, Germany

The Polymer-Assisted Deposition (PAD) route is a deposition route towards an inexpensive, non-vacuum approach for growing long $YBa_2Cu_3O_{7-\delta}$ (YBCO) tapes. The polymer used in this technique is a synthetic organic polymer (polyacrylic acid) that has functional groups with strong complexation affinities for metal ions. The distribution of the metal ions is very homogeneous and, thus, processing times are shorter, leading to good continuous film preparation conditions. The metal polymer precursor films were produced by spin coating a stoichiometric solution (Y:Ba:Cu = 1:2:3) onto $SrTiO_3$ single crystal substrates and subsequently dried at 170 °C in air. The heat treatment was performed in a tube furnace at reaction temperature of 775 °C in a nitrogen atmosphere containing small amounts of oxygen. The quality of the films strongly depends on the precursor solution stability. Furthermore, the effect of metal ions (Sm, Dy) introduced by chemical substitution on the Y site is discussed. The YBCO films were routinely analysed by X-ray Diffraction and Scanning Electron Microscopy. The inductively measured critical current density J_c reached values up to 3.5 x 10^6 A/cm^2 (at 77 K).

TT 18 Superconductivity: Borides, Borocarbides, Carbides, ...

Time: Tuesday 15:00–18:30 Room: HSZ 02

TT 18.1 Tue 15:00 HSZ 02

Three-Dimensional MgB_2-Type Superconductivity in Hole-Doped Diamond — •Jens Kortus[1], Lilia Boeri[2], and Ole K. Andersen[2] — [1]Theoretische Physik, TU Bergakademie Freiberg, Germany — [2]MPI FKF Stuttgart, Germany

We substantiate by numerical and analytical calculations that the recently discovered superconductivity in boron-doped diamond is caused by electron-phonon coupling of the same type as in MgB_2, albeit in three dimensions. Using first-principles linear response methods based on density functional theory we obtain the phonon dispersion and the electron-phonon coupling strength as function of hole doping. As revealed by these calculations, holes at the top of the zone-centered, degenerate sigma-bonding valence-band couple strongly to the optical bond-stretching phonon modes. This mechanism shows several very similar aspects to the one which drives the superconductivity in MgB_2. However, the increase from two dimensions in MgB_2 to three dimensions in diamond reduces the phonon mode softening crucial for the high T_c of 40 K in MgB_2. Even if diamond had the same bare coupling constant as MgB_2, which could be achieved with higher doping, Tc would be limited to only 25 K. Using the same theoretical methods we also investigate the possibility of superconductivity in the isostructural and isoelectronic semiconductors Si and Ge. Superconductivity above 1 K in Si (Ge) requires hole doping beyond 5% (10%).

L. Boeri, J. Kortus, O.K. Andersen, Phys. Rev. Lett. 93, 237002 (2004)

TT 18.2 Tue 15:15 HSZ 02

Superconductivity and electron phonon coupling in doped MgB_2 compounds — •Vivien Petzold[1] and Helge Rosner[2] — [1]TU Dresden — [2]MPI for Chemical Physics of Solids Dresden

Recently, substitutions on the metallic site in MgB_2, e.g. $Mg_{1-x}Sc_xB_2$ [1], $Mg_{1-x}(AlLi)_xB_2$ [2] and $Nb_{1-x}B_2$ [3] were investigated intensively. For the achievable doping levels (x=0.12...0.27) in $Mg_{1-x}Sc_xB_2$, the compound shows only very small structural changes, allowing the separation of lattice and doping effects. On the other hand $Mg_{1-x}(AlLi)_xB_2$ is isoelectronical to MgB_2, but varies in lattice constants depending on x. In order to investigate the influence of the degree of substitution on the electronic properties, we present band structure calculations using different levels of approximation: rigid band and virtual crystal approach as well as supercell calculations and coherent potential approximation. We show that the latter two approaches lead to consistent results with respect to lattice expansion and electronic properties (density of states, Fermi surfaces). We demonstrate that in the transition metal (T) diborides the doping dependent changes in the electronic structure are strongly influenced by the sp^2(B)-d(T) hybridization. The influence of the doping on the electron phonon coupling is discussed.

[1] Agrestini et al. Phys. Rev. B **70** 134514 (2004).
[2] Monni et al. cond-mat 0506162 (2005).
[3] Yamamoto et al. Physica C 383 (2002) 197-206.

TT 18.3 Tue 15:30 HSZ 02

Density functional theory for superconductors: Applications to MgB_2 and Pb — •A. Floris[1], N. Lathiotakis[1], A. Sanna[2], C. Franchini[2], M. Marques[3], M. Lueders[4], G. Profeta[5], A. Continenza[5], S. Massidda[2], and E.K.U. Gross[1] — [1]Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]INFM SLACS and Dipartimento di Scienze Fisiche, Universita' degli Studi di Cagliari, Italy — [3]Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie - Paris VI, France — [4]Daresbury Laboratory, Warrington WA4 4AD, United Kingdom — [5]C.A.S.T.I. - INFM and Dipartimento di Fisica, Universita' degli studi dell'Aquila, Italy

Predicting the properties of superconductors is of both fundamental and technological importance. The discovery of superconductivity in MgB_2 (T_c=39.5 K), with a clear presence of two gaps, has renewed the interest in conventional superconductivity. Here we present two applications of a novel approach to superconductivity that allows one to calculate material-specific properties without using any adjustable parameters. Within this approach, we have obtained the critical temperature and the two gaps of MgB_2 in good agreement with experiment, taking into account the strong anisotropy of both the electron-phonon and the Coulomb interactions. Moreover, in a fully k-resolved formalism, we find two different gaps also in Pb, and we relate this fact to the difference in strength of the electron-phonon coupling associated with the two bands crossing the Fermi level. This calculation shows how our formalism is able to capture, in absence of any ad-hoc model, the features of multi-gap superconductors.

TT 18.4 Tue 15:45 HSZ 02

Specific heat of $Mg(B_{1-x}C_x)_2$: Two Superconducting Gaps — •Niels Oeschler[1,2], Robert A. Fisher[1], Norman E. Phillips[1], William E. Mickelson[1], and Alex Zettl[1] — [1]University of California, Berkeley, CA, USA — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

We present specific heat data of polycrystalline $Mg(B_{1-x}C_x)_2$ with $x = 0.1$ and 0.2 from 1K to 35K in magnetic fields up to 9T.
Recently, MgB_2 was identified as a phonon-mediated two-gap superconductor with remarkably high transition temperature of 39K. The small gap and the large gap open at the same temperature due to interband coupling. Substituting carbon on the boron site has the effect of electron filling and inducing disorder. The superconducting transition temperature decreases monotonically from 39K for MgB_2 to 20K for $Mg(B_{0.8}C_{0.2})_2$. The specific heat of both samples can be accurately fitted with two superconducting energy gaps using the extended α model. The amplitudes of the gaps are found to be larger than the BCS value for the large gap and smaller than the BCS value for the small gap. However, it is observed that the size of both gaps decreases upon increasing the carbon content.
The evolution of the gap sizes, the normal-state Sommerfeld coefficients, the Debye temperatures and the critical fields are compared to those of MgB_2.

TT 18.5 Tue 16:00 HSZ 02

Superconducting properties of the 13 K rare earth carbide superconductor, La_2C_3 — •Jun Sung Kim, Reinhard K. Kremer, Volodymyr Babizhetskyy, Ove Jepsen, and Arndt Simon — MPI-FKF, 70569 Stuttgart

Superconductivity in rare earth carbides has attracted interest again after the recent discovery of the 18 K superconductor Y_2C_3.[1] We have

successfully synthesized the related La system, La_2C_3, and after a careful control of the carbon content and the annealing procedures, optimized the superconducting properties reaching at sharp transition temperature $T_c \sim 13.2$ K. The superconducting properties have been investigated by heat capacity measurements in magnetic fields up to $H = 9$ T, resistivity and magnetization measurements up to $H = 30$ T. The characteristic specific heat anomaly is compared to the predictions of the BCS and the α model, and a quantitative estimate of the electron-phonon coupling strength and the logarithmic average phonon frequency is made. From a detailed analysis including full potential electronic structure calculations based on the refined structure gained from the refinement of low-temperature neutron powder diffraction experiments, La_2C_3 is found to be in the strong electron-phonon coupling regime. The upper critical fields show a clear enhancement with respect to the Werthamer-Helfand-Hohenberg prediction and amount to ~ 20 T at 0 K.

[1] G. Amano, S. Akutagawa, T. Muranaka, Y. Zenitani, and J. Akimutsu, J. Phys. Soc. Jpn. **73**, 530 (2004).

— 15 min. break —

TT 18.6 Tue 16:30 HSZ 02

Soft-mode behavior in superconducting MgB_2-like ternary silicides MAlSi (M=Ca,Sr,Ba) — •R. Heid[1], K.-P. Bohnen[1], B. Renker[1], P. Adelmann[1], D. Ernst[1], and H. Schober[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Institut Laue-Langevin, Grenoble

The discovery of superconductivity with $T_c \approx 39$K in MgB_2 has led to an intensive search for new superconductors with similar layered structures. Among them, the ternary silicides MAlSi with M=Ca,Sr,Ba exhibit interesting electronic and superconducting properties. With increasing mass of the M ion, T_c drops from 7.8K (Ca) to 5.1K (Sr) to <2K (Ba). Electronic structure calculations suggest that all three compounds possess very similar electronic properties [1], thus pointing to significant differences in the phonons and electron-phonon coupling (EPC).

Here we present results of a combined experimental and theoretical investigation of the lattice dynamics and EPC of the series MAlSi, M=Ca,Sr,Ba. Inelastic neutron-scattering measurements of the generalized phonon density of states show evidence for a low-frequency phonon mode in CaAlSi, which stiffens with increasing mass of the M ion. Using density-functional perturbation calculations of the phonons and EPC, we could identify this mode as an out-of-plane Al vibration with a large EPC. Contrary to a previous theoretical study [2], we do not find evidence for a dynamical instability. We will discuss implications for the observed superconducting trends among the MAlSi series.

[1] I. I. Mazin *et al.*, Phys. Rev. B**69**, 180512 (2004)
[2] G. Q. Huang *et al.*, Phys. Rev. B**69**, 064509 (2004)

TT 18.7 Tue 16:45 HSZ 02

Lattice dynamics and electron-phonon interaction in doped small radius nanotubes — •K.-P. Bohnen[1], R. Heid[1], H.J. Liu[2,3], and C.T. Chan[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Dept. of Phys., Univ. of Sci. and Technology, Kowloon, HongKong — [3]Dept. of Phys., Wuhan Univ., Wuhan, People's Republic of China

Recently lattice dynamics of small radius nanotubes has received a lot of attention due to the competition between superconductivity and Peierls transition. So far all ab-initio calculations for isolated nanotubes with diameter of 4 Å have shown a strong tendency to either a Peierls transition (in (3,3)-tubes)[1] or a structural transition to a non-metallic state with a small gap ((5,0)-tube) [2], in contrast to experimental findings of superconductivity in 4 Å tubes [3]. Doping these tubes might offer a possibility to enhance superconductivity, an effect which is well known from intercalated graphite. We present here ab-initio calculations of the lattice dynamics and electron-phonon coupling for doped (3,3)-tubes. The doping level has been chosen to move the Fermi level to a region of high density of states, however so far these calculations still favor the Peierls transition compared to superconductivity.

[1] K.-P. Bohnen, R. Heid, H.J. Liu, C.T. Chan, PRL **93**, 245501 (2004)
[2] D. Connetable et al., PRL **94**, 015503 (2005)
[3] Z.K. Tang et al., Science **292**, 2462 (2001)

TT 18.8 Tue 17:00 HSZ 02

Strong electron-phonon coupling in YNi_2B_2C: Theory and Experiment — •F. Weber[1,2], A. Kreyssig[3], L. Pintschovius[1], K. Hradil[4], K.-P. Bohnen[1], R. Heid[1], and W. Reichardt[1] — [1]Forschungszentrum Karlsruhe, Inst. f. Festkörperphysik — [2]Fak. f. Physik, Univ. Karlsruhe — [3]IAPD, TU Dresden — [4]PCI, Univ. Göttingen

Several compounds of the family $RENi_2B_2C$ (RE=Y, Lanthanoid) exhibit high superconducting transition temperatures (up to about 20 K) which is thought to be due to strong electron-phonon coupling (EPC). We made extensive calculations using density functional theory which indeed predict an EPC strength sufficient to explain the observed T_c's. We note that the strong EPC gives rise to pronounced anomalies in the phonon dispersion curves and concurrently to large line widths of certain phonon modes. In particular, there should be a pronounced phonon anomaly at the zone boundary in the (110)-direction (the so-called M-point) in addition to the already known anomaly in the (100)-direction. Inelastic neutron scattering measurements were performed on YNi_2B_2C on the triple axis spectrometer PUMA, Munich. The data show an extremely good agreement between the predicted and the observed phonon frequencies. Moreover, the measurements confirm the strong line broadening of the anomalous M-point mode predicted by theory. Finally, measurements in different Brillouin zones confirm the theoretical predictions, that in spite of the low frequency of the anomalous mode its eigenvector contains rather large amplitudes of the light atoms B and C.

TT 18.9 Tue 17:15 HSZ 02

Single crystal X-ray diffraction analysis and electron density calculation of YNi_2B_2C — •T. Leisegang[1], D. C. Meyer[1], P. Paufler[1], D. Souptel[2], G. Behr[2], O. Ignatchik[3], A. Ormeci[4], H. Rosner[4], and J. Wosnitza[5] — [1]ISP, TU Dresden, Germany — [2]IFW-Dresden, Germany — [3]IFP, TU Dresden, Germany — [4]MPI-CPfS, Germany — [5]HLD Dresden, FZ Rossendorf, Germany

The quaternary borocarbide YNi_2B_2C, space group (139) $I4/mmm$, exhibits superconductivity ($T_c \approx 15$ K) as was first reported in [1]. This superconducting behaviour depends strongly on the crystal composition within the small homogeneity range and on the crystal growth conditions. Here we report on investigations of two different samples, namely bulk samples grown by a floating zone technique [2] and plate samples grown by a flux-growth method [3]. De Haas-van Alphen (dHvA) measurements were performed to determine the electronic band structure as well as the evolution of a superconducting energy gap at the Fermi surface [4]. To evaluate the exact crystal structure, single-crystal X-ray diffraction measurements at room temperature were performed. Different models of structural disorder were refined and a difference-Fourier analysis was carried out. The experimental electron density will be compared with theoretical calculations. The work was supported by the Deutsche Forschungsgemeinschaft (SFB 463).

[1] Nagarajan et al., Phys. Rev. Lett. 72, 274 (1994).
[2] Souptel et al., J. Cryst. Growth 276, 652 (2005).
[3] Canfield et al., Phys. Today 51, 40 (1998).
[4] Ignatchik et al., J. Magn. Magn. Mat. 290-291, 424 (2005).

TT 18.10 Tue 17:30 HSZ 02

The Fermi surface topology and the superconducting gap function in UPd_2Al_3: a neutron spin-echo study — •Arno Hiess[1], Elizabeth Blackburn[1,2], Maikel C. Rheinstädter[1], Wolfgang Häussler[1,3], Nicholas Bernhoeft[4], and Gerry H. Lander[2] — [1]Institut Laue-Langevin, BP 156, F-38042 Grenoble, France — [2]European Commission, JRC, ITU, Postfach 2340, D-76125 Karlsruhe, Germany — [3]FRM-II, TU München, D-85748 Garching, Germany — [4]DRFMC, CEA-Grenoble, F-38054 Grenoble, France

We report on a single crystal neutron spin-echo investigation of the low-energy dynamic response in the magnetic superconductor UPd_2Al_3 ($T_N = 14$ K, $T_{sc} = 2$ K) in the vicinity of the antiferromagnetic wavevector $Q_0 = (0\ 0\ 0.5)$. Well inside the superconducting phase, antiferromagnetic quasielastic scattering, which is present in the normal state, is absent for relaxation times shorter than 10 ns, equivalent to an energy resolution better than 1 μeV. These observations are related to the geometry of the gap function and the Fermi surface topology. Any nodes present at the Fermi surface do not contribute significant weight to the electronic susceptibility. This places strong constraints on possible models for the origin and role of magnetic excitations in this magnetic superconductor.

TT 18.11 Tue 17:45 HSZ 02

Superconductivity and Lattice Instability in Compressed Lithium from Fermi Surface Hot Spots — •Deepa Kasinathan[1], Jan Kunes[1], Amy Lazicki[1,2], Helge Rosner[3], Choong-shik Yoo[2], Richard Scalettar[1], and Warren Pickett[1] — [1]Dept. of Physics, University of California - Davis, CA 95616, U.S.A — [2]Lawrence Livermore National Labratory, Livermore, CA — [3]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

Lithium, a simple metal not su perconducting above 5mK at ambient pressure, becomes a 20 K superconductor at 50 GPa. This high T_c is shown to arise from critical (formally divergent) electron-phonon coupling to the transverse phonon branch along intersections of Kohn anomaly surfaces with the Fermi surface. First principles linear response calculations of the phonon spectrum and spectral function $\alpha^2F(\omega)$ reveal (harmonic) instability already at 25 GPa. Our results imply that the fcc phase is anharmonically stabilized in the 25-38 GPa range.

TT 18.12 Tue 18:00 HSZ 02

Cooper pairing on a sphere: multielectron bubbles in helium — •Jacques Tempere[1,2], Vladimir Gladilin[1], Jozef Devreese[1], and Isaac Silvera[2] — [1]TFVS, Universiteit Antwerpen, Universiteitsplein 1, 2610 Antwerpen, Belgium — [2]Lyman Laboratory of Physics, Harvard University, Cambridge MA, USA

Electrons on helium constitute a versatile realization of a two-dimensional electron gas. Multielectron bubbles are cavities inside liquid helium, containing electrons that collect at the surface of the bubble, forming a spherical two-dimensional electron gas. In this contribution, we investigate the effects of the electron-ripplon interaction on the spherical electron system. We derive the conditions for which the electron-ripplon interaction can lead to an attractive interaction between the electrons, and to pairing. The paired state is described using Richardson's method. The density of states, the pair-breaking gap, and the ground state level occupations are derived and discussed. The difference between Cooper pairing in a flat electron system and Cooper pairing on a sphere are highlighted. Finally, progress in the experimental realization of this system is discussed.

TT 18.13 Tue 18:15 HSZ 02

Direct observation of non-local effects in superconductors — •Elvezio Morenzoni[1], Andreas Suter[1], Eugenie Kirk[1], Hubertus Luetkens[1,2], Thomas Prokscha[1], Rustem Khasanov[1,3], Michael Horisberger[1], and Nadir Garifianov[4] — [1]Paul Scherrer Institut, CH-5232 Villigen PSI — [2]TU Braunschweig, 38106 Braunschweig — [3]University of Zurich, CH-8057 Zurich — [4]Kazan Physical-Technical Institute, 420029 Kazan, Russian Federation

Applying a small magnetic field parallel to the surface of a superconductor results in the expulsion of the magnetic flux from its interior, except for a small region on the nm scale close to its surface where the local field B(z) (z depth from the surface) is heavily damped. It is very difficult to measure B(z) directly, since it extends only over a few tens of nanometer away from the surface into the material. This requires experimental probes that allow to measure the properties of such regions directly. We used the newly developed low energy muon spin rotation technique at PSI to first microscopically measure B(z) in conventional superconductors (Pb, Ta, Nb). Our measurements show that B(z) clearly deviates from an exponential decay underneath the surface and are a direct, model-independent proof for a non-local response in a superconductor. While $B(z)$ for Nb and Pb is well described within the Pippard and BCS models, for Ta this is true to a lesser degree. We attribute this discrepancy to the fact that the superfluid density is decreased by approaching the surface on a length scale ξ_0 an effect which is not taken self-consistently into account in the mentioned models. From the quantitative analysis London penetration and coherence length are obtained.

TT 19 Correlated Electrons: Low-dimensional Materials

Time: Tuesday 14:00–19:00 Room: HSZ 301

TT 19.1 Tue 14:00 HSZ 301

Heat transport of spin chains in $CaCu_2O_3$ — •A. Waske[1], H. ElHaes[2], C. Hess[1], N. Wizent[1], M. Apostu[1], G. Behr[1], C. Sekar[1], G. Krabbes[1], B. Büchner[1], F. Heidrich-Meisner[3], and W. Brenig[3] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Institut für Theoretische Physik, TU-Braunschweig, Germany

We present experimental results for the magnon thermal conductivity $\kappa_{\rm mag}$ of the ladder-like material $CaCu_2O_3$. Due to the small Cu-O-Cu bonding angle within the ladders ($\sim 120°$) the magnetic rung coupling is much weaker than the magnetic coupling along the legs. Hence, at sufficiently high temperatures the material is expected to behave like independent spin chains. In our experiments, we find a strong signature of magnetic heat transport above ~ 50 K, which appears to be linear in temperature. We estimate the magnetic mean free path which turns out to be of the order of 25 Å.

TT 19.2 Tue 14:15 HSZ 301

Revisiting the magnetism of hole-doped CuO_2 spin chains in $Sr_{14-x}Ca_xCu_{24}O_{41}$ — •Jürgen Schnack[1], Rüdiger Klingeler[2], Vladik Kataev[2], and Bernd Büchner[2] — [1]Universität Osnabrück, Fachbereich Physik — [2]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany

Magnetization measurements of $Sr_{14-x}Ca_xCu_{24}O_{41}$ with $0 \le x \le 12$ in magnetic fields up to 16 T show that the low temperature magnetic response of the CuO_2 spin chains changes strongly upon doping [1]. For $x = 0$ quantum statistical simulations [2] yield that the temperature and field dependence of the magnetization can be well described by an effective Heisenberg model in which the ground state configuration is composed of spin dimers, trimers, and monomers [3]. Reduction of the number of holes in the chains through Ca-doping leads to an additional contribution to the magnetization, which depends linearly on the magnetic field. Remarkably, the slope of this linear contribution increases with the Ca content. We discuss this behavior in the context of an effective Heisenberg model for hole-doped spin chains [2].

[1] R. Klingeler *et al.*, cond-mat/0511110
[2] J. Schnack, Eur. Phys. J. B **45** (2005) 311
[3] R. Klingeler *et al.*, cond-mat/0508626

TT 19.3 Tue 14:30 HSZ 301

Electronic structure of the incommensurate composite crystal $Sr_{14}Cu_{24}O_{41}$ — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, 86135 Augsburg

The incommensurate composite systems $(Ca,Sr)_{14}Cu_{24}O_{41}$ are based on two different structural units, CuO_2 ladders and CuO chains, where the Cu ions have the average valence 2.25. In the Sr compound nearly all Cu^{2+} ions (with $S = 1/2$) are found on the ladders, and nearly all Cu^{3+} ions are located on the chains. The latter form Zhang-Rice singlets, socalled holes. Substitution of Sr by Ca leads to a transfer of holes from the chains to the ladders. The spin order on the chains likewise depends on the doping and ranges from dimers to antiferromagnetic order.

Our calculations are based on density functional theory and take into account the details of the crystal structure [1] by means of an unit cell including 10 chain and 7 ladder units. The LDA results show that the chains and ladders can be treated independently. We present systematic investigations of the local density of states at the chain sites by studying a reduced unit cell without CuO_2 ladders. The crystal structures of the Ca and Sr-rich compound differ in a symmetric or asymmetric alignment of the CuO chains. We find that two bands contribute to the d_{xz}-states near E_F in the asymmetric case, whereas they are degenerate in the symmetric case. A tight binding fit shows that the orbital overlap between nearest and next-nearest neighbours is of the same order of magnitude. Details of the magnetic ordering and the role of electronic correlations result from spin-polarized and LDA+U calculations.

[1] Y. Gotoh et al., Phys. Rev. B 68, 224108 (2003)

TT 19.4 Tue 14:45 HSZ 301

Optical response of the low-dimensional insulator TiOCl under pressure — •S. Frank[1], A. Pashkin[1], C. A. Kuntscher[1], M. Hoinkis[2,3], M. Klemm[2], M. Sing[3], S. Horn[2], and R. Claessen[3] — [1]1.Physikalisches Institut, Universität Stuttgart, Germany — [2]Experimentalphysik 2, Universität Augsburg, Germany — [3]Experimentelle Physik 4, Universität Würzburg, Germany

The role of lattice, spin, and orbital degrees of freedom for the properties of the low-dimensional Mott insulator TiOCl is currently under debate. Upon cooling, the compound undergoes a transition to a non-

magnetic ground state, most probably a spin-Peierls state. The role of the orbital degree of freedom is much less clear: The occurrence of a second phase transition was discussed in terms of strong orbital fluctuation; this picture was questioned by transmission measurements, showing strong absorption features which were interpreted in terms of transitions between the crystal field-split Ti t_{2g} levels [1]. To obtain more information on the orbital excitations in TiOCl and to add new facets to its properties, we studied the polarization-dependent optical response as a function of pressure. The measurements were performed over a broad frequency range (mid-infrared to visible) on very thin crystals, which allowed to determine the position and lineshape of the absorption features as a function of pressure. We also discuss the possibility of a pressure-induced phase transition.

Supported by the DFG, Emmy Noether-program.

[1] R. Rückamp et al., Phys. Rev. Lett. **95**, 097203 (2005)

TT 19.5 Tue 15:00 HSZ 301

A possible dimerized ground state in the spin-1/2 cuprate $Na_3Cu_2SbO_6$ — •Miriam Schmitt[1] and Helge Rosner[2] — [1]TU Dresden — [2]MPI CPfS Dresden

Simulated by the resent discovery of helical ground states in spin-1/2 chain cuprates, we present an electronic structure study of the newly synthesized compound $Na_3Cu_2SbO_6$. This compound contains Cu_2O_6 sub-units build from edge shared CuO_2 plaquettes. The Cu_2O_6 sub-units are arranged in chains along the y-direction, interrupted by SbO_6 octahedra. The Cu-O-Cu bond angle in the Cu_2O_6 units is about 95°, therefore a competition of ferromagnetic and antiferromagnetic interactions can be expected. We investigate the electronic and magnetic structure of $Na_3Cu_2SbO_6$ starting from LDA band structure calculations that are mapped to an effective one-band tight-binding model and subsequently to an extended Heisenberg model. A variety of possible ground states is compared with respect to their total energy including the strong correlation using the LDA+U scheme. Furthermore, we discuss frustration of the magnetic exchange interaction along the chains due to next-nearest neighbor coupling and the influence of inter-chain interaction.

supported by the DFG (Emmy-Noether-program)

TT 19.6 Tue 15:15 HSZ 301

Magneto–elastic effects in Azurite — •Andreas Brühl[1], Katarina Removic–Langer[1], Yeekin Tsui[1], Bernd Wolf[1], Michael Lang[1], and Jürgen Schreuer[2] — [1]Physikalisches Institut, J.W.Goethe–Universität Frankfurt — [2]Institut für Mineralogie, J.W.Goethe–Universität Frankfurt, Frankfurt am Main

Quantum spin systems with frustration exhibit comprehensive phase diagrams with a variety of possible ground states. One of the simplest one-dimensional frustrated quantum systems is the $S = 1/2$ diamond chain. According to recent theoretical calculations for the distorted diamond chain the ground state is either a ferrimagnetic phase, a dimerized phase or a spin liquid phase. So far, experimental work has been hampered by lacking appropriate compounds until recently, when Kikuchi et al. found that the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) is a model substance for the distorted diamond chain. In this contribution we present results of magnetic susceptibility, thermal expansion and pulse field ultrasonic measurements on a high quality azurite single crystal. From the pronounced anomalies in the coefficient of thermal expansion as a function of temperature and the elastic constant as a function of magnetic field around the saturation field of 32 T, we infer an extraordinarily strong magneto–elastic coupling constant. We discuss our results in light of the different possible ground states that have been proposed for this material.

TT 19.7 Tue 15:30 HSZ 301

Electronic structure and magnetic properties of the spin-$\frac{1}{2}$ system Bi_2CuO_4 — •Oleg Janson[1,2] and Helge Rosner[1] — [1]MPI CPfS Dresden — [2]SPbSU St. Petersburg, Russia

Bi_2CuO_4 crystallizes in the tetragonal system, with isolated CuO_4 plaquettes arranged parallel to the xy plane and staggered in chains along the z axis. Initially, Bi_2CuO_4 was treated as 1D compound, but low temperature data, especially the magnetic moment of 0.93 μ_B, show that quantum fluctuations are strongly suppressed and exclude a 1D model. Neutron scattering data reveal FM-ordered chains along z, that are AFM ordered with respect to each other [1]. To elucidate the origin of the surprisingly FM-ordered chains, we performed DFT calculations to evaluate the relevant orbitals and couplings. Total energy calculations yield a magnetic groundstate coinciding with the experimental data. From a tight-binding fit of the LDA band structure we obtained the exchange integrals. The most important result is that the main coupling is between the chains and the in-chain interaction is relatively small. Thus, the FM arrangement of chains is due to strong AFM exchange of neighbouring plaquettes that belong to the different chains. Therefore, Bi_2CuO_4 has to be described as a compound with 3D coupling.

This investigation was supported by the DFG, Emmy Noether-program

[1] J. L. García-Muñoz, J. Rodríguez-Carvajal et al. J. Phys.: Condens. Matter, **2** (1990) 2205–2214

TT 19.8 Tue 15:45 HSZ 301

High Field Magnetization and ESR on a S = 1 Spin Ladder — •C. Mennerich[1], C. Golze[1,2], V. Kataev[2], A. Alfonsov[2], R. Klingeler[2,3], B. Büchner[2], D.J. Price[4], M. Goiran[3], H. Rakoto[3], J.-M. Broto[3], O. Kataeva[5], M. Broekelmann[1], S. Grossjohann[6], W. Brenig[6], and H.-H. Klauss[1] — [1]IPKM,TU Braunschweig, Germany — [2]IfW Dresden, Germany — [3]LNCMP Toulouse, France — [4]U Glasgow, United Kingdom — [5]Arbuzov Institute, RAS, Kazan, Russia — [6]IThP, TU Braunschweig, Germany

The compound $Na_2Ni_2(ox)_2(H_2O)_2$ (ox =C_2O_4) forms a S=1 spin ladder. SQUID measurements show a pronouced maxima at temperatures between 39 K and 47 K along different crystallographic axes. This behaviour results from antiferromagnetic interactions and a single ion anisotropy D in the distorted octahedral surrounding of the Ni(II) ions. To determine the anisotropy D and the g-factor we performed high frequency (up to 740 GHz) high field (up to 30 T) ESR measurements on a powder sample resulting in D = 11.5 K and g = 2.2. Using these results we analysed the susceptibility and magnetization measurements. High field magnetization measurements up to 55 Tesla on a powder sample show typical magnetization steps in very good agreement with our simulations. These results prove that the system is close to the decoupled dimer limit. Further support for this conclusion stems from quantum monte carlo simulations performed for different ratios of intra-dimer to inter-dimer coupling taking into account the single ion anisotropy D.

This work is supported by the DFG within SPP1137 under contract KL1086/6-1.

TT 19.9 Tue 16:00 HSZ 301

Mössbauer Study of the Fe(II) S=2 Spin Chain System $K_2Fe(C_2O_4)_2$ — •H.-H. Klauss[1], F. Gouider[1], F.J. Litterst[1], S. Grossjohann[2], A. Honecker[2], W. Brenig[2], and D.J. Price[3] — [1]IPKM, TU Braunschweig, Germany — [2]IThP, TU Braunschweig, Germany — [3]Department of Chemistry, U Glasgow, United Kingdom

Fe(II) in $K_2Fe(C_2O_4)_2$ is arranged in zig-zag chains in which the magnetic exchange is primarily mediated by the oxalate $(C_2O_4)2-$ anions [1]. Mössbauer spectroscopy proves a well isolated orbital singlet ground state of the Fe in a very unusual trigonal prismatic local symmetry. Magnetic susceptibility measurements reveal a Curie-Weiss like behaviour at high temperatures and a broad cusp at 20 K consistent with dominant 1-D antiferromagnetic interactions. 3-D magnetic order is found below 7 K by Mössbauer spectroscopy. In the magnetic susceptibility an upturn is found below 7 K indicating a weak ferromagnetic component in the dominantly antiferromagnetically ordered state. Using Quantum Monte Carlo the magnetic susceptibility for a S=2 spin chain is calculated and compared with the experimental data. This results in an intrachain magnetic exchange constant of $J||/k_B \approx 6$ K. From an RPA analysis of the 3-D ordering temperature the interchain magnetic exchange constant is estimated to be one order of magnitude smaller consistent with a dominant 1-D character of the magnetic interaction in this system.

[1] M.B. Hursthouse, M.E. Light, and D.J. Price, Angew. Chem. Int. Ed. 43 (2004) 472.

TT 19.10 Tue 16:15 HSZ 301

From weakly coupled tetrahedra to molecular like host guest magnets — •R. Takagi[1], R. Becker[1], M. Johnsson[1], R. K. Kremer[2], R. Valenti[3], and P. Lemmens[4] — [1]Dept. Inorg. Chem., Stockholm Univ., Sweden — [2]MPI-FKF, Stuttgart, Germany — [3]Univ. Frankfurt, Germany — [4]IPKM, TU Braunschweig, Germany

The search for novel weakly coupled or molecular like magnets in the range of lone pair oxohalogenides based on Cu^{2+}, Ni^{2+}, and Mo^{2+} has been very fruitful in recent years. We give an overview on their structural, electronic and magnetic properties. Established magnetic structures have dimers, chains, tetrahedra, 5- and 13-spin centers. The latter are realized as guests in cages of high symmetry host structures.

Work supported by DFG SPP1073 and ESF-HFM.

— 15 min. break —

TT 19.11 Tue 16:45 HSZ 301

Magnetic properties of Vanadium Oxide Nanotubes — •I. Hellmann[1], R. Klingeler[1], E. Vavilova[1,2], Y. Arango[1], A. Popa[1], V. Kataev[1], Ch. Täschner[1], and B. Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, Kazan, Russia

A new class of nanoscale low-dimensional magnets, mixed valent vanadium-oxide multiwall nanotubes (VO_x-NTs), shows up diverse properties ranging from spin frustration and semiconductivity to ferromagnetism by doping with either electrons or holes [1]. To obtain insights into the magnetic properties of these novel nanosize magnets we have studied the static magnetisation M of undoped VO_x-NTs in the temperature range from 2 K to 600 K in magnetic fields up to 14 T. The data provide evidence for the occurrence of two magnetically nonequivalent vanadium sites in the structure. These sites can be presumably attributed to V^{4+}(d^1, S=1/2) ions in the octahedral and tetrahedral oxygen coordination, respectively. The former are strongly antiferromagnetically correlated and exhibit some signatures of a spin-liquid behaviour. The latter are much weaker magnetically coupled and dominate the low-temperature static magnetic response. In addition to $M(H,T)$ measurements we present also ESR and NMR results obtained on the same samples and discuss possible models of spin coupling and low-energy spin dynamics in VO_x-NTs.

[1] L. Krusin-Elbaum *et al.*, Nature **431**, 672 (2004)

TT 19.12 Tue 17:00 HSZ 301

Stripe Correlations in $Na_{0.75}CoO_2$ — •Jochen Geck[1], Martin von Zimmermann[2], Helmuth Berger[3], Sergey Borisenko[1], Helmut Eschrig[1], Klaus Koepernik[1], Martin Knupfer[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]HASYLAB at DESY, Germany — [3]EPF Lausanne, Switzerland

Spin and charge stripes in correlated two-dimensional electron systems are one of the hot spots of today's condensed matter research. So far, stripes have been observed in materials based on square lattices like the nickelates and the high-temperature superconducting cuprates. Here we show, based on high-energy x-ray diffraction data and LDA calculations, that sodium-density stripes are formed in $Na_{0.75}CoO_2$; a material based on a triangular lattice. The LDA calculations show that the sodium order results in a sizeable dip of the density of states at the Fermi level, pointing to band structure effects as a driving force for the ordering. This indicates that the stripe order is an intrinsic feature of the two-dimensional CoO_2-layers. Similarities regarding the pinning of stripe correlations in the high-temperature superconducting cuprates and the Na_xCoO_2-materials will also be discussed.

TT 19.13 Tue 17:15 HSZ 301

Density Functional Calculations of the Total Energy and Electronic Structure of Na_xCoO_2 Using the LDA — •Klaus Koepernik, Helmut Eschrig, Jochen Geck, and Bernd Buechner — IFW Dresden, Germany

We analyze the low temperature electronic structure of $Na_{0.75}CoO_2$. Full potential all-electron density functional calculations within the local density approximation (LDA) have been performed. A number of low symmetry superstructures in the Sodium planes have been compared with respect to the LDA total energy. Our findings support the symmetry recently found in diffraction experiments. The superstructure favoured by LDA calculations shows a Sodium charge density wave (CDW) in aggreement with the experimental results. Besides Coulomb energy arguments in favour of the CDW the density of states indicates a band energy gain due to the CDW. The band energy favorization of the CDW is further supported by a small Sodium offset from its symmetry position, increasing the amplitude of the wave. Comparision with the cuprates shows rather big differences in the doping mechanism and therefore in the low energy physics.

TT 19.14 Tue 17:30 HSZ 301

Magnetically driven microwave absorption in $La_1Sr_1MnO_4$: Pulsed magnetic fieldstudies — •R. Klingeler[1,2], V. Kataev[1], U. Schaufuss[1], B. Büchner[1], P. Reutler[1,3], A. Revcolevschi[3], M. Goiran[2], H. Rakoto[2], J.M. Broto[2], and B. Raquet[2] — [1]IFW Dresden, Germany — [2]LNCMP Toulouse, France — [3]UniversitéParis-Sud, France

Spin degrees of freedom are expected to dominate the magnetism in layered hole-free $La_1Sr_1MnO_4$ as the orbital momentum of the Mn ions is quenched by the anisotropic crystal field. Surprisingly, our thermal expansion and NEXAFS data indicate that orbitals are still relevant. There is a temperature driven reorientation of the orbital states. Recent inelastic neutron scattering (INS) data reveal a large spin gap of ∼2.2 THz and two in-gap excitations at 0.8 THz and 1.7 THz in the antiferromagnetically (AF) ordered ground state. The origin of the large anisotropy and the in-gap excitations is unclear. Here we report high frequency electron spin resonance, magnetization and electrical conductivity measurements in magnetic fields up to 60 T. In the AF ordered state we observe a surprisingly strong absorption of sub-Terahertz electromagnetic radiation in fields above 15 T. In the DC limit conductivity measurements yield a significant negative magnetoresistance $R(H)$ as well. However, there are no anomalies in $R(H)$ as well as in the magnetization $M(H)$ in the field range where strong microwave absorption is observed. At still larger fields $M(H)$ reveals the anomaly which can be associated with the lower in-gap spin excitation found in the INS. We discuss our results in terms of an unusual interplay between structure, orbitals and spins.

TT 19.15 Tue 17:45 HSZ 301

Phase transition of β-$MoTe_2$ studied by transport measurements and soft x-ray photoemission spectroscopy — •Thorsten Zandt, Robert Heimburger, Lenart Dudy, Beate Müller, Alica Krapf, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Inst.f.Physik, Humboldt-Universität zu Berlin

$MoTe_2$ undergoes a phase transition at about 1125 K from a low-temperature semiconducting β-phase (hexagonal) to a high-temperature metallic β-phase (monoclinic). Upon cooling, for monoclinic β-$MoTe_2$ an additional phase transition is observed at 250 K. This transition is accompanied by a discontinuous structural change, i.e. the monoclinic angel β of 93°55′ changes to 90° [1] resulting in an orthorhombic Td-$MoTe_2$ structure. In this contribution we present a detailed temperature dependent study of the transport and electronic properties of the 250K-phase transition of the $MoTe_2$ single crystals. The in-plane resistivity as well as the magnetic susceptibility reveal a distinct hysteretic behavior at the phase transition. In addition, temperature dependent soft x-ray photoemission of Te 4d core levels show a large splitting, which could indicate the occurrence of charge density wave (CDW) formation in β-$MoTe_2$, although there is no direct evidence yet like superlattice spots in the electron diffraction pattern. This will be discussed within a model in which the competition between Coulomb and elastic interactions may drive the first-order lock-in transition to Td-$MoTe_2$ at 250 K.

[1] Clarke, R, Marseglia E and Hughes H P 1978 Phil. Mag. 38 121

TT 19.16 Tue 18:00 HSZ 301

Two-Dimensional Electron-Electron Scattering in the Inherent Conducting Polymer $\{(CH_3)_{0.92}ReO_3\}_\infty$ — •R. Miller[1], E.–W. Scheidt[1], G. Eickerling[1], Ch. Helbig[1], R. Herrmann[1], W. Scherer[1], and P. Schwab[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]Theoretische Physik II, Universität Augsburg,

The metal-oxide system polymeric methyltrioxorhenium $\{(CH_3)_{0.92}ReO_3\}_\infty$ (*poly*-MTO) is a unique representative of an inherent conductive organometallic polymer. In particular the $\{ReO_2\}_\infty$ planes characterize *poly*-MTO as a prototype for a purely two-dimensional system. The resistivity data of pure *poly*-MTO exhibit a crossover from metallic ($d\rho/dT > 0$) to insulating ($d\rho/dT < 0$) behavior at a characteristic temperature $T_{min} \cong 38$ K. Above T_{min} the resistivity $\rho(T)$ is remarkably well described by a two-dimensional electron system. Below T_{min} an unusual resistivity behavior, similar to that found in doped cuprates, is observed. The resistivity increases as $\rho \sim \ln(1/T)$ before it follows a $\sqrt{T}$ temperature dependence below 2 K. We suggest a crossover from purely two-dimensional charge-carrier diffusion within the $\{ReO_2\}_\infty$ planes to three-dimensional diffusion at low temperatures in a disorder-enhanced electron-electron interaction scenario (Altshuler-Aronov correction).

TT 19.17 Tue 18:15 HSZ 301

Sample-dependent resistivity profiles in κ-(ET)$_2$Cu[N(CN)$_2$]Br organic superconductors - interrelations with other normal- and superconducting-state properties — •C. Strack[1], C. Akinci[1], V. Paschenko[1], B. Wolf[1], E. Uhrig[1], W. Assmus[1], M. Lang[1], J. Schreuer[2], L. Wiehl[2], J. Schlueter[3], J. Wosnitza[4], D. Schweitzer[5], and J. Wyckhoff[6] — [1]Physikalisches Institut, J.W. Goethe-Universität Frankfurt, FOR 412 — [2]Institut für Mineralogie, J.W. Goethe-Universität Frankfurt, FOR 412 — [3]Materials Science Division, Argonne NL, Illinois, USA — [4]Institut für Festkörperphysik, TU Dresden — [5]3. Physikalisches Institut, Universität Stuttgart — [6]Max Planck Institut für Chemische Physik fester Stoffe, Dresden

The organic superconductor κ-(ET)$_2$Cu[N(CN)$_2$]Br shows striking sample-to-sample variations in the electrical resistivity [1]: While most of the crystals reveal a ρ(T) maximum around 90 K with a semiconducting behaviour above, some remain metallic for $T < 300$ K. In the absence of significant differences in the crystals' structural parameters, chemical composition and ESR spectra, these results indicate that real structure phenomena, i.e. disorder and/or defects, strongly affect the inelastic scattering [1]. Here we report on a comparative resistivity study on a variety of crystals with quite different ρ(T) profiles. The work aims at seeking out interrelations between the anomalous scattering contributions at intermediate temperatures and features of the normal- and superconducting-state, such as the glass transition at $T_g \approx 77$ K, the temperature $T^* \approx 40$ K [1], as well as the superconducting transition temperature. [1] C. Strack et al., Phys. Rev. B 72, 054511 (2005)

TT 19.18 Tue 18:30 HSZ 301

Coulomb parameters and spectral function for TTF-TCNQ — •Erik Koch — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

The key ingredient for a realistic description of strongly correlated materials by a model Hamiltonian is the reliable determination of the Coulomb repulsion parameters. For molecular crystals this is possible. For the example of the quasi one-dimensional organic conductor TTF-TCNQ we show how to calculate the Coulomb repulsion energies between charges in the HOMO/LUMO orbitals. As these molecules, like most π-systems, are planar, we find that a description by a standard Hubbard model with only on-site interaction U is not sufficient. Instead, interactions between charges on different molecules have to be taken into account. Including these longer range interactions has a strong effect on the spectral function, giving results consistent with the photoemission data, without having to assume unrealistically large band-width, as is necessary when when neglecting the Coulomb terms between neighboring molecules.

TT 19.19 Tue 18:45 HSZ 301

Infrared and Raman studies of the competition between spin and charge order in quasi-1D conductors — •Michael Dumm[1], Matteo Masino[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Dipartimento di Chimica and INSTM-UdR, Università di Parma, Parma, Italy

Charge order (CO) phenomena and their competition with spin order are one focus of recent research on low-dimensional highly correlated materials like organic conductors or transition-metal oxides. In the quasi-1D (TMTTF)$_2X$ charge-transfer salts charge disproportionation (CD) on the (TMTTF)$_2$-dimers leads to a ferroelectric CO state. Subsequently, at lower T a transition into a spin-Peierls ground state is observed. Up to now, issues like the charge-order patterns and the coexistence of charge- and spin-ordered ground states in this class of materials remain unclear. We address these issues with T-dependent polarized infrared and Raman spectroscopy on single crystals of (TMTTF)$_2X$.

In the mid-IR spectra, we observed a splitting of several vibronic modes below the charge-order transition which can be directly linked to the CD on the molecules. At far-IR frequencies below 100 cm^{-1}, new intradimer vibrations get IR active along all three crystal axes in the CO state due to the unequal charge distribution on the TMTTF molecules. Above the CO transition, these modes are Raman active. We performed a detailed analysis of the temperature dependence of these modes. We find for the first time clear evidence that the charge order coexists with the spin-Peierls ground state at low temperatures despite the fact that both are competing ground states.

TT 20 Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts - Part 2

Time: Tuesday 14:00–16:00 Room: HSZ 105

Invited Talk

TT 20.1 Tue 14:00 HSZ 105

Theory of inelastic scattering from magnetic impurities — •Gergely Zarand[1,2], Laszlo Borda[1], Natan Andrei[3], and Jan von Delft[4] — [1]Budapest Univ. of Technology and Economics, Ungarn — [2]Institut für Theoretische Festkörperphysik, Universität Karlsruhe — [3]Rutgers University — [4]LM Universität München

Inelastic processes play a crucial role in mesoscopic structures, where these processes destroy quantum interference effects. Recent experiments on quantum wires seem to support that much of these inelastic processes originate from magnetic impurities. Here we provide a framework that - at least at $T = 0$ temperature - allows one to give a precise definition for the inelastic scattering rate and we show how this can be obtained for general quantum impurity models. As an example, we compute the full energy dependence of the inelastic scattering rate for the single channel Kondo problem using the non-perturbative machinery of numerical renormalization group. In contrast to naive expectations, we find a broad plateau of almost constant inelastic scattering rate for energies above the Kondo temperature, $E > T_K$, and a quasi-linear behavior below T_K, which crosses over to the expected Fermi liquid behavior, $\sigma_{\rm inel}(E) \sim E^2/T_K$ only at very small energies. This behavior compares well with recent experimental observations.

TT 20.2 Tue 14:30 HSZ 105

A comment on the universality of transmission distribution of a diffusive conductor — •Mihajlo Vanevic[1] and Wolfgang Belzig[2] — [1]Department of Physics and Astronomy, University of Basel, Switzerland — [2]Department of Physics, University of Konstanz, Germany

We find the distribution of transmission eigenvalues in a series of identical junctions between chaotic cavities using the circuit theory of mesoscopic transport. We show that this distribution rapidly approaches the diffusive limit as the number of junctions increases, independent of the specific scattering properties of a single junction. We obtain the cumulant generating function and the first three cumulants of the charge transfer through the system both in the normal and superconducting case.

TT 20.3 Tue 14:45 HSZ 105

Non-Equilibrium Dynamics in Donor-Bridge-Acceptor Systems: A time dependent Numerical Renormalization Group Study — •Sabine Tornow[1], Ralf Bulla[1], and Frithjof Anders[2] — [1]Theoretische Physik III, Elektronische Korrelationen und — [2]Institut für Theoretische Physik

We investigate the relaxation dynamics of multiple electrons in a donor-bridge-acceptor system (DBA) with a coupling of the electronic degrees of freedom to a common bosonic bath. The model allows to study many-particle effects and the influence of the local and non-local Coulomb interactions. Non-perturbative methods are needed to calculate the non-equilbrium and equilibrium properties in the full parameter space. We are using the time dependent Numerical Renormalization Group to calculate transfer rates. Furthermore we discuss the possibility of many-particle (bipolaronic) and Coulomb-assisted transfer. .

TT 20.4 Tue 15:00 HSZ 105

Linear response conductance of strongly interacting nanostructures using DMRG — •Dan Bohr[1,2], Peter Schmitteckert[2], and Peter Wölfle[2] — [1]MIC, Department of Micro and Nanotechnology, Technical University of Denmark — [2]TKM, Institut für Theorie der Kondensierten Materie, Universität Karlsruhe

In this contribution we present a novel approach for the calculation of transport properties of strongly correlated systems: a direct evaluation of the Kubo expression for the linear conductance by using the states and operator expectation values computed with the Density Matrix Renormalization Group (DMRG). Two different correlation functions are used to evaluate the conductance. The electrons are treated as one-dimensional spinless fermions, and the interactions are confined to

a finite line segment which couples to two tight-binding leads. The developed method is benchmarked against the non-interacting limit, where the conductance can be calculated either by Green's functions or by exact diagonalization. In the interacting case we present DMRG data for an extended nanostructure either in the Luttinger liquid regime or in the charge density wave regime. Finally we analyze the strongly interacting conductance using a simple model of hard-core particles on a reduced size lattice and emphasize the difference compared to an effective charging model.

TT 20.5 Tue 15:15 HSZ 105

Differential Conductance using Real-Time Dynamics in DMRG — •Peter Schmitteckert and Günter Schneider — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Germany

In this work we apply the Real-Time Density-Matrix-Renormalization Group Method (RT-DMRG) to calculate the differential conductance of an interacting nano-structure attached to one-dimensional, non-interacting leads. We first discuss our approach to extract the differential conductance. We then explain the difficulties arising from finite size effects, and how they can be addressed. Finally, we present results for the linear conductance vs. an applied gate voltage and the non-equilibrium differential conductance vs. source-drain voltage for weakly and strongly interacting nano-structures.

TT 20.6 Tue 15:30 HSZ 105

Fano interference and Kondo correlations in the non-linear regime of simple mesoscopic models. — •Alexandru Aldea, Viorel Dinu, and Mugurel Tolea — National Institute of Materials Physics, Bucharest-Magurele, Romania

The Fano effect in mesoscopic systems consists in the asymmetric shape of electron transmittance peaks due to the interference of electron waves propagating along channels with strongly different properties. The tunneling process is additionally affected by the Kondo-type correlation between the spin of the dot and the spin of the incoming electron. The consequences of correlations can be noticed in the local density of states and in changes of the shape of Fano lines. This effect is known as the Fano-Kondo effect and combines the main ingredients of meso-systems: the geometry and interaction . In this work we analyze simple models like the T-shape and triangle model in order to identify specific contributions of the interaction and geometry for the transport properties in the linear and non-linear regime; the triangle model allows also for the magnetic field effects. We calculate the local DoS and conductance in a large range of relevant parameters by the use of the tight-binding Hamiltonian description [1] and non-equilibrium Green function formalism. The equation of motion method is used along with [2].

[1] V.Moldoveanu, M.Tolea, A.Aldea, and B.Tanatar, Phys. Rev. B **71**, 125338 (2005).
[2] O.Entin-Wohlman et al, Phys. Rev. B **71**, 035333 (2005).

TT 20.7 Tue 15:45 HSZ 105

Transport in disordered quantum wires: the global phase diagram — •Thomas Nattermann[1], Michael Fogler[2], and Sergey Malinin[3] — [1]Institut für Theoretische Physik der Universität zu Köln — [2]Department of Physics, UCSD, USA — [3]Department of Chemistry, Wayne State Univ. Detroit, USA

We calculate the tunnel current in a Luttinger liquid with a finite density of strong impurities using using a combined RG and instanton approach. For very low temperatures T (or electric fields E) the (nonlinear) conductivity is of variable range hopping type as for weak pinning. Rare events - usually important in one dimensions - result in logarithmic corrections. For higher fields but low T the conductivity shows power law behavior corresponding to a crossover from multi- to single-impurity (Kane-Fisher) tunneling. For higher T and small fields rare events lead to a number of new results for the conductivity. The discussion of the the various cross-overs in the T-E plane as well as a function of the pinning strength allow a complete determination of the various relevant regimes, including previously found isolated results.

TT 21 Transport: Nanoelectronics II - Spintronics and Magnetotransport - Part 2

Time: Tuesday 16:15–19:00 Room: HSZ 105

TT 21.1 Tue 16:15 HSZ 105

Coherent Spin Ratchets — •Klaus Richter, Andreas Pfund, and Dario Bercioux — Fakultät für Physik, Universität Regensburg

We propose a new class of quantum ratchet devices, namely spin-orbit based ratchets which act as sources for pure spin currents. To this end we demonstrate that the combined effect of a spatially periodic electrostatic potential, lateral confinement and spin-orbit interaction in a two-dimensional coherent conductor gives rise to a quantum ratchet mechanism for spin-polarized currents. Upon external ac-driving, and in the absence of a static bias, the system generates a directed spin current, while the total charge current is zero. We analyze the underlying mechanism by employing symmetry properties of the scattering matrix, and we numerically verify the effect for different setups relevant for experiment. We further show that the spin current directions can be changed upon tuning the Fermi energy or the relative strength of Rashba and Dresselhaus spin orbit coupling.

TT 21.2 Tue 16:30 HSZ 105

Spin-dependent Transport through Quantum Dots connected to Three Ferromagnetic Leads — •Daniel Urban, Matthias Braun, and Jürgen König — Ruhr-Universität Bochum, 44780 Bochum, Germany

Transport through a non-magnetic, single-level quantum-dot with ferromagnetic leads is investigated in the sequential tunneling regime by a real-time diagrammatic technique. If a current is forced through the system, spin accumulates on the dot, which reduces transport (spin-valve effect). The interplay of Coulomb interaction and ferromagnetism gives rise to an exchange field [1], in which the spin precesses so that transport is enhanced.

We consider setups in which a current flows only between two of the leads. The third lead is kept current-free and enters only by its ferromagnetic properties.

The two systems analyzed are a quantum dot spin-flip transistor with coplanar magnetizations and a setup with pairwise orthogonal lead magnetizations. In both cases spin precession due to the third lead further enhances transport while in the latter we additionally observe asymmetries in the conductances under current reversal.

[1] M. Braun, J. König, and J. Martinek, Phys. Rev. B **70**, 195345 (2004)

TT 21.3 Tue 16:45 HSZ 105

Signature of spin-related phases in transport through regular polygones — •Dario Bercioux[1], Diego Frustaglia[2], and Michele Governale[3] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]NEST-INFM & Scuola Normale Superiore, Pisa, Italy — [3]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Germany

We address the subject of transport in one-dimensional ballistic polygon loops subject to spin-orbit interactions. The polygons are modeled in the framework of the spin quantum-network technique [1]. We identify the role played by the polygon vertices in the accumulation of spin-related phases by studying interference effects as a function of the spin-orbit interaction strength. We find that the vertices act as strong spin-scattering centers that hinder the developing of Aharovov-Casher and Berry phases. In particular, we show that the oscillation frequency of interference pattern can be doubled by modifying the shape of the loop from a square to a circle [2].

[1] D. Bercioux *et al.*, Phys. Rev. Lett. **93**, 56802 (2004).
[2] D. Bercioux, D. Frustaglia, and M. Governale, Phys. Rev. B **72**, 113310 (2005).

TT 21.4 Tue 17:00 HSZ 105

Tunneling current through Tomonaga-Luttinger liquid ring with spin-orbit coupling — •Mikhail Pletyukhov[1], Nicolas Pauget[1], and Vladimir Gritsev[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

We calculate dc conductance of an interacting quantum ring with spin-orbit coupling which is attached to normal leads. We consider the linear response regime and assume a weak coupling to the leads. Electron-

electron interaction in the ring is described non-perturbatively by means of the multicomponent Tomonaga-Luttinger liquid model. We study how the positions of the conductance peaks depend on the system parameters (magnetic flux, gate voltage, spin-orbit coupling strength) and observe the features arising due to electron correlations.

TT 21.5 Tue 17:15 HSZ 105

Sequential and Co-Tunneling Shot Noise in Quantum Dot Spin Valves — •Matthias Hettler[1], Axel Thielmann[1], Jürgen König[2], and Gerd Schön[1,3] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [3]Institut für Theoretische Festkörperphysik, Universität Karlsruhe

For a single level quantum dot coupled to ferromagnetic electrodes transport is sensitively dependent on the magnetic orientation and degree of polarization of the electrodes. If in addition a magnetic field leads to Zeemann split states on the quantum dot, the additional energy scale of inelastic co-tunneling processes comes into play. Co-tunneling processes strongly influence the transport not only in the Coulomb-blockade regime, but also around the resonances and above the sequential tunneling threshold, even at quite small dot-electrode coupling. In particular, the shot noise displays rich behavior that can only be understood by dealing with sequential and co-tunneling processes on equal footing. We present a diagrammatic approach to this problem that is valid for for arbitrary Coulomb interaction and accounts for non-Markovian memory effects relevant to the shot noise [1]. We observe spin-accumulation and spin-inversion on the quantum dot and predict strongly non-monotonic behavior of the shot noise with peaks and peak-dip features as well as various regimes where the noise is anomalously enhanced (super-Poissonian noise).

[1] A. Thielmann, M. H. Hettler, J. König, and G. Schön, Phys. Rev. Lett. 95, 146806 (2005).

— 15 min. break —

TT 21.6 Tue 17:45 HSZ 105

Fingerprints of spin polaron states in quantum transport through mesoscopic wires — •Herbert Schoeller, Frank Reininghaus, and Thomas Korb — Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen

Using the Keldysh formalism in combination with a self-consistent diagrammatic approach, we investigate the possibility to find fingerprints of spinpolaron states in quantum transport trough a mesoscopic quantum wire coupled via local exchange to a ferromagnetic spin chain. The spin polaron state occurs due to a hybridization between electronic states and magnons. Due to its low decoherence rate we find coherent transport and a new peak in the differential conductance as function of bias voltage. In addition we find peaks from the usual scattering states and inelastic tunneling. We discuss the peak structure as function of an external magnetic field, polarization of the leads, and the level spacing on the quantum wire.

TT 21.7 Tue 18:00 HSZ 105

Effects of Disorder and Reduced Adiabaticity on the Topological Hall Effect — •Michael Wimmer, Tobias Breu, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

In the Topological Hall Effect (THE), a non-vanishing Hall effect is introduced not by a magnetic field, but by the Berry phase of spins adiabatically following a magnetic texture. Based on theoretical considerations on a clean, perfectly adiabatic system, an experimental realization was proposed in [1]. However, a real system might not be perfectly adiabatic: For example, elastic scattering has shown to be impairing adiabaticity [2].

We have developed a recursive Green's function algorithm to calculate the conductance of a four-terminal structure and present numerical studies on the THE. Our main focus is on the effects of disorder and on parameters outside the perfectly adiabatic regime. First results indicate that the THE persists for scattering lengths in reach of experiment.

[1] P. Bruno, V. K. Dugaev, and M. Taillefumier, Phys. Rev. Lett **93**, 096806 (2004)
[2] M. Popp, D. Frustaglia, K. Richter, Phys. Rev. B **68**, 041303 (2003).

TT 21.8 Tue 18:15 HSZ 105

Magnetotransport along a barrier: multiple quantum interference of edge states — •Anatoli M. Kadigrobov, Mikhail V. Fistul, and Konstantin B. Efetov — Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum Germany

Transport in a two-dimensional electron gas subject to an external magnetic field is analyzed in the presence of a *longitudinal barrier*. Similar systems have been produced by using a split-gate technique or cleaved edge fabrication method. We show that *quantum interference of the edge states* bound by the longitudinal barrier results in a drastic change of the electron motion: the degenerate discrete Landau levels are transformed into an alternating sequence of energy bands and energy gaps. The spectrum $\epsilon_n(p_x)$ is characterized by a nearly periodic dependence on the momentum p_x along the barrier. The width of the bands and the gaps can be tuned by the magnetic field and the gate voltage. These features of the electron spectrum should result in a high sensitivity of thermodynamic and transport properties of the 2D electron gas to external fields. In particular, we predict giant oscillations of the ballistic conductance and discuss nonlinear current-voltage characteristics, coherent Bloch oscillations and effects of impurities.

TT 21.9 Tue 18:30 HSZ 105

Magnetic Switching of the Superconducting Transition Temperature Ferromagnetic/Superconducting Bi- and Tri-Layers — •Roland Steiner, Alfred Plettl, and Paul Ziemann — Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm

Superconductivity and ferromagnetism are two antagonistic phenomena. The interplay between these two phenomena in multilayer systems is currently under intensive research [1].

In the present contribution results are presented on the magnetoresistance R(H) of ferromagnet/superconductor double- and trilayer-systems in their superconducting state with a typically 30 nm thick Niobium film as superconductor in all cases. It is demonstrated that the R(H)-curve exhibits a non-monotonous behaviour in the range of the coercitive field H_{coe} of the involved ferromagnets close to the superconducting transition at T_c. The T_c(H)-curves show a local minimum at H_{coe}. In contrary to theoretical results based on the Proximity-effect in trilayer systems [2], in the present system, switching into a parallel oriented magnetization of the sandwiching FM-layers leads to a T_c increase ($\Delta T_c \approx 50$ mK) as compared to the corresponding antiparallel alignement.

Additional experiments on FM/SC double layers deliver clear indications that the observed behaviour can be attributed to stray fields acting on the superconducting Niobium layer. To underline this conclusion micromagnetic simulations (oommf-code) will be discussed.

[1] A. Buzdin, Nat. Mat. (3), 751 (2004)
[2] I. Baladié et al., Phys. Rev. B 63, 54518 (2001)

TT 21.10 Tue 18:45 HSZ 105

Transport through anisotropic magnetic molecules — •Florian Elste[1] and Carsten Timm[2,1] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, USA

We theoretically investigate inelastic transport through anisotropic magnetic molecules, weakly coupled to metallic leads. The differential conductance shows characteristic fine-structure splitting of the Coulomb blockade peaks originating from excitations involving nondegenerate spin multiplets. Magnetic anisotropy is found to be crucial for slow spin relaxation. In the presence of anisotropy we find giant spin amplification: If a bias voltage is applied to a molecule prepared in a spin-polarized state the spin accumulated in the leads can be made exponentially large. If the molecule is coupled to one ferromagnetic and one paramagnetic lead the molecular spin can be reversed by applying a bias voltage even in the absence of a magnetic field. For this case, the current-voltage characteristics reveal wide voltage ranges where the current is strongly suppressed due to selection rules for the spin. Spin blockade behavior is accompanied by negative differential conductance and super-Poissonian shot noise. Based on our findings, we propose schemes for reading and writing spin information in molecular memory devices.

TT 22 Symposium Quantum Fluids

Time: Tuesday 15:00–17:45 Room: HSZ 304

Invited Talk TT 22.1 Tue 15:00 HSZ 304

A-B Transition and Anisotropic Scattering in Superfluid ^{3}He in Aerogel — •Yoonseok Lee — Department of Physics, University of Florida, PO Box 118440, Gainesville, FL 32611, USA

For last 10 years, liquid ^{3}He impregnated in high porosity silica aerogel has been investigated extensively. The structure and relevent length scales of the aerogel allow us to investigate the effects of disorder on a p-wave superfluid in a systematic manner. In 98% porosity aerogel, three distinct phases have been observed experimentally. These three phases are conveniently named as A-, B-, and A_1-phase as in the bulk, although only spin structures of the superfluid phases have been identified. Especially, the verdict on the so called A-phase is by no means conclusive. However, a considerable modification in the phase diagram has been reported such as the supression of superfluid transition and a severe alteration in the A-B transition line. In this talk, we will review recent experimental results on the A-B transition in 98% aerogel including our own results and discuss the importance of anisotropic scattering provided by the strand-like structure of aerogel on the A-B transtion.

Keynote Talk TT 22.2 Tue 15:30 HSZ 304

Quantum Turbulence in superfluid ^{3}He — •Shaun Fisher — Department of Physics, Lancaster University, Lancaster LA1 4YB, UK

For the first time, we have access to the study of turbulence in a pure superfluid, at low temperatures, without any viscous effects from the normal fluid. In such a system, turbulence takes the simple form of a tangle of quantised vortex lines having self induced motion in an ideal inviscid fluid. Of particular interest in the quantum system is how turbulence may be generated, how it evolves, and how it decays in the complete absence of viscous forces. Vortices are readily detectable in superfluid ^{3}He-B in the low temperature limit via the Andreev reflection of ballistic quasiparticle excitations. We describe recent measurements of the production and decay of quantum turbulence and compare the observations with classical expectations.

Invited Talk TT 22.3 Tue 16:00 HSZ 304

The Transition in the Vortex Dynamics of Superfluid ^{3}He-B — •V.B. Eltsov, R. Blaauwgeers, R. de Graaf, J. Kopu, and M. Krusius — Low Temperature Laboratory, Helsinki University of Technology, FIN-02015 HUT, Finland

In recent years the field of vortex dynamics in quantum

fluids has wittnessed a flurry of important advances. In superfluid ^{3}He-B quantum turbulence has been investigated from the lowest temperatures up to $0.6\,T_c$, the temperature of the transition from turbulent dynamics at low temperatures to the superconductor-like highly dissipative dynamics at high temperatures. We have studied the evolution of vortex loops injected in vortex-free flow in a rotating cylindrical bucket of ^{3}He-B and have traced with NMR a complete path to the final lowest energy configuration of rectilinear vortex lines stretched parallel to the rotation axis. With decreasing mutual friction damping injected loops become unstable towards formation of new vortices. Depending on vortex density this process proceeds either through rapid turbulent vortex multiplication due to inter-vortex interactions or via growth and reconnection to the boundary of Kelvin wave excitations on individual vortex lines. In the final stage a bundle of vortex lines expands along the rotating column into the vortex-free regions in the form of a propagating vortex front followed by a helically twisted cluster of vortex lines.

— 15 min. break —

Keynote Talk TT 22.4 Tue 16:45 HSZ 304

Stable textures and defects in slabs of superfluid 3He-A — •Paul Walmsley and Andrei Golov — School of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, UK

We have studied, both experimentally and numerically, various stable textures of the order parameter in superfluid 3He-A in a slab geometry. These textures include continuous vortices and three different types of domain wall as well as specific textures such as the inhomogeneous textures in the centre of a disk-shaped volume where a cylindrical pipe enters the volume along its axis. Our experiments consisted of torsional oscillators, containing disk-shaped slabs of 3He-A, mounted on a rotating nuclear demagnetization cryostat. We were able to detect the response of the orbital texture to applied counterflow which when combined with numerical calculations enabled us to identify the texture present. We found that the texture depended on how it had been prepared. Oriented textures could be prepared by cooling while rotating but domain walls were always present if we cooled (or warmed from the B-phase) without rotation. We will present our measurements of flow-induced critical velocities and compare them to numerical calculations.

Keynote Talk TT 22.5 Tue 17:15 HSZ 304

Molecular Spectroscopy in Helium Droplets at Low Temperatures — •Alkwin Slenczka — Institute for Physical and Theoretical Chemistry, Uni Regensburg, 93040 Regensburg, Germany

About a decade ago helium droplets created in a cold supersonic expansion have been established as a new matrix for molecular spectroscopy. The new expermental technique unifies advantages of matrix isolation and supersonic jet experiments. The unique advantage of ^{4}He droplets is the superfluid phase. It explains the very gentle nature of this host system which becomes apparent in rotationally fully resolved molecular spectra. We will review experimental observations revealing physical details of helium droplets and of the solvation of molecules in helium droplets which were obtained in high resolution spectra of molecules in helium droplets.

TT 23 Solids At Low Temperature: Cryogenics

Time: Wednesday 14:30–16:15 Room: HSZ 02

Invited Talk TT 23.1 Wed 14:30 HSZ 02

Electronic micro-refrigeration and thermometry — •Jukka Pekola[1], Alexander Savin[1], Matthias Meschke[1], Tero Heikkilä[1], Francesco Giazotto[2], Wiebke Guichard[3], and Frank Hekking[3] — [1]Low Temperature Laboratory, Helsinki University of Technology, P.O. Box 3500, 02015 HUT, Finland — [2]SNS, Pisa, Italy — [3]CNRS, Grenoble, France

Electronic thermometry is based on determining the energy distribution of electrons in a conductor. Refrigeration, in turn, is equivalent to narrowing this distribution. We discuss various relaxation mechanisms that determine the distribution under different experimental conditions. Particular devices to be described include thermometers based on Coulomb blockade, tunneling in hybrid tunnel junctions, interplay between thermal noise and shot noise, and refrigerators based on tunneling in normal-metal/superconductor and superconductor/superconductor tunnel junctions. Perspectives of miniaturized refrigerators between ambient and milli-kelvin temperatures are discussed. Observations of distributions beyond the equilibrium Fermi distribution will be reviewed as well. We conclude by a report of our recent observations of electron cooling by radiation through a superconducting line.

TT 23.2 Wed 15:00 HSZ 02

Low temperature confocal microscopy with a 4 K closed-cycle cryostat — •Christoph Boedefeld[1], Angelika Kueng[1], Christian Schulhauser[1], Matthias Buehler[2], and Jens Hoehne[2] — [1]attocube systems AG, Koeniginstrasse 11a (Rgb), 80539 Munich, Germany — [2]VeriCold Technologies GmbH, Bahnhofstrasse 21, 85737 Ismaning

Low temperature confocal microscopy is a technique of major interest with regard to research fields ranging from material and surface science to single molecule spectroscopy. Common setups involve the usage of expensive liquid helium and suffer from the lack of coarse positioning units at cryogenic temperatures. We present for the first time a highly flexible confocal microscope combined with a 4 K closed-cycle cryostat.

This complete system solution enables plug-and-play high resolution confocal microscopy at low temperatures without the need of liquid helium. The low-vibration pulse tube based cryostat has been specially adapted for very low vibrations as required for applications in combination with scanning probe microscopy. Furthermore, extremely short cool down times of less than 2 hours for standard samples can be achieved. The developed confocal microscope is thermally compensated guaranteeing ultra-high stability at low temperature providing at the same time very high optical resolution as will be shown in various examples. Furthermore, nanopositioning units based on the slip-stick principle allow coarse positioning over centimeters. The system allows operation at extreme conditions as high magnetic fields and high vacuum.

TT 23.3 Wed 15:15 HSZ 02

Modified Closed Cycle Refrigerator for Neutron Diffraction Study at Temperatures around and below 1 K — •Bastian Klemke and Michael Meissner — BENSC, Hahn-Meitner Institut Berlin

A Joule-Thomson (J/T) Helium gas expansion stage has been designed to operate as a third stage attached to the second stage of a closed cycle refrigerator. Room temperature Helium gas (injection pressure p = 1...10 bar) is cooled by heat exchangers mounted to the cold heads of the first and the second stage, respectively. Inside the J/T unit the Helium gas is liquefied and simultaneously evaporated by an external rotary pump via an attached pumping tube. Using ^{4}He-gas results in a base temperature of 1.3 K and in a precise temperature regulation up to 50 K. Operation with ^{4}He-gas proved to be very simple and reliable as no gas handling system is needed. For closed loop circulation with ^{3}He-gas we set up a small gas handling system which operates with the same J/T unit. Base temperatures down to 0.6 K have been observed stable over long times and easy temperature regulation has been achieved, too. Because in neutron and x-ray scattering experiments sample change and cooling time from 300 K are an important issue, the J/T unit and heat exchangers have small thermal masses. Due to these construction details our present design can be operated in HUBER 5020 Euler cradles in all goniometer orientations.

TT 23.4 Wed 15:30 HSZ 02

Setup für in-situ ac-susceptibility measurements during neutron scattering at low temperatures — •Enrico Faulhaber[1], Oliver Stockert[2], and Michael Loewenhaupt[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden — [2]Max-Planck-Institut für Chem. Physik fester Stoffe, D-01187 Dresden

Neutrons are a valuable microscopic probe to investigate magnetic ordering phenomena but are insensitive to superconductivity. Driven by our needs to directly correlate magnetism with superconductivity, we designed an in-situ ac-susceptibility setup for use in neutron scattering experiments at low temperatures. The setup follows the classical setup with one excitation coil and two pickup coils. The sample is placed beneath one pickup coil in the neutron beam to reduce the neutron background originating from scattering on the coils. Further, the coils were shielded against neutrons with boron nitride.

The setup has been used successfully in several experiments at the HMI in Berlin and at the ILL in Grenoble. Superconducting transitions could easily be traced. In addition, a recent experiment has shown that the setup is even able to detect magnetic ordering transitions. We will present the realised setup and selected results.

TT 23.5 Wed 15:45 HSZ 02

Thermally robust noise thermometer for milli-kelvin temperatures — •Astrid Netsch, Elena Hassinger, Christian Enss, and Andreas Fleischmann — Kirchhoff-Institut fuer Physik, Universitaet Heidelberg, INF 227, D-69210 Heidelberg, Germany

The temperature dependence of thermally driven voltage fluctuations of an electrical resistor is described by the dissipation-fluctuation theorem. This fundamental law of statistical physics provides a direct relation between temperature and independently measurable quantities, making the measurement of noise an attractive option for primary thermometry. However, the realization of such thermometers for the measurement of very low temperatures has often been problematic, preventing this technique from being widely used in low temperature laboratories. We present a setup for Johnson-noise thermometry that uses a commercial dc-SQUID as preamplifier. The noise to be measured is generated by the thermal motion of electrons in a bulk sample of a high purity metal such as gold or copper. These random currents cause fluctuations of magnetic flux in a pickup coil which is connected to the input coil of a current-sensor dc-SQUID. The thermometer is easy to fabricate and rather insensitive to typical sources of parasitic heating. We discuss general design considerations as well as the dependence of the temperature uncertainty upon measurement time. To characterize the thermometer we compared it to a superconducting standard reference device (SRD1000) which represents the temperature scale PLTS-2000. The spectral power density of flux noise was measured as a function of temperature and found to be linear in the investigated range from 6 mK to 4 K.

TT 23.6 Wed 16:00 HSZ 02

Low mechanical loss materials at cryogenic temperatures for interferometric gravitational wave detectors — •Anja Zimmer, Ronny Nawrodt, Sandor Nietzsche, Ralf Neubert, Matthias Thürk, Wolfgang Vodel, and Paul Seidel — Institut für Festkörperphysik, FSU Jena, Helmholtzweg 5, 07743 Jena

High precision instruments like gravitational wave detectors require components with very low thermal noise. This noise can be reduced by cooling down and using materials providing low mechanical loss even at the operating temperature. A special cryogenic measuring setup was used for investigation of the mechanical loss within the temperature range of 5 to 300 K. Experimental results on different materials are discussed focussing on microscopic processes in solids.

This work was supported by the German DFG under contract SFB TR7.

TT 24 Superconductivity: Cryodetectors

Time: Wednesday 16:30–19:00 Room: HSZ 02

Invited Talk

TT 24.1 Wed 16:30 HSZ 02

Cryogenic detectors — •Gabriel Chardin — DAPNIA/SPP, CEA/Saclay, F-91191 Gif-sur-Yvette, France

Over the last 15 years, cryogenic detectors have developed rapidly, resulting in devices with unprecedented energy resolutions and identification properties of the experimental background. I will present some of the major developments involving massive detectors (dark matter and double beta decay searches) and microcalorimeters (neutrino mass, X-ray spectroscopy). I will also briefly review some of the developments involving cryogenic detector matrices for X-ray, infrared and CMB missions.

TT 24.2 Wed 17:00 HSZ 02

Detector Development for Calibration Measurements in CRESST — •Wolfgang Westphal, Chiara Coppi, Franz von Feilitzsch, Christian Isaila, Jean-Côme Lanfranchi, Sebastian Pfister, Walter Potzel, Wolfgang Rau, Michael Stark, and Doreen Wernicke — Physik Department E15, Technische Universität München, James-Franck-Straße, D-85748 Garching

In the CRESST experiment the simultaneous measurement of the heat signal and the scintillation light from events in $CaWO_4$ is used to discriminate the background electron recoil events from nuclear recoil events. The detectors consist of $CaWO_4$ crystals equipped with transition edge sensors (TES) for the measurement of the heat signal and a light detector made of silicon, also equipped with a TES. The two detector parts are mounted together in a reflective housing for improved light collection. A potentially harmful background in CRESST are recoiling nuclei from surface alpha decays. At the TU München we are performing calibration measurements to characterize that background. For this purpose we are developing modified detectors capable of measuring the expected higher count rates in these experiments.

TT 24.3 Wed 17:15 HSZ 02

Reproduzierbare Herstellung supraleitender W-Dünnschichten als Detektorkomponenten für das CRESST Experiment — •Sebastian Pfister[1], Godehard Angloher[2], Chiara Coppi[1], Franz von Feilitzsch[1], Dieter Hauff[2], Christian Isaila[1], Jean-Côme Lanfranchi[1], Emilja Pantic[2], Federica Petricca[2], Walter Potzel[1], Franz Pröbst[2], Wolfgang Seidel[2], Michael Stark[1], and Wolfgang Westphal[1] — [1]Physik Department E15, Technische Universität München, James-Franck-Strasse, D-85748 Garching — [2]Max-Planck-Institut für Physik, Föhringer Ring 6, D-80805 München

Die notwendige Sensitivitätssteigerung von Experimenten zur direkten Suche nach Dunkler Materie erfordert u.a. eine Vergrösserung der Detektormasse. Da die Detektormodule nicht beliebig in der Grösse skaliert werden können muss zwangsläufig ihre Anzahl erhöht werden. Für den Ausbau des CRESST-Experimentes ist somit die reproduzierbare Herstellung supraleitender W-Dünnschichten, die als supraleitendes Phasenübergangsthermometer verwendet werden, von grosser Bedeutung. Untersuchungen zur Reproduzierbarkeit von W-Dünnschichten auf $CaWO_4$-Kristallen (Phonondetektor) und Silizium-beschichteten Al_2O_3-Substraten (Szintillationslichtdetektor) werden durchgeführt.

TT 24.4 Wed 17:30 HSZ 02

Cryogenic light detectors with Neganov-Luke amplification — •Christian Isaila[1], Oliver Boslau[2], Chiara Coppi[1], Franz von Feilitzsch[1], Peter Goldstrass[2], Josef Kemmer[2], Jean-Come Lanfranchi[1], Andreas Pahlke[2], Sebastian Pfister[1], Walter Potzel[1], Wolfgang Rau[1], Michael Stark[1], Doreen Wernicke[3], Wolfgang Westphal[1], and Florian Wiest[2] — [1]Technische Universität München, Physik Department E15, James-Franck Str., 85748 Garching — [2]Ketek GmbH, Gustav Heinemann Ring 125, 81739 München — [3]VeriCold Technologies GmbH, Bahnhofstr. 21, 85737 Ismaning

CRESST (Cryogenic Rare Event Search with Superconducting Thermometers) searches for nuclear recoils induced by particle dark matter. For an active suppression of the background due to electron recoils both phonons and scintillation light generated in a CaWO4 crystal are detected simultaneously. While the phonon signal is read out by a transition edge sensor (TES) on the CaWO4 crystal, the scintillation light is measured by a cryogenic light detector consisting of a silicon absorber equipped with a TES. As only a small fraction (about 1%) of the energy of the incident particles is transferred into light, very sensitive light detectors are needed. The threshold of the light detectors can be improved by applying an electric field to the silicon crystal leading to an amplification of the thermal signal due to the Neganov-Luke effect. Measurements with an applied Neganov-Luke voltage will be presented.

TT 24.5 Wed 17:45 HSZ 02

Metallic Magnetic Calorimeters (MMC) for high-resolution spectroscopy of x-ray quanta and energetic particles — •Andreas Burck, Markus Linck, Hannes Rotzinger, Tim Scarbrough, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Heidelberg, Germany

Metallic magnetic calorimeters (MMC) are non-dispersive low temperature particle detectors. They combine the high spectral resolution of dispersive spectrometer and the high efficiency of solid state spectrometer. Their calorimetric detection principle allows for a variety of absorber materials and detector geometries. Metallic magnetic calorimeters consist of an absorber and a metallic paramagnetic temperature sensor which is situated in a weak magnetic field. The deposition of energy in the absorber causes a rise in temperature and results in a change of magnetization of the paramagnetic sensor which is measured by using a low-noise high-bandwidth dc-SQUID. We present the state of development of the current prototype detectors. The observed noise contributions and the energy resolution in MMC's will be discussed. Furthermore the results achieved with prototype detectors for some applications such as high resolution spectroscopy and absolute activity measurements of low-energy emitting radionuclides in metrology will be shown.

TT 24.6 Wed 18:00 HSZ 02

3D-scanning microscopy for microwave frequencies with Josephson cantilevers — •Andre Kaestner, Felix Stewing, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, TU Braunschweig, Hans-Sommer-Straße 66, 38106 Braunschweig

In recent semiconductor communication technology frequencies between a few GHz up to 100 GHz are employed. In the future much higher frequencies up to the THz regime are in reach. Therefore we develop a new method for measuring the near-field radiation of a microwave source with small dimensions. We use a scanning microscope equipped with a Josephson junction on a cantilever to measure a near-field power distribution in three dimensions around a microwave chip.

To detect the microwave radiation we use Josephson junctions sensitive to frequencies between several GHz to a few THz. The Josephson junctions are made of the high-temperature superconductor $YBa_2Cu_3O_7$ on $LaAlO_3$ bicrystal substrates. The 3D-positioning stage of the scanning microscope system allows us to measure the power distribution in a volume of 15x15x15 mm^3 with a spatial resolution of 100 nm. For demonstration first results for the power distribution of a 98 GHz source are presented.

TT 24.7 Wed 18:15 HSZ 02

Development of an array of calorimetric low temperature detectors for heavy ion physics — •S. Ilieva[1,2], A. Bleile[1,2], P. Egelhof[1,2], A. Kiseleva[1], O. Kiselev[1], S. Kraft-Bermuth[1,2], and J. P. Meier[1,2] — [1]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [2]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany

Calorimetric low temperature detectors (CLTDs) for heavy ion detection have been frequently demonstrated to achieve an excellent relative energy resolution of $\Delta E/E$ = 1–5 x 10^{-3} in a wide range of ions and energies (E = 0.1–360 MeV/u). The application of a CLTD in accelerator mass spectrometry achieved an improvement in sensitivity by one order of magnitude. In superheavy element research, CLTDs as high-resolution energy detectors combined with time-of-flight detectors may potentially be used for identification of superheavy nuclei with $Z \geq 113$. The CLTDs developed up to now have an active area of approximately 2x3 mm^2, not sufficient to fully exploit their potential. To increase the active area, an array of CLTDs for heavy ion research is currently subject of design and investigation of performance. The array is designed to provide an active area of 30 x 80 mm^2, consisting of about 100 pixels. For this purpose, a special windowless ^{4}He bath cryostat with large cooling power has been constructed and adapted to the needs of heavy ion research. As a first step, a 2 x 2 pixel prototype array with four individually temperature-regulated pixels and a total area of 6 x 6 mm^2 is realized and its performance under heavy ion irradiation is investigated. First results of these investigations and perspectives will be discussed.

TT 24.8 Wed 18:30 HSZ 02

First test experiment for precise Lamb shift measurements on hydrogen-like heavy ions with low temperature calorimeters — •V. Andrianov[1], K. Beckert[1], P. Beller[1], A. Bleile[1], P. Egelhof[1], A. Gumberidze[1], C. Kilbourne[2], H. J. Kluge[1], S. Kraft-Bermuth[1], D. McCammon[3], J. P. Meier[1], U. Popp[1], R. Reuschl[1], T. Stöhlker[1], and S. Trotsenko[1] — [1]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [2]Goddard Space Flight Center, Greenbelt, USA — [3]Univ. of Wisconsin, Madison, USA

The precise determination of the Lamb shift in hydrogen-like heavy ions provides a sensitive test of quantum electrodynamics in very strong Coulomb fields, not accessible otherwise. To increase the accuracy of the Lamb shift measurement on stored $^{238}U^{91+}$ ions at the ESR storage ring at GSI, a high-resolution calorimetric low temperature detector for hard X-rays was developed. The experimental requirements for the detector are a high absorption efficiency and a relative energy resolution of about 10^{-3} for 50–100 keV X-rays. The detector consists of arrays of silicon thermistors and X-ray absorbers made of high-Z material. A test array consisting of 4 pixels was recently applied in a first test experiment for Lamb shift measurement at the ESR. A 89 MeV/u $^{238}U^{92+}$ beam stored in the ESR interacted with a 10^{11} cm^{-3} internal argon gas-jet target. The Lyman-α lines emitted from the charge-exchanged $^{238}U^{91+}$ ions were clearly identified. An energy resolution of ΔE = 149 eV was obtained at E_γ = 70 keV and a total detection efficiency of 1 x 10^{-7} was reached. The results of this test experiment as well as future perspectives will be discussed.

TT 24.9 Wed 18:45 HSZ 02

Energy loss in down-conversion process in thin superconducting films — •Alexander Kozorezov — Department of Physics, Lancaster University, Lancaster, UK

We have developed theory of photoelectron energy down-conversion in thin superconducting films. Presence of interfaces at a distance which

may be comparable to mean free paths for pair-breaking phonons is an important factor allowing pair breaking phonons to escape from the film. Both mean number of quasiparticles generated in the down-conversion process and their fluctuations depend on details of down-conversion process in the vicinity of interface. Theory predicts important contributions to both statistical fluctuations of generated quasiparticles through phonon escape noise and inhomogeneous broadening effects originating from the initial spatial distribution of photoelectrons. We discuss extra limitations to resolving power of single photon detectors based on superconducting tunnel junctions and TES microcalorimeters. Good agreement between theory and experiment for Ta/Al/AlO_x/Al/Ta superconducting tunnel junctions is demonstrated. Implications for optimum design of single photon spectroscopic arrays are discussed.

TT 25 Correlated Electrons - Poster Session

Time: Wednesday 14:30–18:30 Room: P1

TT 25.1 Wed 14:30 P1

Charge-order metal-insulator transition in the two-dimensional α- (BEDT-TTF)$_2$I$_3$: a Raman scattering study — •M. Masino[1], N. Drichko[2], M. Dressel[2], D. Schweitzer[2], C. Ulrich[3], and B. Keimer[3] — [1]Dip. Chimica GIAF, Universitá di Parma, Italy — [2]Physikalisches Institut, Univetsität Stuttgart, Germany — [3]MPI für Festkörperforschung, Stuttgart, Germany

A charge order metal-insulator transition is a widely studied phenomenon in low-dimensional solids. Two-dimensional organic conductor α-(BEDT-TTF)$_2$I$_3$ (T_{CO}=135 K) is a model compound to investigate the change of the vibronic and electronic Raman response on this transition. We studied polarized Raman spectra of the single crystals as a function of temperature. We focus our attention on the low-frequency spectral region (10-500 cm^{-1}) where the insulating single particle gap is expected in the electronic response. We found a strong dependence of the spectra on excitation-line and polarization: resonant behavior of the linear I_3 anion is found with λ=514 nm excitation polarized parallel to I_3 axis (*i.e.* approximately parallel to the *a* axis); while the Raman response from the BEDT-TTF conducting layer is seen with the λ=647 nm polarized in the perpendicular direction. This allows us to improve the assignment of the BEDT-TTF phonons. In the charge ordered phase the most strongly coupled molecular vibrations split due to the different charge distribution on the molecules. Moreover, the overall spectral background decreases, and a broad band at 400 cm^{-1} appears below T_c. The nature of these anomalous spectral features is discussed in terms of electronic scattering response, and vibronic Raman enhancement.

TT 25.2 Wed 14:30 P1

Optical response of the low-dimensional organic compound (TMTTF)$_2$AsF$_6$ at the pressure-induced deconfinement transition — •A. Pashkin, C. A. Kuntscher, and M. Dressel — 1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The organic (TMTTF)$_2X$ salts consist of weakly coupled, half-filled molecular stacks and are prime examples of one-dimensional Mott-Hubbard insulators. In the (TMTSF)$_2X$ analogs, where sulfur is substituted by selenium, the coupling along and between the stacks is enhanced, causing a deconfinement transition, i.e., a crossover from a Mott-Hubbard insulator to a higher-dimensional metallic state. Optical spectroscopy was shown to be a key tool to monitor such a deconfinement transition induced by chemical pressure. Similar effects as induced by chemical pressure can also be achieved by applying external pressure.

We studied the pressure dependence ($<$ 6 GPa) of the mid-infrared reflectivity of (TMTTF)$_2$AsF$_6$ for the polarization of the incident radiation along and perpendicular to the molecular stacking axis *a*. With increasing hydrostatic pressure the infrared response along the stacking axis *a* approaches that of the highly-conducting TMTSF analogs. The onset of an appreciable Drude-like response for the b' direction, along which the interstack hopping occurs, is observed above 2.5 GPa suggesting a deconfinement transition. The pressure dependence of the transfer integral $t_{b'}$ has been extracted. Furthermore, the pressure-dependent optical response along the least conducting axis, c^*, is presented.

Supported by the DFG, Emmy Noether-program.

TT 25.3 Wed 14:30 P1

Charge order fluctuations in 1/4- filled conductors α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ (M=NH$_4$,K,Tl,Rb) investigated by infrared spectroscopy. — •Natalia Drichko[1], Martin Dressel[1], Jaime Merino[2], and Andres Greco[3] — [1]1. Physikalisches Institut Universität Stuttgart, Germany — [2]UAM, Spain — [3]UNR-CONICET, Argentina

Electron-electron interactions determine the properties of the two-dimensional organic conductors α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ in a wide temperature range and can be tuned by variation of the charge reservoir layer: M=NH$_4$, K, Tl, Rb. We study electronic properties of these compounds by infrared reflectance spectroscopy and compare our results with calculations performed for strongly correlated 1/4-filled conductors close to charge order transition. The observed Drude-like peak has only 10 % of the total spectral weight; we assign the shift of the spectral weight to higher frequencies to the fluctuations of charge order. For NH$_4$ compound, influence of electronic correlations decrease with temperature. For the stronger correlated K and Tl salts, spectral indications of the short-range charge order at low temperatures are observed. The charge-carriers scattering rate exhibits the temperature dependence as predicted for fluctuating charge order. We suggest a generic phase diagram for α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ compounds depending on the strength of the electronic correlations. We further discuss its relevance to the superconducting ground state observed in NH$_4$ material below 1 K and the density-wave ground state, observed below 10 K for the other members of this family.

TT 25.4 Wed 14:30 P1

Spin-zero anomaly in the magnetic quantum oscillations of a two-dimensional metal — •B. Bergk[1], O. Ignatchik[2], M. Jäckel[1], J. Wosnitza[2], V. M. Gvozdikov[3], J. A. Schlueter[4], J. Mohtasham[4], R. W. Winter[5], and G. L. Gard[5] — [1]Institut für Festkörperphysik, Technische Universität Dresden — [2]Dresden High Magnetic Field Laboratory, Forschungszentrum Rossendorf — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [4]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, USA — [5]Department of Chemistry, Portland State University, Portland, Oregon

We present de Haas–van Alphen (dHvA) and Shubnikov-de Haas (SdH) measurements on the quasi-two-dimensional organic superconductor β''-(BEDT-TTF)$_2$SF$_5$CH$_2$CF$_2$SO$_3$. The measurements were carried out by the torque method and by four-point low-frequency ac-resistance measurements in magnetic fields up to 15 T. Unlike theoretical expectations for two-dimensional metals the dHvA signal shows an unconventional sawtooth wave-form, i. e., an 'inversed sawtooth' wave form is observed. In order to investigate the behaviour in more detail we performed angle-dependent dHvA and SdH measurements. The SdH effect displays the behaviour predicted by the grand-canonical Lifshitz-Kosevich theorie. In contrast, the dHvA signal can be explained by a theory, which includes a slightly oscillating chemical potential. Even for simultaneous measurements of both effects the behaviour does not change. This means that the dHvA signal is not affected by an external charge carrier reservoir.

TT 25.5 Wed 14:30 P1

Field-induced charge-density-wave transitions under pressure in the organic metal α-(BEDT-TTF)$_2$KHg(SCN)$_4$ — •Werner Biberacher[1], Dieter Andres[1], Mark Kartsovnik[1], Ilya Sheikin[2], Harald Müller[3], and Natalia Kushch[4] — [1]Walther-Meissner-Institut, Garching, Germany — [2]LNCMI, CNRS, BP 166, Grenoble, France — [3]ESRF, BP 220, Grenoble, France — [4]Institute of Problems of Chemical Physics, Chernogolovka, Russia

Hydrostatic pressure is a parameter that tunes the nesting conditions of the charge-density-wave (CDW) state existing in the organic metal α-(BEDT-TTF)$_2$KHg(SCN)$_4$. With pressure the CDW gradually becomes suppressed and above 2.5 kbar it does not exist any more at zero magnetic field. The orbital effect of the magnetic field is demonstrated to re-establish the density wave, while the orbital quantization induces different CDW states in different field intervals. In particular, we have found that hysteretic features characteristic of the first order field-induced CDW transitions become visible at much higher temperatures at certain orientations of the magnetic field. This is a direct evidence for the existence of this theoretically predicted effect.

TT 25.6 Wed 14:30 P1

Anomalous magnetoresistance of a layered conductor in the weakly incoherent interlayer coupling regime — •Mark Kartsovnik[1], Dieter Andres[1], Sergei Simonov[2], Werner Biberacher[1], Harald Mueller[3], Natalia Kushch[4], and Ilya Sheikin[5] — [1]Walther-Meissner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]Institute of Solid State Physics, 142432 Chernogolovka, Russia — [3]ESRF, BP 220, F-38043 Grenoble, France — [4]Institute of Problems of Chemical Physics, 142432 Chernogolovka, Russia — [5]LNCMI, CNRS, BP 166, F-38042, Grenoble, France

Owing to a high crystal quality and an extremely weak interlayer coupling in the layered organic conductor α-(BEDT-TTF)$_2$KHg(SCN)$_4$, it is possible to realize, by selecting a sample with an appropriate electron scattering rate, either the coherent or incoherent interlayer transport regime while the strong-field criterion, $\omega_c\tau > 1$, is achieved at conventional magnetic fields of a few tesla. We report on striking differences in the angle-dependent interlayer resistance of this compound observed on samples characterized by different sample quality. In the cleanest samples, the magnetoresistance is a complex function of the magnetic field orientation, bearing the information about the geometry of the well defined three-dimensional Fermi surface. By contrast, the lower quality samples are essentially insensitive to the strength and orientation of the magnetic field component lying in the plane of the conducting layers. We attribute this anomalous behavior to the breakdown of the coherent charge transport across the layers in the lower quality samples.

TT 25.7 Wed 14:30 P1

Determination of the phase diagram of the spin ladder system $(C_5H_{12}N)_2CuBr_4$ by caloric and magnetic measurements — •Klaus Kiefer[1], Christian Rüegg[2], Thomas Wand[1], Michael Meissner[1], Des McMorrow[2], Karl Krämer[3], Daniel Biner[3], and Hans U. Güdel[3] — [1]BENSC, Hahn-Meitner-Institut Berlin — [2]Department of Physics and Astronomy, University College London, UK — [3]Universität Bern

The phase diagram of the S=1/2 spin ladder system $(C_5H_{12}N)_2CuBr_4$ was determined by measurements of the specific heat, the magnetocaloric effect and the magnetisation in magnetic fields up to 14.5 T. The exponential temperature dependence of the low temperature specific heat clearly reveals the existence of an energy gap between the non magnetic ground state and the magnetic excitations. The field driven closing of this gap is found to occur at about 7 T. In the Luttinger liquid regime the expected linear temperature dependence of the specific heat was confirmed. Down to the lowest accessible temperature of 0.3 K no additional transition to long-range 3D-order could be detected.

TT 25.8 Wed 14:30 P1

Collective modes in electron Fermi-liquid of organic layered conductors — •Dmitrii Stepanenko, Olga Kirichenko, and Valentin Peschansky — B.I.Verkin Institute for Low Temperature Physics and Engineering,

We have studied theoretically the propagation of electromagnetic waves in organic layered conductors at low temperature, when the charge carriers mean free path is the largest parameter of the dimensionality of length. It is shown that the specific of the Q2D charge carriers energy spectrum in layered conductors results in the oscillatory dependence of the electron drift velocity v_D upon the angle θ between the magnetic field vector and the normal to the layers. In a strong magnetic field, when the cyclotron frequency of electrons is much greater than their collision frequency, for the entire series of the values $\theta = \theta_c$ the velocity v_D is vanishingly small everywhere at the Fermi surface. This is the case when the collisionless absorption of the wave is absent and propagation of weakly damping modes is possible for an arbitrary orientation of the wave vector. The spectrum of the collective modes have been analyzed with regard to the Fermi liquid interaction between electrons.

TT 25.9 Wed 14:30 P1

Electron Spin Resonance in sine-Gordon Spin Chains in the Perturbative Spinon Regime. — •S. Zvyagin[1], J. Wosnitza[1], A. Kolezhuk[2], J. Krzystek[3], and R. Feyerherm[4] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Rossendorf, 01314 Dresden, Germany — [2]Institut fuer Theoretische Physik, Universitaet Hannover, 30167 Hannover, Germany — [3]National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA — [4]Hahn-Meitner-Institut (HMI), 14109 Berlin, Germany

We report on low-temperature multi-frequency ESR studies of copper pyrimidine dinitrate, a spin-1/2 antiferromagnetic chain with alternating g-tensor and the Dzyaloshinskii-Moriya interaction, allowing us to test a new theoretical concept proposed recently by Oshikawa and Affleck [Phys. Rev. Lett. 82, 5136 (1999)]. Their theory, based on bosonization and the self-energy formalism, can be applied for precise calculation of ESR parameters of S = 1/2 antiferromagnetic chains in the perturbative spinon regime. Excellent quantitative agreement between the theoretical predictions and experiment is obtained. Results of the presentation are published in: S.A. Zvyagin et al., Phys. Rev. Lett. 95, 017207, 2005.

TT 25.10 Wed 14:30 P1

Heat transport in one-dimensional quantum magnets — •C. Hess[1], P. Ribeiro[1], A. Waske[1], N. Wizent[1], R. Klingeler[1], D. Elefant[1], C. Sekar[1], G. Krabbes[1], B. Büchner[1], H. ElHaes[2], G. Roth[2], F. Heidrich-Meisner[3], and W. Brenig[3] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Institut für Theoretische Physik, TU-Braunschweig, Germany

We present experimental results for the magnon thermal conductivity $\kappa_{\rm mag}$ of several one-dimensional S=1/2 spin systems, like spin ladders and chains. We put a focus on spin chain materials such as $SrCuO_2$ and $CaCu_2O_3$. $SrCuO_2$ exhibits a strong signature of $\kappa_{\rm mag}$ from spinons. However, the size of $\kappa_{\rm mag}$ is difficult to determine due to its coincidence with the peak of the phonon thermal conductivity $\kappa_{\rm ph}$. In order to obtain a better separation of $\kappa_{\rm mag}$ and $\kappa_{\rm ph}$ we selectively suppress $\kappa_{\rm ph}$ by substituting Ca for Sr. A strong signature of magnetic heat transport is also present in $CaCu_2O_3$ along its chains. Since $\kappa_{\rm ph}$ is strongly suppressed in this material the temperature dependence of $\kappa_{\rm mag}$ can be well extracted. We estimate the magnetic mean free path which turns out to be of the order of 25 Å.

TT 25.11 Wed 14:30 P1

Magnetic heat conduction in Ca-doped $SrCuO_2$ spin chains — •P. Ribeiro[1], A. Waske[1], C. Hess[1], G. Behr[1], R. Klingeler[1], D. Elefant[1], B. Büchner[1], and G. Roth[2] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany

We present new results on the heat conduction of the spin-chain system $Sr_{1-x}Ca_xCuO_2$. The structure of this material contains two parallel antiferromagnetic $S = 1/2$ copper chains with a $J_\parallel \approx 2100$ K. They are decoupled from each other due to a frustration arising from the displacement of half a Cu-Cu distance between them. In addition to the regular phonon heat conduction this material possesses spinon contributions in the chain direction. A separation of both contributions is most ambiguous, since the spinon contribution appears in form of a shoulder on the low-temperature phonon peak. In order to achieve a better separation of both contributions we isovalently substituted Ca for Sr, which leads to a suppression of the phonon heat conduction, while a strong affect on the magnetic system in the substance is not expected.

TT 25.12 Wed 14:30 P1

Quantum Critical Spin Dynamics of a Cu(II) S=1/2 antiferromagnetic Heisenberg chain studied by ^{13}C-NMR spectroscopy — •H. Kuehne[1], J. Litterst[1], H.-J. Grafe[2], C. Baumann[2], J. Haase[2], B. Buechner[2], C. P. Landee[3], M.M. Turnbull[3], and H.-H. Klauss[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Leibniz-Institut für Werkstoffforschung, Dresden, Germany — [3]Departments of Physics and Chemistry, Clark University, Worcester, USA

The antiferromagnetic S=1/2 Heisenberg chain is a model system for quantum many-body physics. It allows a direct comparison between exact theoretical results and experiment for ground state properties and excitations. In this work we study the spin dynamics of a Cu(II) S=1/2 spin chain system by means of ^{13}C-NMR. The actual compound, $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN), is one of the best experimental realizations of an unperturbed S=1/2 chain [1]. It has been characterized by thermodynamic measurements as well as inelastic neutron scattering [1,2]. The full parameter range from the low field limit to beyond the critical magnetic field strength of H_{crit} =13.9 Tesla for ferromagnetic polarization can be accessed. We present field and temperature dependent studies of the T_1 relaxation rate at the Carbon site.

[1] P. Hammar et al., PRB. 59, 1008 (1999).
[2] M.B. Stone et al., PRL 91, 037205 (2003).

TT 25.13 Wed 14:30 P1

$Sr_2Cu(PO_4)_2$: A real material realization of the 1D nearest neighbor Heisenberg chain — •M.D. Johannes[1], J. Richter[2], S.-L. Drechsler[3], A. A. Belik[4], E. Takayama-Muromachi[4], S. Uji[4], and H. Rosner[5] — [1]Naval Research Laboratory, Washington D.C — [2]Institute for Theoretical Physics, Magdeburg, Germany — [3]Leibnitz Institute for Solid State and Materials Research, Dresden, Germany — [4]National Institute for Materials Science, Ibaraki, Tsukuba, Japan — [5]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany

The search for one-dimensional magnets began with the advent of quantum mechanics and the discovery that fluctuation effects, enhanced by low-dimensionality, could lead to novel ground states and exotic effects not accessible in higher dimensions. We present evidence that $Sr_2Cu(PO_4)_2$ is a nearly perfect one-dimensional (1D) spin 1/2 Heisenberg chain with nearest neighbor only interactions. Combining experimental measurements down to T=30mK with first principles and model calculations, we demonstrate that the one dimensionality of $Sr_2Cu(PO_4)_2$, as measured by the ratio k_BT_N/J_1, exceeds that of prototype 1D compound Sr_2CuO_3 by an order of magnitude. Surprisingly, $Sr_2Cu(PO_4)_2$ lacks clear structural chains, achieving magnetic one-dimensionality instead via isolated CuO_4 plaquettes coupled along a single direction. This unusual geometry also strongly suppresses frustrating interactions between second neighbors along the spin chain direction, thereby providing an ideal physical realization of an exactly solvable theoretical model.

TT 25.14 Wed 14:30 P1

Structural and magnetic properties of oxalate-bridged low-dimensional Cu^{2+} spin systems — •Katarina Remović-Langer[1], Volodymyr Pashchenko[1], Andrey Prokofiev[1], Bernd Wolf[1], Michael Lang[1], Jürgen Schreuer[2], Leonore Wiehl[2], Eiken Haussühl[2], and Björn Winkler[2] — [1]Physikalisches Institut, J. W. Goethe-Universität, FOR 412, Max-von-Laue-Str. 1, D-60438 Frankfurt(M), Germany — [2]Institut für Mineralogie/Kristallographie, J. W. Goethe-Universität, FOR 412, Senckenberganlage 30, D-60054 Frankfurt(M), Germany

Our study focused on the structural and magnetic properties of two 1,1′-bicoordinated oxalate-bridged Cu^{2+} spin chains, $[Cu(\mu\text{-ox})\text{-}(H_2O)(4\text{-apy})_2]_n$ (**1**) and $[(pyOH)Cu(ox)\text{-}H_2O]_n$ (**2**). While in **1** all oxalate molecules are in the bis-monodentate configuration, compound **2** is built from two non-equivalent ox molecules which alternate in the bis-bidentate form along the chain. The Cu atoms of compound **1** are in a distorted square-pyramidal environment while those in compound **2** are in a distorted octahedral configuration. Magnetic measurements reveal the behavior of a uniform Heisenberg spin chain with a small antiferromagnetic (AF) exchange coupling constant of $J \approx 3K$ for **1**, consistent with [1], and that of a dimer system with predominant AF intradimer interaction of $J \approx 403K$ and only weak interdimer couplings for **2**. The nature and magnitude of the magnetic coupling through the oxalate bridges in **1** and **2** will be discussed in the light of available structural data.

[1] O. Castillo et al., Inorg. Chem. 39, 6142 (2000).

TT 25.15 Wed 14:30 P1

High-field ESR study of the quantum spin magnet $CaCu_2O_3$ doped with nonmagnetic Zn — •U. Schaufuss, C. Sekar, G. Krabbes, N. Tristan, S.-L. Drechsler, V. Kataev, and B. Büchner — Leibniz Institute for Materials Research IFW Dresden

$CaCu_2O_3$ is a low-dimensional $s = 1/2$ antiferromagnet with a structurally well defined two-leg ladder topology. However, no spin gap characteristic of a two-leg $S = 1/2$-ladder is observed in this material. Instead, $CaCu_2O_3$ orders antiferromagnetically at $T_N = 25\,\mathrm{K}$ and exhibits a small magnetic anisotropy gap at $T < T_N$ [1]. Our recent high-field ESR study of a single crystal of $CaCu_2O_3$ reveals an important role of a few percent of 'extra' spins residing at the structural imperfections for the low-temperature magnetism of the bulk spin lattice in this compound [1]. To obtain a deeper insight into a complex interplay between the host and the 'extra' spins we studied static magnetization and high-field ESR of a series of $CaCu_2O_3$ single crystals doped with nonmagnetic Zn. We discuss the influence of the nonmagnetic defects on the properties of the strongly correlated low-dimensional spin lattice focussing on the doping dependence of T_N and of the anisotropy gap.

[1] M. Goiran *at al.*, cond-mat/0501647.

TT 25.16 Wed 14:30 P1

Excitation spectrum and magnetic properties of the layered $Na_5RbCu_4(AsO_4)_4Cl_2$ — •V. Gnezdilov[1], P. Scheib[2], P. Lemmens[2], Yu. Pashkevich[3], D. Chervinskii[3], K. Lamonova[3], S. Zvyagin[4], M. Ulutagay-Kartin[5], S.-J. Hwu[5], and J.A. Clayhold[5] — [1]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [2]IPKM, TU Braunschweig, D-38106 Braunschweig, Germany — [3]A.A. Galkin Donetsk Phystech, NASU, Ukraine — [4]Hochfeld-Magnetlabor, Forschunszentrum Rossendorf, 01328 Dresden, Germany — [5]Dept. Chem., Clemson Univ., Clemson, South Carolina 29634, USA

We report on a Raman scattering study on the $Na_5RbCu_4(AsO_4)_4Cl_2$ compound with a remarkable layered lattice structure comprised of antiferromagnetically coupled square Cu_4O_4 tetramers and a magnetic transition at T_N=17K. Due to the asymmetric exchange paths and the missing inversion centers an unique spectrum of magnetic excitations is observed and analyzed theoretically. This work has been supported partly by the ESF-HFM.

TT 25.17 Wed 14:30 P1

Excitation spectrum of the novel frustrated 2D s=1/2 system $(CuCl)LaNb_2O_7$ — •V. Gnezdilov[1], P. Scheib[2], P. Lemmens[2], Yu.G. Pashkevich[3], T. Kitano[4], Y. Ajiro[4], N. Oba[4], K. Yoshimura[4], and H. Kageyama[4] — [1]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [2]IPKM, TU Braunschweig, D-38106 Braunschweig, Germany — [3]A.A. Galkin Donetsk Phystech, NASU, 83144 Donetsk, Ukraine — [4]Dept. Chem., Kyoto Univ., Kyoto 606-8502, Japan

We report on the magnetic properties and Raman scattering data of the double-layered perovskite $(CuCl)LaNb_2O_7$ with a square lattice of s=1/2, prepared by topotactic ion-exchange reactions. Thermodynamic and spectroscopic experiments show a spin gap of $\approx$ 2 meV. Evidence for competing ferro- and antiferromagnetic exchange pathes connecting nearest and second-nearest-neighbors, respectively, exist. The role of the lattice system for the magnetic properties is critically discussed. This work has been supported partly by the ESF-HFM.

TT 25.18 Wed 14:30 P1

^{51}V NMR Study of Vanadium Oxide Nanotubes — •E. Vavilova[1,2], V. Kataev[1], I. Hellmann[1], R. Klingeler[1], C. Täschner[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, 420029 Kazan, Russia

Mixed valent vanadium oxide nanotubes VO_x-NT have recently attracted much attention as they exhibit a number of unusual magnetic properties, ranging from ferromagnetism at room temperature to spin-liquid phenomena [1]. In these nanoscale magnets one finds structurally well defined V-O-V-... chains, but also isolated V-sites. In order to get an insight into the spin dynamics of this complex system we performed NMR measurements on ^{51}V nuclei in a magnetic field of 7.05 T at temperatures between 15 K and 285 K. We find a broad NMR spectrum centered at a frequency $\sim$ 78.9 MHz with a partially relsoved quadrupole structure. Measurements of transversal and longitudinal nuclear-spin relaxation times, T_2 and T_1, respectively, reveal two sites of V with distinctly different relaxation rates. These two sites are assigned to vanadium in 4+ (d^1, $S = 1/2$) and 5+ (d^0, $S = 0$) oxidation states, respectively. Though T_1 at both sites exhibit a strong temperature dependence we find no evidence for a spin gap of the order $\sim$ 700 K which possible occurrence in VO_x-NT is suggested in Ref. [1]. In addition to NMR results we present also our magnetization data and discuss possible mechanisms of vanadium nuclear spin relaxation and their interplay with the static magnetic properties.

TT 25.19 Wed 14:30 P1

Spectroscopic investigations of 2D J1-J2 quantum spin systems — •P. Scheib[1], V. Gnezdilov[2], P. Lemmens[1], S. Gonthier[3], P. Millet[3], E. Kaul[4], and Ch. Geibel[4] — [1]IPKM, TU Braunschweig, Germany — [2]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [3]CEMES, Toulouse, France — [4]MPI-CPfS, Dresden, Germany

The interest in frustrated 2D quantum spin system is increasing as novel system have been discovered that enlarge the parameter space from 2D AF to mixed AF/FM systems. We report Raman scattering results on Li_2VOSiO_4, $Pb_2VO(PO_4)_2$, and $(Sr,Ba)ZnVO(PO_4)_2$ to compare the effect of the local structure on the resulting AF and AF/FM couplings. This work has been supported partly by the ESF-HFM.

TT 25.20 Wed 14:30 P1

Spectroscopic investigation of the crossover behavior in $TeVO_4$ — •V. Gnezdilov[1], G. Caimi[2], L. Degiorgi[2], P. Lemmens[3], R.K. Kremer[4], and H. Berger[5] — [1]B.I. Verkin Inst. for Low Temp. Phys., NASU, Kharkov, Ukraine — [2]LfF, ETH Zürich, Switzerland — [3]IPKM, TU Braunschweig, Germany — [4]MPI-FKF, Stuttgart, Germany — [5]IPMC, EPFL, Lausanne, Switzerland

The magnetic susceptibility of $TeVO_4$ shows a crossover at T*=75K with different slopes of the reciprocal susceptibility. Using infrared absorption and Raman scattering we investigate the correlation of structural and electronic properties of this compound to understand the reason for this peculiar behavior. Spin-wave excitations are observed and analyzed for $T<T_c$=17K. This work has been supported by ESF-HFM.

TT 25.21 Wed 14:30 P1

Magnetic investigation on a new one-dimensional Fe(II)-triazole complex — •Katarina Remović-Langer[1], Volodymyr Pashchenko[1], Bernd Wolf[1], Michael Lang[1], Chunhua Hu[2], Jürgen Brüning[2], Kibrom Arefe[2], Jens Kühne[2], Juste E. Djanhan[2], and Martin U. Schmidt[2] — [1]Physikalisches Institut, J. W. Goethe-Universität, FOR 412, Frankfurt (M), Germany — [2]Institut für Anorganische und Analytische Chemie, J. W. Goethe-Universität, Frankfurt (M), Germany

A new one-dimensional triazole complex of Fe(II) ($S = 2$) with the general formula $\{[Fe(C_4H_7N_3O)_3](p\text{-}ClC_6H_4SO_3)_2\}_n$ has been synthesized and characterized magnetically. The structure of this polymeric compound consists of linear chains in which the neighboring Fe(II) atoms are triply bridged by pairs of bonded N atoms of the triazole ligands. Each Fe^{2+} ions have a thermodynamically stable high-spin state. The obtained magnetic properties of Fe-triazole complex can be satisfactorily explained by using a magnetic model for a one-dimensional spin $S = 2$ chain with weak antiferromagnetic Fe-Fe coupling of $J/k \approx 2.2K$.

TT 25.22 Wed 14:30 P1

Comparing the electronic structure of the quantum magnets TiOBr and TiOCl — •Michael Sing[1], Markus Hoinkis[1,2], Leonardo Pisani[3], Roser Valenti[3], Sander van Smaalen[4], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg,D-97074 — [2]Experimentalphysik II, Universität Augsburg, D-86135Augsburg, Germany — [3]Institut für Theoretische Physik, UniversitätFrankfurt, D-60054 Frankfurt, Germany — [4]Laboratory of Crystallography, University of Bayreuth,D-95440 Bayreuth, Germany

The layered Mott insulators TiOBr and TiOCl were recently interpreted as spin-Peierls compounds. They undergo two successive phase transitions with a non-magnetic spin-Peierls ground state and an intermediate state, in which an incommensurate order develops. In an extended temperature regime above the transitions the compounds display large fluctuation effects. It is still unclear how to interpret the electronic dispersions of TiOCl measured by photoelectron spectroscopy in the high temperature regime.[1] In order to elucidate the behavior of these compounds in the high temperature phase we studied the electronic structure of TiOBr and TiOCl by photoelectron spectroscopy and density-functional calculations. The experimentally and theoretically obtained density of states of both compounds are compared. Furthermore, we present momentum-resolved measurements and discuss the quasi-one-dimensional nature of the electronic dispersions. A detailed comparison of the two compounds makes the interpretation of the dispersions in a Mott-Hubbard picture appear less plausible.

[1] M. Hoinkis *et al.*, Phys. Rev. B. **72**, 125127 (2005)

TT 25.23 Wed 14:30 P1

Spatial Localization Behavior in the Two-Dimensional Inherent Conducting Polymer $\{(CH_3)_{0.92}ReO_3\}_\infty$ — •E.–W. Scheidt[1], R. Miller[1], G. Eickerling[1], Ch. Helbig[1], F. Mayr[1], R. Hermann[1], W. Scherer[1], and H.–A. Krug von Nidda[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]EP V, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany

Polymeric methyltrioxorhenium, $(CH_3)_{0.92}ReO_3$ (*poly*-MTO), is the first member of a new class of inherent conductive organometallic hybrids and represents a prototype for a purely two-dimensional system, confirmed by X-ray- and IR-studies as well as by specific-heat and resistivity measurements. Below a characteristic temperature the resistivity changes from metallic to insulating behavior, where in the latter a positive magnetoresistance is observed. These properties are intensified by intercalation studies of *poly*-MTO with donor and acceptor molecules leading to a preliminary phase diagram. The increasing temperature range of the insulating regime is accompanied by an increasing amount of localized magnetic moments at the Re^{VI} (d^1)-ions as revealed by susceptibility and magnetization measurements and ascertained by ESR studies. Magnetic field dependent susceptibility measurements also clarify the role of the magnetic field as a tuning parameter for localization. This may be the reason for the positive magnetoresistance in these systems. This scenario is also corroborated by the magnetic field dependent electrical field gradient V_{zz} determined from the specific heat contribution of the quadrupole moments and confirmed by DFT calculations.

TT 25.24 Wed 14:30 P1

Pressure studies on the polymeric compound methyltrioxorhenium (poly-MTO) $(CH_3)_{0.9}ReO_3$ — •Valdeci Mariano de Souza[1], Michael Lang[1], Robert Miller[2], Christian Helbig[2], Ernst-Wilhelm Scheidt[2], and Wolfgang Scherer[2] — [1]Physikalisches Institut, J.W. Goethe-Univeristät, Frankfurt am Main, Germany — [2]Chemische Physik und Materialwissenschaften, Universität Augsburg, Germany

Transport measurements on the polymeric compound methyltrioxorhenium (poly-MTO) $(CH_3)_{0.9}ReO_3$ have been performed in the temperature range 2-300 K and under ^{4}He-gas pressure up to 10 kbar. The structural motive and transport properties of poly-MTO are reminiscent of those of classical perowskites in two dimensions. The metallic conductivity has been attributed to the presence of demethylated Re atoms giving rise to excess electrons which delocalize within the Re-5d bands. Upon cooling, the system remains metallic down to about 30 K, below which the resistivity starts to increase. In this non-metallic low-temperature range, the resistivity follows a log(1/T) dependence over one decade in temperature. Attempts to increase the electrical conductivity by intercalation with the organic donor molecule tetrathiafulvalene (TTF) showed that with increasing amount of TTF donors, the system becomes less conducting in the metallic high-temperature range and the low-T resistivity upturn is strongly reinforced. In contrast, the application of hydrostatic pressure results in a reduction of the resistivity over the whole T-range investigated, while the metal-to-insulator crossover around 30 K remains unaffected.

TT 25.25 Wed 14:30 P1

Thermodynamics of two-dimensional spatially anisotropic Heisenberg model — •Tatiana Antsygina, Marina Poltavskaya, Konstantin Chishko, and Igor Poltavsky — B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine

Using the formalism of two-time Green's functions and the decoupling procedure by Kondo and Yamaji we have investigated thermodynamic and magnetic properties of the 1/2-spin Heisenberg antiferromagnet on a spatially anisotropic triangular lattice with nearest neighbor exchange constant J_1 along one direction and J_2 along other two directions. The thermodynamic functions are expressed in terms of correlation functions which obey the self-consistent system of equation. At arbitrary temperatures the system can be solved only numerically, and temperature dependences of the energy, heat capacity and magnetic susceptibility at different relations between J_1 and J_2 can be calculated in the wide temperature range. We have analyzed the case $\nu = J_1/J_2 \ll 1$ and found that with the increase of ν the height of the peak on the heat capacity decreases and the peak position shifts to lower temperatures. It is shown that the temperature dependence of the magnetic susceptibility is in excellent agreement with the high temperature series expansions [1]. Possible applications of the theoretical results for the interpretation of physical properties of real low-dimensional magnets are discussed.

1. W. Zheng, R.R.P. Singh, R.H. McKenzie, R. Coldea, cond-mat/0410381.

TT 25.26 Wed 14:30 P1

Heat capacity and spin susceptibility of two-dimensional t-J model — •Marina Poltavskaya, Tatiana Antsygina, Konstantin Chishko, and Igor Poltavsky — B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine

Thermodynamic properties of the two-dimensional t-J model on square and triangular lattices near half-filling are investigated theoretically within an analytical approach based on the Kondo and Yamaji's Green function decoupling scheme. The assumption is made that in the sys-

tem under study two types of elementary excitations exist: "spin wave-like"ones and those corresponding to the correlated motion of the holes. It is shown that these excitations are effectively separated if the hopping amplitude t is less than the exchange constant J. For this case the temperature dependences of the heat capacity and spin susceptibility are calculated in the wide temperature range. It was found, that with the increase of doping from the half-filling the maximum of the spin susceptibility increases and its position shifts to lower temperatures for both types of lattices. Such behavior is in agreement with the qualitative predictions made in [1]. Heat capacity demonstrates a double peak shape. The high temperature peak is associated with the "spin wave-like"excitations and shifts to lower temperatures with doping. The low temperature peak appears due to the holes and its height and position depend on both the doping and ratio t/J.

1. E. Dagotto Rev. Mod. Phys., 66, 763 (1994).

TT 25.27 Wed 14:30 P1

Mesoscopic BCS pairing in the repulsive 1d-Hubbard model — •Andreas Osterloh[1], Luigi Amico[2], and Andrea Mastellone[2] — [1]Institut für theoretische Physik, Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany. — [2]MATIS-INFM & Dipartimento di Metodologie Fisiche e Chimiche (DMFCI), Universita' di Catania, viale A. Doria 6, I-95125 Catania, Italy

We study mesoscopic pairing in the one dimensional repulsive Hubbard model and its interplay with the BCS model in the canonical ensemble. The key tool is comparing the Bethe ansatz equations of the two models in the limit of small Coulomb repulsion. For the ordinary Hubbard interaction the BCS Bethe equations with infinite pairing coupling are recovered; a finite pairing is obtained by considering a further density-dependent phase-correlation in the hopping amplitude of the Hubbard model. We find that spin degrees of freedom in the Hubbard ground state are arranged in a state of the BCS type, where the Cooper-pairs form an un-condensed liquid on a "lattice" of single particle energies provided by the Hubbard charge degrees of freedom; the condensation in the BCS ground state corresponds to Hubbard excitations constituted by a sea of spin singlets.

TT 25.28 Wed 14:30 P1

Hubbard model in a magnetic field at weak coupling — •Carsten Knecht and P.G.J. van Dongen — University of Mainz, Institut für Physik, 55099 Mainz, Germany

The phase diagram of the half-filled Hubbard model is studied at weak coupling in two spatial dimensions. A homogeneous magnetization in the z-direction and a staggered magnetization in the x-direction are assumed. We apply perturbation theory at fixed order parameter (PTFO) to this system. The results are compared with the well know Hartree-Fock solutions that usually overestimate the order parameters. This calculation is also relevant for superconductivity in the doped two-dimensional negative-U Hubbard model.

TT 25.29 Wed 14:30 P1

Collective spin excitations within the time-dependent Gutzwiller approximation for the Hubbard model — •Falk Günther and Götz Seibold — BTU Cottbus

We use a spin-rotational invariant slave-boson-formulation of the Hubbard model, in order to investigate the collective excitations of itinerant ferromagnets. The expansion of the resulting spin-rotational invariant Gutzwiller energy functional around the saddle point allows the computation of dynamic correlation functions using the random-phase approximation (RPA). We evaluate ferromagnetic and antiferromagnetic instabilities from the transverse magnetic susceptibility and compute the dispersion relation for the spin waves. Results for one- and two-dimensional systems are presented and compared with the convetional Hartree-Fock+RPA theory.

TT 25.30 Wed 14:30 P1

Doping dependence of spin excitations in the stripe phase of high-Tc superconductors — •Götz Seibold[1] and Jose Lorenzana[2] — [1]Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany — [2]SMC-INFM,ISC-CNR, Dipartimento di Fisica, Universita di Roma La Sapienza, P. Aldo Moro 2, 00185 Roma, Italy

Based on the time-dependent Gutzwiller approximation of the extended Hubbard model we calculate the energy and momentum dependence of spin excitations for striped ground states. Since our approach correctly reproduces the experimentally obtained incommensurability vs. doping behavior in La-based cuprates the present investigation allows to quantitatively predict the energy ω_{res} and intensity of the 'resonance peak' as well as the spin velocity of high energy (optical) magnons in this compound. In the underdoped regime $\delta < 1/8$ we find a linear dependence ofω_{res} on doping whereas the resonance energy significantly shifts to higher values when the charge concentration in the stripes starts to deviate from half filling for $\delta > 1/8$.

TT 25.31 Wed 14:30 P1

Spectral properties of RVB superconductor — •Bernhard Edegger[1], Claudius Gros[1], and V.N. Muthukumar[2] — [1]Institut für Theoretische Physik, Universität Frankfurt, D-60438 Frankfurt, Germany — [2]Department of Physics, City College of the City University of New York, New York, NY 10031

We use a Gutzwiller renormalized mean field theory to study properties of projected quasiparticles within the tJ model. We calculate the one-particle spectral function and discuss the relevance for tunneling and photoemmision spectroscopies in doped Mott insulators like the high T_C superconductors. Besides we consider incoherent excitations and emphasise their importance in describing the striking asymmetry seen in the tunneling experiments.

TT 25.32 Wed 14:30 P1

Competing phases of the $t-J$ model on the triangular lattice. — •Irakli Titvinidze[1] and Matthias Vojta[2] — [1]Institut fuer Theoretische Physik A, RWTH Aachen, Templergraben 55, 52056 Aachen, Germany — [2]Institut fuer Theorie der Kondensierten Materie,Universitaet Karlsruhe, Postfach 6980, 76128 Karlsruhe, Germany

Our aim is to study the $t-J$ model on a triangular lattice, employing the Sp($2N$) large-N mean-field theory used previously [1,2] for the square-lattice geometry.

Our calculations show that for low doping a spin-Peierls state is realized in the system, while for high doping s-wave superconductivity occurs. For intermediate doping two different phases with a single-site unit cell appear: For small t/J we find a symmetry-broken phase with links fields $|Q_1| = |Q_2| > |Q_3|$, whereas for large t/J a "120° phase" is realized, with $Q_1 = Q_2\, e^{2\pi i/3} = Q_3\, e^{4\pi i/3}$. This is in qualitative agreement with published results of Kumar and Shastry [3] and Ogata [4].

[1] S. Sachdev and N. Read, Int. J. Mod. Phys. B 5, 219 (2000)
[2] M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B 62, 6721 (2000)
[3] B. Kumar and B. S. Shastry, cond-mat/0304210
[4] M. Ogata, cond-mat/0304405

TT 25.33 Wed 14:30 P1

VCA-approach to the magnetic properties of the 2-D Hubbard Model — •Sascha Brehm[1], Michael Potthoff[1], Markus Aichhorn[1,2], Enrico Arrigoni[2], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria

A new scheme for calculating two-particle (here spin-) response functions within the Variational Cluster Approach (VCA) [1] is presented and applied to the 2D-Hubbard model. The magnetic suszebility is calculated from the normal and superconducting one-particle Green's functions extracted from the VCA for the infinite-sized system and the q- and omega-dependent 2-particle vertex obtained from a cluster calculation. It is shown that this approach reproduces some characteristic features of the neutron-scattering data for the magnetic excitations in high-Tc cuprates. [1]PRL 91,206402 (2003)

TT 25.34 Wed 14:30 P1

Competing magnetic interactions in 1D and 2D cuprates - an electronic structure study — •Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and Helge Rosner[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]MPI CPfS Dresden

In many copper oxygen networks, especially for Cu-O-Cu bond angles close to 90°, ferromagnetic interactions play an important role in addition to the well known superexchange $J \sim t^2/U$. We present a systematic study of the electronic structure and the exchange integrals for different types of 1D and 2D spin 1/2 cuprate systems: edge and corner shared single-chain (Li_2CuO_2, Sr_2CuO_3), double-chain ($SrCuO_2$), and planar ($CaCuO_2$, $Sr_2CuO_2Cl_2$) arrangements. Based on full potential LSDA and LSDA+U band structure calculations and subsequently derived tight-binding models we estimate sign and magnitude of the most

relevant exchange integrals. We compare the results of total energy calculations with those of various tight-binding (TB) models from one-band and multi-band approaches. The ferromagnetic contributions can be estimated from the difference between the TB and the total energy results. We investigate the effect of the network configuration (edge shared vs. corner shared CuO_2 plaquettes) and of the dimensionality on the coupling strength.

TT 25.35 Wed 14:30 P1

Thermoelectric effects in layered conductors with a multisheet Fermi surface — •Olga Kirichenko and Valentin Peschansky — B.I.Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, Kharkov, Ukraine

Thermoelectric effects in layered organic conductors with the Fermi surface consisting of topologically different sheets in the form of cylinders and planes with weak corrugation of an arbitrary form, are studied theoretically. It is shown that at low enough temperatures, when account of the quantization of charge carriers orbital motion in a magnetic field is essential, the dependence of thermoelectric field upon reciprocal magnetic field takes the form of giant oscillations. Thermomagnetic coefficients of a layered conductor are shown to depend periodically upon the angle between the magnetic field direction and the normal to the layers. The presence of a group of charge carriers with a Q1D dispersion relation results in the strong anisotropy of thermoelectrical coefficients due to the existence of preferred direction for velocities of electrons belonging to this group. Experimental investigations of thermoresistanse and thermo-emf at different orientations of the magnetic field with respect to the layers allows to study in detail the energy spectrum of conduction electrons, in particular to determine electron effective masses and the distribution of their velocities at the Fermi surface.

TT 25.36 Wed 14:30 P1

Hall effect in quasi-two-dimensional conductors — •Valentin G. Peschansky[1] and Raed Hasan[2] — [1]B.I.Verkin institute for low temperature and Egineering, 61103 Kharkov, Ukraine — [2]V.N.Karazin Kharkov national university, 4 Svoboda sq., 61077 Kharkov, Ukraine

Galvanomagnetic phenomena have been studied theoretically in layered conductors with a quasi-two-dimensional electron energy spectrum of an arbitrary form in a strong magnetic field B. At low enough temperature, when the smearing of the Fermi distribution function for charge carriers is much less than the separation between quantized Landau levels the Hall field oscillates with 1/B. It is shown that in conductors with the Fermi surface consisting of topologically different elements the amplitude of quantum oscillations of the Hall field is sufficiently large and comparable to the amplitude of the Shubnikov-de Haas magnetoresistance oscillations. In the case when the Fermi surface has the form of a single corrugated cylinder there are no quantum corrections to the Hall field in the collisoinless limit. Experimental studies of the Hall field along with the B-dependence of the magnetoresistance at different orientations of the magnetic field permits one to restore the Fermi surface completely.

TT 25.37 Wed 14:30 P1

Fermionic renormalization group flow into phases with broken discrete symmetry: charge-density wave mean-field model — •Roland Gersch[1], Carsten Honerkamp[2], Daniel Rohe[3], and Walter Metzner[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Institut für Theoretische Physik, Uni Würzburg, Am Hubland, 97074 Würzburg — [3]Ecole Polytechnique - CPhT, F91128 Palaiseau Cedex, France

We generalize the application of the functional renormalization group (fRG) method for the fermionic flow into the symmetry-broken phase to finite temperatures. We apply the scheme to the case of a broken discrete symmetry: the charge-density wave (CDW) mean-field model at half filling. We show how an arbitrarily small initial CDW order parameter starts to grow at the CDW instability and how it flows to the correct final value, suppressing the divergence of the effective interaction in the fRG flow. The effective interaction peaks at the instability and saturates at low energy scales. The relation to the mean-field treatment and the prospects of the new method are discussed.

TT 25.38 Wed 14:30 P1

Analytical approach to the quantum-phase transition in the one-dimensional spinless Holstein model — •Steffen Sykora[1], Arnd Hübsch[2], and Klaus W. Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Department of Physics, University of California, CA 95616, USA

We study the one-dimensional Holstein model of spinless fermions interacting with dispersion-less phonons by using a recently developed projector-based renormalization method (PRM). At half-filling the system shows a metal-insulator transition to a Peierls distorted state at a critical electron-phonon coupling where both phases are described within the same theoretical framework. The transition is accompanied by a phonon softening at the Brillouin zone boundary and a gap in the electronic spectrum. For different filling, the phonon softening appears away from the Brillouin zone boundary and thus reflects a different type of broken symmetry state.

TT 25.39 Wed 14:30 P1

Dimerization effect on Luttinger liquid behavior — •Satoshi Ejima[1], Satoshi Nishimoto[2], and Florian Gebhard[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Max-Planck-Institut für Physik Complexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

A number of organic conductors exhibit a variety of electronic phases and some of them show a Luttinger liquid behavior due to strong one-dimensionality. For instance, a description by a Luttinger liquid seems to be more appropriate to analize experimental results (optical conductivity, photoemission spectroscopy, the dc resistivity, etc.) in $(TMTCF)_2X$. However, theoretical investigation with one-dimensional extended Hubbard model at quarter filling has been more puzzling.

Very slow carrier density fluctuations have been observed by recent NMR experiments. A key factor for such fluctuations can be *dimerization* along the TMTCF stacks. We study a dimerized Hubbard chain for various band filling with density-matrix renormalization group method. We suggest that the Luttinger liquid properties are drastically affected by the dimerization especially around quarter filling.

TT 25.40 Wed 14:30 P1

Time Evolution of a Luttinger Liquid through a correlated insulator — •Salvatore R. Manmana[1,2], Alejandro Muramatsu[1], and Reinhard M. Noack[2] — [1]Institut f. Theoretische Physik III, Universität Stuttgart, Germany — [2]AG Vielteilchennumerik, Fachbereich Physik, Philipps-Universität Marburg, Germany

We investigate the time evolution of a system of spinless fermions on a one-dimensional lattice with nearest-neighbor repulsion V and nearest-neighbor hopping t at half filling. Starting from the ground state of the Luttinger liquid phase, we study the time evolution after the system is perturbed by suddenly increasing the interaction to a value associated with an insulating ground state. Using a variant of the time-dependent density-matrix renormalization group method that approximates the time-evolution operator within a Krylov subspace, we calculate the *full* time evolution of the system. In the atomic limit, $t = 0$, the density and the density-density correlation function are time-independent, while the momentum distribution $\langle n_k \rangle$ shows behavior characteristic of periodic collapse and revival of the initial Luttinger liquid state. Therefore, the density-density correlations and one-particle propagators are no longer connected by a single anomalous dimension as in the equilibrium case. For parameter values away from this classical limit, we find relaxation phenomena when the perturbed interaction is near the quantum critical point. For intermediate values new nonequilibrium states are found.

TT 25.41 Wed 14:30 P1

The spectral properties and the metal-insulator transition in the spin-fermion and s-d exchange model: equation of motion approach — •Andrey Katanin[1,2] and Valentin Irkhin[2] — [1]Max-Planck-Institut für Festkörperforschung, 70569, Stuttgart, Germany — [2]Institute of Metal Physics, 620219 Ekaterinburg, Russia

The classical s-d exchange and the spin-fermion models are studied within the equation-of-motion approach combined with the $1/N$ expansion (N is the number of spin components, $N = 3$ for physical spins). The local and magnetic splitting in the electronic spectral functions is discussed. In the $d \to \infty$ limit, where only local fluctuations are important, the s-d model yields a metal-insulator transition with increasing interaction strength, while the spin-fermion model yields nonvanishing

spectral weight at the Fermi level at any finite interaction. For $d = 2$ in the presence of strong ferromagnetic fluctuations the self-energy at low temperatures T has a non-Fermi liquid form in the energy window $|\omega| < \Delta_0$ near the Fermi level, where Δ_0 is the spin splitting for magnetically ordered ground state, and $\Delta_0 \propto T^{1/2} \ln^{1/2}(v_F/T)$ in the quantum critical regime (v_F is the Fermi velocity). In the renormalized classical regime the spectral functions have a two-peak structure at finite T, which implies quasisplitting of the Fermi surface due to strong magnetic fluctuations. The role of dynamic spin fluctuations in the spin-fermion model is discussed.

TT 25.42 Wed 14:30 P1

Orbital Waves versus Vibronic Excitations — •Kai P. Schmidt[1], Markus Grüninger[2], and Götz S. Uhrig[3] — [1]Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne, CH 1015 Lausanne, Switzerland — [2]II. Physikalisches Institut der RWTH Aachen, Templergraben 55, 52056 Aachen, Germany — [3]Theoretische Physik, Geb. 38, FR 7.1, Universität des Saarlandes, D-66123 Saarbrücken, Germany

A large number of transition-metal compounds show orbital ordering at low temperatures. But the experimental observation of the corresponding elementary excitations of an orbitally ordered state, the so-called orbital waves (orbitons), turned out to be rather difficult, and a watertight experimental proof for the existence of orbitons is still lacking. It is therefore natural to ask whether other degrees of freedom are involved in transition-metal compounds which complicates the search for orbital waves. In this contribution the coupling of orbital and lattice degrees of freedom is investigated. We calculated the kinetic and the spectral properties of the orbital waves for a one-dimensional toy-model. The elementary excitations are orbital-wave-like for small orbiton-phonon coupling. In contrast, the excitations are vibronic when the coupling between orbital and lattice degrees of freedom is large. The most interesting case is the crossover regime at intermediate couplings. Here the most important spectral contribution is a continuum build by one orbiton and by one phonon. Surprisingly, the spectral density displays rather sharp resonances inside the continuum which form a shadow-like image of the one-orbiton dispersion.

TT 25.43 Wed 14:30 P1

Variational cluster approach to superconducting and antiferromagnetic phases in hole- and electron-doped cuprates — •Markus Aichhorn[1,2], Enrico Arrigoni[1], Michael Potthoff[2], and Werner Hanke[2] — [1]Institute for Theoretical and Computational Physics, Graz University of Technology — [2]Institute for Theoretical Physics, University of Würzburg

Using the recently proposed Variational Cluster Approach (VCA), we study the competition between d-wave superconductivity and antiferromagnetism in hole- and electron-doped cuprates. In both cases, our thermodynamic consistent results for the t-t'-U Hubbard model suggest the occurrence of phase separation into a mixed antiferromagnetic-superconducting phase at low doping and a pure superconducting phase at higher doping, although the energy scale for phase separation is an order of magnitude smaller on the electron-doped side. We argue that this can explain the different pseudogap and superconducting transition scales in hole- and electron-doped materials. The cluster calculations reproduce qualitatively the ground-state phase diagram of high-temperature supercondutors. In particular, they include salient features such as the enhanced robustness of the anitferromagnetic phase for electron-doping, compared to the hole-doped case.

TT 25.44 Wed 14:30 P1

Kondo Shadows in Hybrid Magnetic Molecular Solids — •Mikhail Kiselev[1] and Konstantin Kikoin[2] — [1]Universität Würzburg, Germany — [2]Ben Gurion University, Beer Sheva, Israel

We discuss the properties of layered Anderson/Kondo lattices with metallic electrons confined in 2D xy planes and local spins in insulating layers forming chains in z direction. Each spin in this model possesses its own 2D Kondo cloud, so that the Nozieres' exhaustion problem does not occur. The high-temperature perturbational description is matched to exact low-T Bethe-ansatz solution. The excitation spectrum of the model is gapless both in charge and spin sectors. The disordered phases and possible experimental realizations of the model are briefly discussed.

TT 25.45 Wed 14:30 P1

DMFT/NRG Studies of the Transport Properties of Heavy Fermion Systems — •Claas Grenzebach[1], Frithjof B. Anders[1,2], and Gerd Czycholl[1] — [1]Institut für Theoretische Physik, Universität Bremen — [2]Theoretische Physik, Universität des Saarlands, Saarbrücken

Heavy fermion systems (HFS) are described by the periodic Anderson model (PAM), which is mapped onto an effective single impurity Anderson model (SIAM) by dynamical mean field theory (DMFT). The SIAM is treated with the non-perturbative method of numerical renormalization group (NRG). This has the advantage that the correct Kondo scale is obtained. We investigate the (electronic) transport properties and the characteristic low temperature scales of HFS within this DMFT/NRG approach and calculate the temperature dependence of the resistivity and the thermoelectrical power as well as the frequency and temperature dependence of the dynamical conductivity and compare our results with experimental results typical for HFS. An extension of the model and method to take into account substitutional disorder by means of the coherent potential approximation (CPA) is discussed. Furthermore, we compare our results with the corresponding results obtained by using modified perturbation theory (MPT) as impurity solver. The MPT is exact up to second order in the Coulomb correlation U and reproduces the atomic limit ($V = 0$).

TT 25.46 Wed 14:30 P1

DCA Calculations of the Kondo Lattice Model — •Lee Martin and Fakher Assaad — Universität Würzburg

We consider the two-dimensional Kondo Lattice model with exchange J and hopping t within the framework of the Dynamical Cluster Approximation. Results at different temperatures and different cluster sizes will first be compared with existing BSS results (1) at half-filling. We then move on to the doped lattice with the ultimate aim of mapping out the magnetic phase diagram as a function of doping and coupling J/t.
(1) S. Capponi, F.F. Assaad, Phys. Rev. B 63, 155114, (2001)

TT 25.47 Wed 14:30 P1

Two-particle excitations in the Dynamical Cluster Approximation — •Stephan Hochkeppel, Fakher Assaad, and Werner Hanke — Theoretische Physik, Am Hubland, D-97074 Würzburg

The two-particle properties of the two-dimensional Hubbard model in the strong-coupling regime $U = 8t$ are investigated by using the Dynamical Cluster Approximation (DCA) [1]. In the DCA approach the original lattice problem is mapped to a self-consistently embedded cluster in momentum space. The crucial approximation of the DCA approach is to use the irreducible quantities, e.g the self-energy and irreducible vertices of a cluster as a good approximation of the lattice problem. We utilize a simplified Bethe-Salpeter equation with a renormalized Coulomb coupling $U_{eff}(\vec{q}, i\omega)$ which is determined in the DCA scheme. First results are presented for the spin-excitation spectrum.
[1] M. Jarrell, Th. Maier, C. Huscroft, and S. Moukouri, Phys. Rev. B (2001).

TT 25.48 Wed 14:30 P1

Green functions for t-t' hopping on the Bethe lattice — •M. Kollar[1], M. Eckstein[1], K. Byczuk[1,2], N. Blümer[3], P. van Dongen[3], M. Radke de Cuba[4], W. Metzner[5], D. Tanasković[6], V. Dobrosavljević[6], G. Kotliar[7], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute of Theoretical Physics, Warsaw University, Poland — [3]Institute of Physics, KOMET 337, University of Mainz — [4]Aachen — [5]MPI for Solid-State Research, Stuttgart — [6]Dept. of Physics and NHMFL, Florida State University, USA — [7]Dept. of Physics and Astronomy, Rutgers University, USA

We calculate the local Green function for a quantum-mechanical particle with hopping between nearest (t) and next-nearest neighbors (t') on the Bethe lattice, where the on-site energies may alternate on sublattices [1]. For infinite connectivity the renormalized perturbation expansion is carried out by counting all non-self-intersecting paths, leading to an implicit equation for the local Green function. By integrating out branches of the Bethe lattice the same equation is obtained from a path integral approach for the partition function. This also provides the local Green function for finite connectivity. Finally, a recently developed topological approach [1] is extended to derive an operator identity which maps the problem onto the case of only nearest-neighbor hopping. We find that t' hopping leads to an asymmetric spectrum with additional van-Hove singularities.

[1] M. Kollar *et al.*, Ann. Phys. (Leipzig) **14**, 642 (2005).
[2] M. Eckstein *et al.*, Phys. Rev. B **71**, 235119 (2005).

TT 25.49 Wed 14:30 P1

Phase diagram of the Hubbard model with t-t' hopping on the Bethe lattice — •M. Eckstein[1], M. Kollar[1], M. Potthoff[2], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg

Recently an efficient method for solving hopping Hamiltonians on the Bethe lattice was developed [1]. For infinite coordination number this provides the dynamical mean-field equations for the Hubbard model with nearest-neighbor hopping t and next-nearest-neighbor hopping t'. We solve these equations using the self-energy functional approach [2] and compute the phase diagram. We find that t' hopping strongly influences the Mott-Hubbard metal-insulator transition in the paramagnetic phase. Results for the antiferromagnetic phase, which is suppressed by t' hopping, are also discussed.
[1] M. Eckstein *et al.*, Phys. Rev. B **71**, 235119 (2005); M. Kollar *et al.*, Ann. Phys. **14**, 642 (2005).
[2] M. Potthoff, Eur. Phys. J. B **32**, 429 (2003).

TT 25.50 Wed 14:30 P1

Doping an antiferromagnetic Mott insulator in two dimensions: A variational cluster approach — •Matthias Balzer, Michael Potthoff, and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

The two-dimensional single-band Hubbard model at zero temperature is studied within the variational cluster approach (VCA) [1] using clusters with up to 8 sites. A ficticious staggered magnetic field and an overall shift of the single-particle energies in the reference clusters are used as variational parameters to ensure a thermodynamically consistent determination of the staggered magnetization and the average particle number [2]. Static quantities as well as the one-particle spectral density are calculated as functions of the chemical potential. The system undergoes a transition from the antiferromagnetic Mott insulator at half-filling to a paramagnetic metal at small doping. The critical dopings on the hole- and on the electron-doped side as well as the order of the phase transition are determined. An additional next-nearest-neighbor hopping is taken into account to study a possible phase separation into macroscopically large antiferromagnetic metallic and paramagnetic metallic regions.
[1] M. Potthoff, M. Aichhorn, and C. Dahnken, PRL 91, 206402 (2003)
[2] M. Aichhorn, E. Arrigoni, M. Potthoff, and W. Hanke, preprint

TT 25.51 Wed 14:30 P1

Curie temperature in the Hubbard model with binary alloy disorder — •Krzysztof Byczuk[1], Martin Ulmke[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — [2]FGAN-FKIE, Neuenahrer Str. 20, 53343 Wachtberg, Germany

Magnetic and electric properties of the Hubbard model with binary alloy disorder are studied within the dynamical mean-field theory. A paramagnet-ferromagnet phase transition and a Mott-Hubbard metal-insulator transition is found upon varying the alloy concentration. An enhancement of the Curie temperature due to disorder is demonstrated and is explained by the effects of band splitting and subband filling.
K. Byczuk and M. Ulmke, Eur. Phys. J. B 45, 449-454 (2005)
K. Byczuk, M. Ulmke, and D. Vollhardt, Phys. Rev. Lett. 90, 196403 (2003)

TT 25.52 Wed 14:30 P1

Energy gap in asymmetric Hubbard model — •Ihor V. Stasyuk and Orest B. Hera — Institute for Condensed Matter Physics, 1 Svientsitskii Street, 79011 Lviv, Ukraine

Energy band structure of the asymmetric Hubbard model with hopping integrals dependent on an electron spin (particle sort) is studied using an approximate analytic method within the dynamical mean-field theory. To solve the single-site problem, we use the equation of motion approach. Irreducible parts are separated by projecting on the basis of Hubbard operators, and are calculated using different-time decoupling. Our approximation is a generalization of the Hubbard-III approximation, and it includes the scattering responsible for the additional mechanism (due to the hopping of particles with different spin) of the band formation. When the single-site Coulomb repulsion U is increased, a gap appears in the spectrum. In the Falicov-Kimball limit (when particles of one sort are localized), our approach gives the exact result for the critical value of U corresponding to the alloy-analogy approximation. When a small nonzero hopping of localized particles is introduced, the spectrum is broadened and that leads to the increase of critical U.

TT 25.53 Wed 14:30 P1

Low-temperature phase diagram of the two-orbital Hubbard model — •Robert Peters and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We study the two-orbital Hubbard model by means of the dynamical mean-field theory using Wilson's numerical renormalization group to solve the effective impurity. As additional degree of freedom we include a localized spin coupled via Hund's exchange to the two orbitals, as e.g. necessary to properly describe $La_{1-x}Ca_xMnO_3$.

We investigate ferro-, antiferromagnetic and orbital order and their interplay as function of local Coulomb interaction parameters, filling and the additional localized spin degree of freedom. Comparison to generic features of the phase diagram of $La_{1-x}Ca_xMnO_3$ will be made.

TT 25.54 Wed 14:30 P1

Systematic Study of the Grüneisen-ratio near Quantum Critical Points — •Robert Küchler[1], Philipp Gegenwart[1], Niels Oeschler[1], Christoph Geibel[1], Frank Steglich[1], Karsten Heuser[2], and Ernst-Wilhelm Scheidt[2] — [1]Max-Planck Institut for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany

Recent theoretical work has shown that the Grüneisen ratio $\Gamma \propto \beta/C$ of thermal expansion , $\beta(T)$, to specific heat, $C(T)$, is a highly sensitive probe of quantum criticality. This is because Γ is divergent as T goes to zero at any quantum critical point (QCP) and the associated critical exponent can be used to distinguish between different types of QCPs. We report thermal expansion and Grüneisen ratio measurements in the temperature range 50 mK $\leq$ $T \leq$ 6 K on different Heavy-fermion systems close to magnetic QCPs. Our studies revealed the first-ever observation of a Grüneisen ratio divergence in four heavy fermion systems, which are located in the vicinity of antiferromagnetic QCPs. For $CeNi_2Ge_2$ and $Ce_xIn_{3-x}Sn_x$, $\Gamma \propto 1/T$ in accordance with the SDW scenario for three-dimensional critical spinfluctuations. By contrast, the observed singularity of Γ for $YbRh_2(Si_{0.95}Ge_{0.05})_2$ cannot be explained by the SDW theory, but is consistent with not yet published theoretical results of the locally scenario. Furthermore, the system $CeCu_{5.8}Ag_{0.2}$ has been studied, which shows a similar temperature dependence as found in $YbRh_2(Si_{0.95}Ge_{0.05})_2$ on a reduced temperature scale T/T_0, with $T_0 \approx T_K$, the Kondo temperature.

TT 25.55 Wed 14:30 P1

Hall Effect in $YbRh_2Si_2$ — •Sven Friedemann[1], Niels Oeschler[1], Silke Paschen[1,2], and Frank Steglich[1] — [1]Max-Planck-Institut for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany — [2]Vienna University of Technology, Karlsplatz 13, 1040 Wien, Austria

The heavy-fermion metal $YbRh_2Si_2$ exhibits pronounced non-Fermi liquid behaviour due to its vicinity to a quantum critical point (QCP). At zero magnetic field, the system orders antiferromagnetically at very low temperatures (T_N=70 mK). By applying a small magnetic field, $YbRh_2Si_2$ is driven through the QCP towards the paramagnetic state. Currently, two scenarios for a system at this type of QCP are discussed: The spin-density-wave scenario at which heavy electrons are expected on both sides of the QCP and the locally QCP at which the heavy electrons on the paramagnetic side disintegrate into localised magnetic moments and light conduction electrons on the magnetic side of the QCP. The field-dependent Hall effect as a measure of the Fermi volume turns out to be the appropriate method to characterize the QCP in $YbRh_2Si_2$. Low-temperature Hall-effect measurements of $YbRh_2Si_2$ show a rapid change of the Fermi volume and thus strongly hint at the existence of a locally QCP with a small Fermi surface at the magnetic side and a large one at the paramagnetic side [1]. We present similar measurements of the Hall coefficient on $YbRh_2Si_2$ and on the reference substance $LuRh_2Si_2$ in an extended temperature range.
[1] S. Paschen et al., Nature 432, 881 (2004)

TT 25.56 Wed 14:30 P1

Thermal Transport Properties of the Heavy Fermion Compound $YbRh_2Si_2$ — •Stefanie Hartmann[1], Ulrike Köhler[1], Niels Oeschler[1], Cornelius Krellner[1], Christoph Geibel[1], Samuel Maquilon[2], Zachary Fisk[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, University of California, Davis, CA 95616, USA

The heavy-fermion compound $YbRh_2Si_2$ orders antiferromagnetically at $T_N = 70$ mK and reveals non-Fermi-liquid (NFL) behavior in the vicinity of a (magnetic field induced) quantum critical point (QCP).

Thermal conductivity κ and thermopower S measurements on high-purity single-crystalline samples of $YbRh_2Si_2$ as well as of the nonmagnetic reference compound $LuRh_2Si_2$ in the temperature range between 30 mK and room temperature are presented and discussed within the framework of current theoretical models.

The high temperature transport properties are dominated by the transition from incoherent to coherent Kondo scattering and furthermore by the crystal electric field splitting of the Yb^{3+} ions, as the first excited doublet is situated at 200 K. The low temperature regime is governed by the strong NFL behavior due to the proximity of the antiferromagnetic instability.

TT 25.57 Wed 14:30 P1

Single crystal growth and investigation of the magnetism of the alloy $CePd_{1-x}Rh_x$ for concentrations $x \geq 0.6$ — •M. Deppe[1], P. Pedrazzini[2], N. Caroca-Canales[1], C. Geibel[1], and J.G. Sereni[3] — [1]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]DPMC-Université de Genève, Q. Ernest - Ansermet, 1211 Genève, Switzerland — [3]Lab. Bajas Temperaturas, Centro Atómico Bariloche (CNEA), 8400 S.C. de Bariloche, Argentina

In the orthorhombic alloy $CePd_{1-x}Rh_x$ the continuous decrease of the ferromagnetic ground state $T_C(x)$ can be followed over more than a decade in T, from 6.6 K for $x = 0$ to 0.25 K at $x = 0.8$. Additional low temperature measurements suggest a smeared ferromagnetic quantum-critical point (QCP) for x_{cr} between 0.87 and 0.9.
All these results were based on $CePd_{1-x}Rh_x$ polycrystals. In order to get a more precise insight into the magnetic behaviour in the critical region we grow $CePd_{1-x}Rh_x$ single crystals in the range $x \geq 0.6$. We used the Bridgman technique with a pulling rate of 3-5 mm. Differential thermoanalysis measurements indicate a low melting point $T_m = 1090 \pm 15$ °C. The lattice parameters were defined with X-ray powder diffraction and the composition was investigated with microprobe analysis. We performed specific heat and resistivity measurements down to 0.4 K and compare our results with the previous results on polycrystalline samples. Further we studied the decrease of the magnetic anisotropy with x by susceptibility and magnetization measurements. These results will be discussed in relation to the scenario for the critical concentration.

TT 25.58 Wed 14:30 P1

Ultra-low-temperature specific heat of $CePd_{1-x}Rh_x$ – smeared ferromagnetic quantum phase transition — •Adam Pikul, Tanja Westerkamp, Robert Kuechler, Nubia Caroca-Canales, Philipp Gegenwart, Julian Sereni, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The $CePd_{1-x}Rh_x$ system exhibits a continuous evolution from ferromagnetic (FM) order in CePd ($T_C = 6.5$ K) to an intermediate–valence ground state in CeRh [1]. In the present contribution we report on results of low-temperature specific-heat measurements performed for polycrystalline samples of $CePd_{1-x}Rh_x$, with the compositions $0.8 \leq x \leq 0.95$, which are supposed to be close to a FM quantum critical point [1].

In contrast to $CePd_{0.2}Rh_{0.8}$, still demonstrating the FM phase transition at $T_C = 370$ mK, the $C(T)$ curve measured for $CePd_{0.15}Rh_{0.85}$ does not show any anomaly at least down to 70 mK. In the latter compound $C/T \sim -\ln T$, characteristic of a non-Fermi-liquid (NFL) system, and achieves a value of almost 1 J/(mol K^2) at 70 mK. Upon further increasing of the Rh-content the value of C/T decreases, but the NFL behavior is still well visible in the samples with $0.87 \leq x \leq 0.95$, for which $C/T \sim T^{-\alpha}$ ($\alpha \approx 0.5$). Upon applying magnetic fields FL behavior $C/T(T) \sim const.$ is recovered in all different samples.

The above-mentioned results indicate that the NFL behavior is observed down to mK-temperatures over an extended x-range ($0.85 \div 0.95$). This would be compatible with a smeared quantum phase transition.

A. Pikul's attendance at this conference was sponsored by the Humboldt Foundation.

[1] J. G. Sereni, R. Küchler, C. Geibel, Physica B 359–361 (2005) 41

TT 25.59 Wed 14:30 P1

Hall effect near the quantum critical point of $CeCu_{6-x}Au_x$ — •M. Röger[1], M. Uhlarz[1], S. Putselyk[1], O. Stockert[2], and H. v. Löhneysen[1,3] — [1]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe — [2]Max-Planck-Institut für chemische Physik fester Stoffe, D-01187 Dresden — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The heavy-fermion system $CeCu_{6-x}Au_x$ orders antiferromagnetically above $x_c = 0.1$. The quantum phase transition at x_c displays unusual features, e.g., low-dimensional spin fluctuations and locally critical slowing down of these spin fluctuations suggestive of a breakdown of the Kondo coupling between $4f$ and conduction electrons [1]. This breakdown should be reflected in the Hall effect [2]. The Hall effect of $CeCu_{6-x}Au_x$ ($0 \leq x \leq 0.2$) as measured in a finite field ($B = 0.3$ T) along the magnetically easy c axis has shown Fermi-liquid behavior at low T, i.e. a temperature-independent Hall constant R_H below ~ 0.3 K [3]. Applying the magnetic field parallel to the magnetically hard b-axis (anisotropy factor ~ 10) allows to detect the effect of magnetic order on R_H for $x = 0.2$ and of quantum criticality for $x = 0.1$.

[1] A. Schröder et al., Nature **407**, 6802 (2000)
[2] P. Coleman et al., J. Phys. Cond. Matt. **13**, R723 (2001)
[3] H. Bartolf et al., Physica B **359-363**, 86 (2005)

TT 25.60 Wed 14:30 P1

Experimental Study of the Hall Effect and Magnetoresistance in MnSi — •Andreas Neubauer, Christian Pfleiderer, Philipp Niklowitz, and Peter Böni — Physik Department E21, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany

The itinerant-electron magnet MnSi orders magnetically at $T_c = 29.5$ K. The magnetic state is characterised by a helical modulation along the $\langle 111 \rangle$ space diagonal in the cubic B20 structure. Magnetic field suppresses the helical order above 0.6 T. The properties of MnSi are in various ways remarkable. The temperature dependence of the electrical resistivity suggests the emergences of an extended non-Fermi liquid phase above $p_c = 14.6$ kbar. Neutron scattering at ambient pressure shows an anomalous field dependence of helical fluctuations which may indicate certain similarities with the presence of partial magnetic order akin liquid crystals observed in a pocket of the NFL-phase. Here we report a detailed study of the Hall effect and the magnetoresistance of MnSi. We focus in particular on normal and anomalous contributions to the Hall effect and consider similarities and differences with conventional ferromagnets.

TT 25.61 Wed 14:30 P1

Magnetocaloric effect and Grüneisen parameter of thespin-gap system $TlCuCl_3$ — •S. Stark[1], N. Johannsen[1], T. Zabel[1], O. Heyer[1], A. Oosawa[2], H. Tanaka[3], A. Vasiliev[4], and T. Lorenz[1] — [1]II. Physikalisches Institut, Universität zuKöln, Germany — [2]Advanced Science Research Center,Japan Atomic Energy Research Institute, Japan — [3]Dep. ofPhysics, Tokyo Institute of Technology, Japan — [4]LowTemp. Physics Dep., Moscow State University, Russia

$TlCuCl_3$ is a S = $\frac{1}{2}$ quantum system with a nonmagnetic singlet ground state and a small energy gap to the excited triplet states. A magnetic field $H > 6$ T induces 3D antiferromagnetic order with a staggered magnetization perpendicular to the applied field. This transition can be described by a Bose-Einstein condensation of magnons and represents an example for a field-induced quantum phase transition. We present a study of the magnetocaloric effect, the thermal expansion α, the specific heat c_p and the magnetostriction. There exist clear predictions for the behavior of these quantities near a quantum critical point [1]. The differential magnetocaloric effect $\theta = \frac{dT}{dB}$ and the Grüneisen parameter $\Gamma = \frac{\alpha}{c_p}$ are very convenient to determine a possible quantum critical behavior of $TlCuCl_3$, since one anticipates that both Γ and $\frac{\theta}{T}$ diverge ($\sim \frac{1}{T}$) for $T \to 0$ and $B \to B_c$. Using Ehrenfest relations we also derive the uniaxial pressure dependence of the phase boundary [2]. We performed our measurements down to 0.3 K and compare our results to the existing theory.

[1] L. Zhu *et al.*, Phys. Rev. Lett. 91 (2003) 066404.
[2] N. Johannsen *et al.*, Phys. Rev. Lett. 95 (2005) 017205.

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TT 25.62 Wed 14:30 P1

Bulk and Surface Photoemission in Ytterbium Compounds — •Stefan W. Schmidt[1], Friedrich Reinert[2], and Stefan Hüfner[1] — [1]Universität des Saarlandes, 7.2 Experimentalphysik, D-66041 Saarbrücken, Germany — [2]Universität Würzburg, Experimentelle Physik II, D-97084 Würzburg, Germany

We have investigated a broad range of intermetallic intermediate-valent Yb compounds with high-resolution UPS. The results lead to interesting correlations between the binding energy ε_0 and the linewidth Γ_0 of the near-E_F spectroscopic structure and the ytterbium valence υ_{Yb} in these systems, and we discuss the influence of crystal field effects to the interpretation of our data.

From an investigation of the first order valence phase transition observed in the $4f$- and $4d$-XPS data of the prototypical compound $YbInCu_4$ [1] and a comparison to existing PE data [2, 3], we conclude that a surface-near region of thickness $d \approx$ 20–40 Å with different physical properties could be common to these materials. Therefore, the theoretical modelling of these systems on the base of UPS data has to consider the systematic differences between bulk and surface sensitive PES measurements, especially in comparison to thermodynamic measurements or bulk sensitive methods.

[1] S. Schmidt, S. Hüfner, F. Reinert and W. Assmus, Phys. Rev. B **72**, 195110 (2005).
[2] H. Sato *et al.*, Phys. Rev. Lett. **93**, 246404 (2004).
[3] H. Sato *et al.*, Phys. Rev. B **69**, 165101 (2004).

TT 25.63 Wed 14:30 P1

Spin-phonon coupling in Cr-based thiospinel systems probed by infrared spectroscopy — •Torsten Rudolf[1], Joachim Hemberger[1], Peter Lunkenheimer[1], Franz Mayr[1], Andrei Pimenov[1], Vladimir Tsurkan[1,2], and Alois Loidl[1] — [1]Center for Electronic Correlation and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, 2028 Chisinau, Republic of Moldova

We investigated several Cr-based thiospinels ACr_2S_4 with A=Mn, Fe, Zn, Cd, and Hg. In these magnetic semiconductors interesting physical features were found as e.g. relaxor ferroelectricity and colossal magnetocapacitance [1] in $CdCr_2S_4$, colossal magnetoresistance in $Fe_{1-x}Cu_xCr_2S_4$ or an orbital glass state in $FeCr_2S_4$ [2]. Beside the magnetic and thermodynamic properties we focus on the interplay between magnetism and phonon properties. We systematically studied the temperature and magnetic field dependence of the phonon spectra employing Fourier Transform Infrared Spectroscopy in a range from 5 K to 300 K and in fields of up to 7 T.

[1] J. Hemberger *et al.*, Nature **434**, 364 (2005)
[2] R. Fichtl *et al.*, Phys. Rev. Lett. **94**, 027601 (2005)

TT 25.64 Wed 14:30 P1

Detection of percolation-depercolation phase transition in silver rich Ag_xSe thin films by magneto transport measurements — •Marc von Kreutzbruck[1], Kai Allweins[1], Gertrud Lembke[1], Boris Mogwitz[2], Carsten Korte[2], and Jürgen Janek[2] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 58, D-35392 Gießen, Germany

In this work we investigate the galvanomagnetic transport properties of polycrystalline Ag_xSe thin films with a thickness ranging from 6 nm to 200 nm and a silver excess of about $x = 2.3$. The latter is near the percolation-depercolation phase transition, where the transport is mainly mediated by silver paths and silver clusters on the nanoscale. Sample characterization by measuring the conductivity, Kohler Slope, and temperature behavior yielded no clear indication whether a sample is in the percolative regime. A more reliable characterization of the semiconductor/metal heterostructure was obtained by measuring weak localization effects. The determination of the corresponding characteristic scattering lengths, such as the spin-orbit length L_{so} and the inelastic length $L_i(T)$, divided the Ag_xSe films clearly into two groups. We interpret these findings as an indication that the weak localization approach can be used as a sound method to determine the percolative nature of a 2D-heterostructure. An analytical model with predictive power is proposed.

TT 25.65 Wed 14:30 P1

Non-equilibrium properties of quantum impurity systems from the functional renormalization group approach — •Riccardo Gezzi, Thomas Pruschke, and Volker Meden — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The functional renormalization group approach is extended to handle stationary non-equlibrium problems. As first application we study a quantum-dot system subject to a finite bias voltage. As approximations to the flow-equation scheme we employ truncation at zero and one-loop order, ignoring energy dependencies in the latter.

Since in the limit of vanishing bias voltage an analytical solution to the differential equation generated in the zero-loop approximation exists, we can discuss the analytic structure of the solution to the flow equations obtained and show that in contrast to the equilibrium formulation poles in the right hand side can lead to an ill-conditioned problem for numerical differential equation solver.

First results for non-equilibrium properties of the single-impurity Anderson model will be discussed.

TT 25.66 Wed 14:30 P1

Equilibrium dynamics of the Anderson Impurity Model from functional RG methods — •Ralf Hedden, Volker Meden, Thomas Pruschke, and Kurt Schönhammer — Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We calculate the single-particle Greens-function of quantum multi impurity systems with local correlations modelled by the Anderson Impurity Model using a functional renormalization group scheme. Systems of one, two and three impurities coupled by hopping matrix elements are studied. The influence of an Ising-like Hund's-coupling is investigated. For special parameter sets we can even treat systems with an arbitrary number of impurities. We investigate how the different parameters effect the behaviour of the local spectral function.

TT 25.67 Wed 14:30 P1

Spin-boson model dynamics for non-equilibrium initial preparation — •Andreas Hackl[1] and Stefan Kehrein[2] — [1]Theoretische Physik III, Center for Electronic Correlations and Magnetism, Department of Physics, Universitaet Augsburg — [2]Department of Physics, LMU Muenchen Theresienstr. 37, 80333 Muenchen

The spin-boson model as a paradigm for quantum dissipation is well-understood in equilibrium. [1] However, many interesting questions regarding its dynamics are still open if the spin-boson model is initially prepared in a quantum state that is not its ground state. We use infinitesimal unitary tranformations (flow equation method) [2] to eliminate the system-bath coupling in a controlled nonperturbative approximation. In this way we are able to solve the Heisenberg equations of motion for the spin operators analytically with good accuracy, which allows us to study such non-equilibrium dynamics. We discuss various correlation functions, their equilibration properties and the fluctuation-dissipation theorem for different classes of initial states.

[1] S. Kehrein und A. Mielke, Annalen der Physik (Leipzig) 6, 90 (1997)
[2] F. Wegner, Annalen der Physik (Leipzig) 3, 77 (1994)

TT 25.68 Wed 14:30 P1

Phase Diagram of the Non-Equilibrium Anisotropic Kondo Model — •Peter Fritsch and Stefan Kehrein — LMU München, Department für Physik

Using the method of infinitesimal unitary transformation (flow equations), we derive a perturbative scaling picture of the anisotropic Kondo Model in a non-equilibrium state due to an applied dc-voltage bias. The scaling picture generically contains both the equilibrium and the non-equilibrium physics of the model, thereby allowing us to study the effect of decoherence on the Kosterlitz-Thouless quantum phase transition found in the equilibrium model.

This work is a generalization of the previous flow equation analysis of the isotropic non-equilibrium Kondo Model [1].

[1] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005)

TT 25.69 Wed 14:30 P1

Kondo Effect in Bosonic Spin Liquids — •Lars Fritz, Serge Florens, and Matthias Vojta — Theorie der Kondensierten Materie, Universitaet Karlsruhe

In a metal, a magnetic impurity gets fully screened at low temperatures by the conduction electrons. In contrast, an impurity coupled to spin-1 bulk bosons, such as triplet excitations in paramagnets, is only partially screened, even at the bulk quantum critical point, where the excitations are gapless. We argue that this difference is not due to the statistics of the host particles, but instead related to the structure of the impurity-bulk coupling. We show that in frustrated quantum magnets with bosonic spinon excitations one can observe a bosonic version of the Kondo effect.

TT 25.70 Wed 14:30 P1

Nonequilibrium Transport through a Double Quantum Dot System in the Kondo Regime — •V. Koerting and P. Wölfle — Institut fuer Theorie der Kondensierten Materie, Universitaet Karlsruhe, Karlsruhe

We consider nonequilibrium electron transport through a quantum dot in the Kondo regime coupled by exchange interactions to a second quantum dot connected to a third reservoir. The current is evaluated in perturbation theory. In a magnetic field it is shown to depend on the nonequilibrium magnetization in an essential way. The dependence of the magnetizations of both quantum dots on the exchange coupling, the magnetic field and temperature is calculated.

TT 25.71 Wed 14:30 P1

Weak Itinerant Ferromagnetism and Half-Metallicity in the New Filled Skutterudite $TlFe_4Sb_{12}$ — •Andreas Leithe-Jasper[1], Walter Schnelle[1], Helge Rosner[1], Michael Baenitz[1], Raul Cardoso-Gil[1], John A. Mydosh[2], and Yuri Grin[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

The chemical, structural and magnetic properties of the new filled skutterudite $TlFe_4Sb_{12}$ are described. X-ray diffraction and elemental analysis established the cubic crystal structure ($a = 9.1959(2)$ Å) without defects and disorder at the cationic site. The electronic structure is calculated by FPLO methods. Electronic structure calculations within the LDA exhibit a band ferromagnetic ground state and predict a nearly perfect half metallic state (97.5 %) similar to the isotypic compounds $M Fe_4Sb_{12}$ (M = Na, K) [1,2,3].

From experiments, $TlFe_4Sb_{12}$ is an itinerant electron ferromagnet with small magnetic moments ($M_r = 0.30\mu_B$/Fe atom) and $T_C \approx 85$ K. A Curie-Weiss behaviour with a paramagnetic moment per Fe-atom of $1.69\,\mu_B$ and $\Theta \approx T_C$ is observed above T_C, similar to $M Fe_4Sb_{12}$ (M = Na, K). The results of an NMR study are discussed.

[1] A. Leithe-Jasper *et al.,* Phys. Rev. Lett. 91, 037208 (2003).
[2] A. Leithe-Jasper *et al.,* Phys. Rev. B 70, 214418 (2004).
[3] G. Sheet *et al.,* Phys. Rev. B RC, in print (2005).

TT 25.72 Wed 14:30 P1

Magnetic order in thin films of the heavy fermion superconductor UNi_2Al_3 — •Martin Jourdan[1], Andrey Zakharov[1], Arno Hiess[2], Tim Charlton[3], Nick Bernhoeft[4], Danny Mannix[5], and Hermann Adrian[1] — [1]Institut für Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut Laue Langevin, BP 156, F-38042 Grenoble, France — [3]Rutherford Appelton Laboratory, ISIS facility, UK — [4]Dépt. de Recherche Fond. sur la Matière, France — [5]XMaS UK CRG beamline, ESRF, BP 220, F-38043 Grenoble Cedex 9, France

In the case of the heavy fermion superconductor UNi_2Al_3 a strong interconnection between its superconducting and magnetic properties is expected. Thus a careful characterization of the magnetic state of thin film samples primarily prepared for the investigation of the unconventional superconducting properties of this compound is necessary.
Resonant magnetic x-ray scattering was employed to investigate the magnetic state of epitaxial a^* oriented thin films UNi_2Al_3. The observed incommensurate propagation vector as well as the Neél temperature correspond to those of bulk samples. The 1200Å film shows magnetic order with a correlation length > 800Å parallel to the growth axis. Out of the three possible magnetic domains the one with the moment direction perpendicular to the film surface is not realized.

TT 25.73 Wed 14:30 P1

Growth of heavy-fermion superconductor $CeCoIn_5$ thin films — •Oleksiy K. Soroka, Gabriele Blendin, and Michael Huth — Physikalisches Institut, Max-von-Laue-Str. 1, D-60438, Frankfurt am Main

Heavy-fermion superconductors develop superconductivity out of a normal state in which electronic correlations cause a large increase of the conduction electrons' effective mass. The superconductive state is strongly affected by the magnetic excitations in these materials and is insofar unconventional. The most direct technique to investigate the spectrum of these excitations is tunneling spectroscopy which benefits strongly from well-defined surface as presented by epitaxial thin films. $CeCoIn_5$ is a member of the heavy-fermion family with the general formula $CeMIn_5$ (M=Co, Ir, Rh). It has the highest transition temperature of all heavy-fermion superconductors discovered up to date and is close to a quantum critical point. Thin films of $CeCoIn_5$ were deposited on different substrates by using molecular beam epitaxy. The growth characteristics were studied by means of x-ray diffraction. The chemical composition of the films was examined by energy dispersive x-ray analysis.

TT 25.74 Wed 14:30 P1

Metamagnetic transition in the cubic heavy fermion compound $CeIn_{3-x}Sn_x$ — •J. Arndt[1], N. Caroca-Canales[2], M. Dörr[1], C. Geibel[2], O. Stockert[2], and M. Loewenhaupt[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden

We report on magnetisation measurements on single crystals of the heavy fermion alloy $CeIn_{3-x}Sn_x$ at low temperatures. $CeIn_3$ orders antiferromagnetically below $T_N = 10.2$ K. Substituting tin for indium suppresses the magnetic order until $T_N = 0$ at a critical concentration $x_c = 0.67$ [1]. In the vicinity of this quantum critical point the system shows non-Fermi liquid behaviour [2]. Magnetisation measurements on single crystals with $x \leq 0.8$ were performed in static magnetic fields up to $B = 13.5$ T and pulsed fields up to $B = 47$ T at temperatures $T > 2$ K. The susceptibility $\chi = \mathrm{d}M/\mathrm{d}B$ as a function of magnetic field displays a kink at low fields ($B < 10$ T) in the paramagnetic state of samples with $0.4 \leq x \leq 0.65$. This anomaly, observed for the first time, seems to be related to a metamagnetic transition where magnetic intersite correlations are destroyed. The critical field $B^\star$, at which the transition occurs in paramagnetic $CeIn_{3-x}Sn_x$, is lowered with increasing x, i. e. with decreasing strength of the correlations in the system. In high magnetic fields ($B > 35$ T) we observed effects ascribed to the population of the excited crystal field state.

[1] T. Rus *et al.*, Physica B, **359-361**, 62 (2005)
[2] J. Custers *et al.*, Acta Phys. Pol. B **34**, 379 (2003)

TT 25.75 Wed 14:30 P1

Crossover from Ferro- to Antiferromagnetism in the Layered Kondo Systems CeTPO (T=Ru, Os) — •Cornelius Krellner[1], Nagesh S. Kini[2], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Applied Chemistry, Hiroshima University, Kagamiyama 1-4-1, Higashi-Hiroshima 739-8527, Japan

Intermetallic Kondo lattice systems have attracted considerable attention in the last decades. While their exist many Ce-based compounds showing antiferromagnetical ground states, only very few systems are known with ferromagnetic order. On the way to find new Ce-based Kondo lattices close to a ferromagnetic quantum phase transition, the CeTPO (T=transition metal) compound series attracted our interest, because of the rather unusual crystal structure with alternating layers of TP_4 and OCe_4 tetrahedra. In this contribution we will present the first investigation of the physical properties of CeTPO (T=Ru, Os) crystallizing with the tetragonal ZrCuSiAs type structure (P4/nmm). Measurements of the magnetic susceptibility reveal that in both compounds Cerium is in a trivalent state. A pronounced decrease of the resistivity below 50 K indicates the coherence effects of a Kondo scale of order $T_K = 10$ K. But whereas CeRuPO shows a ferromagnetic transition at 15 K both in temperature dependent susceptibility and specific heat, the isoelectronic CeOsPO becomes antiferromagnetic below 4.4 K. The possible origin of these effects will be discussed.

TT 25.76 Wed 14:30 P1

Electronic structure, thermodynamics and transport properties of $CeRh_2Sn_4$ — •Monika Gamza[1], Walter Schnelle[2], Andrzej Slebarski[1], and Helge Rosner[2] — [1]Institute of Physics, University of Silesia, Katowice, Poland — [2]MPI CPfS Dresden

In the last years, CeRhSn was intensively investigated because it exhibits a non-Fermi-Liquid (NFL) character of the physical properties in a region of low temperatures. Recent results [1,2] confirm that CeRhSn is placed in the vicinity of an antiferromagnetic instability and indicate the significant role of atomic disorder in the formation of the NFL state.

Here, we present a study of the compound $CeRh_2Sn_4$ which has not yet been investigated so far. The Ce 3d x-ray photoelectron spectroscopy (XPS) spectrum indicates a mixed valence of Ce suggesting similarities to the above mentioned CeRhSn. We present a combined experimental and theoretical study based on thermodynamic data (heat capacity, magnetic susceptibility and resistivity) and spectroscopic data (XPS) together with ab-initio band structure calculations.
For a clear presentation of the unusual electronic properties we compare $CeRh_2Sn_4$ with the non-magnetic isostructural reference system $LaRh_2Sn_4$.
Supported by the State Commitee for Scientific Research (KBN) through Grant No. 1 P03B 052 28 and by the DFG, Emmy Noether-program.
[1] A. Ślebarski et al., Phys. Rev. B **72** (2005), 085443.
[2] H. Tou et al., Phys. Rev. B **70** (2004), 100407.

TT 25.77 Wed 14:30 P1

^{119}Sn solid state NMR as a local probe for correlations in $CeRu_4Sn_6$ — •Eva Maria Brüning[1], Michael Baenitz[1], Andrei Gippius[2], André Strydom[3], Silke Bühler-Paschen[1], and Frank Steglich[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Moscow State University, Faculty of Physics, Moscow, Russia — [3]Department of Physics APK, University of Johannesburg, South Africa

A ^{119}Sn NMR study on the tetragonal semimetal $CeRu_4Sn_6$ and the metallic structural homologue $LaRu_4Sn_6$ is presented. At low fields (1.8 T, 28.5 MHz) a broad NMR line with small (-0.33%) and nearly independent negative Knight shift $K(T)$ is observed, whereas at larger fields (up to 7.5 T) a structure in the spectra could be resolved. The NMR spectra are well represented by a superposition of two broadened anisotropic S=1/2 lines, consistent with the two different Sn sites in the tetragonal structure. The behavior of the spin-lattice relaxation rate $1/T_1$ at 28.5 MHz above approximately $T = 20$ K is consistent with a narrow-gap semiconductor ($1/T_1 \sim T\exp(-\Delta/k_BT), \Delta/k_B = 33$ K). The formation of correlations become apparent below $T^* = 10$ K where an upturn is observed in $1/T_1T$. This is consistent with the specific heat results in the framework of the Korringa model where $(T_1T)^{-1} \propto K^2 \propto N_{EF}^2 \propto (C/T)^2$ is valid. $1/T_1$ investigations at higher fields show the supression of the low-temperature upturn. In conclusion the results for $CeRu_4Sn_6$ suggest the formation of a ground state of strongly correlated quasiparticles within a low-carrier density.

TT 25.78 Wed 14:30 P1

Quantum Critical Behavior in $CeNi_{9-x}Cu_xGe_4$. — •E. –W. Scheidt[1], W. Scherer[1], G. Hilscher[2], and H. Michor[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040

$CeNi_9Ge_4$ exhibits unusual non-Fermi liquid (nFl) behavior with the largest ever recorded value of the electronic specific heat $\Delta c/T \cong 5.5\,\mathrm{JK^{-2}mol^{-1}}$ without showing any trace of magnetic order [1]. Specific heat measurements show that the logarithmic increase of the Sommerfeld coefficient flattens off below 200 mK indicating coherent effects, whereas substitution of Ce by La in $CeNi_9Ge_4$ supports a single ion scenario as the main reason for the nFL behavior. Here we report on new substitution experiments replacing Ni by Cu. Specific heat and susceptibility results will discussed in the framework of a quantum critical phase transition scenario.
[1] U. Killer, E.-W. Scheidt, G. Eickerling, H. Michor, J. Sereni, Th. Pruschke, S. Kehrein, Phys. Rev. Lett. **92**, 27003 (2004)

TT 25.79 Wed 14:30 P1

Suppression of magnetic order in $YbNiSi_{3-x}Ge_x$ — •K. Grube[1], W. Knafo[1], C. Meingast[1], S. Drotziger[2], M. Uhlarz[2], Th. Wolf[1], P. Adelmann[1], and H. v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), Germany

$YbNiSi_3$ shows moderately heavy-fermion behaviour with antiferromagnetic long-range order below $T_N = 5.1$ K. We have studied the thermodynamic and transport properties of single crystals grown using the flux method with specific heat, DC magnetization, and resistivity measurements in magnetic fields up to 14 T. The magnetic order is suppressed in a magnetic field of 8 T. On the other hand, $YbNiGe_3$ shows a very small magnetic susceptibility and no sign of magnetic order down to the lowest measured temperature of 1.9 K, indicating an intermediate-valent state. Preliminary experiments on polycrystalline $YbNiSi_2Ge$ samples exhibit signs of magnetic ordering below 3 K. We report on the magnetic phase diagram of $YbNiSi_3$ and the dependence of the specific heat on the Ge content.

TT 25.80 Wed 14:30 P1

High temperature specific heat and crystal field of the non-Fermi-Liquid system $YbRh_2Si_2$ — •J. Ferstl, C. Geibel, O. Stockert, and F. Steglich — Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

The heavy fermion system $YbRh_2Si_2$ has attracted considerably interest in the last years, being located very close to a quantum critical point (QCP). Strong Kondo-like fluctuations lead to a very weak magnetic order with a transition temperature of only $T_N = 70$ mK at ambient pressure. A lot of physical investigations were done in the low temperature region, but much less investigations and analysis were devoted to the behaviour at higher temperatures. We shall present measurements of the specific heat C_p at higher temperatures. The results are analysed in view of crystal field (CEF) effects and discussed in comparison with results from inelastic neutron scattering. C_p of $YbRh_2Si_2$ and $LuRh_2Si_2$ were measured in the temperature range $2\ \mathrm{K} \leq T \leq 300$ K. From the difference we deduced the contribution C_{4f} of the Yb-4f-electrons. We confirm the presence of a broad maximum between 40 K and 80 K in C_{4f}. This maximum can be related to the first excited CEF level which, according to neutron data, is located around 17 meV. While C_{4f} is more conclusive than neutron data for this lowest excited CEF level, $C_{4f}(T)$ is less conclusive for the higher levels, for which neutron data gave rather precise excitation energies of 25 meV and 43 meV. Thus the combination of specific heat and neutron data allows a more reliable determination of the whole CEF scheme.

TT 25.81 Wed 14:30 P1

How many Kondo-ions are seen by the electron spin resonance in $Yb_{1-x}R_xRh_2Si_2$? — •J. Wykhoff[1], J. Sichelschmidt[1], S. MaQuilon[2], L. Pham[2], Z. Fisk[2], C. Krellner[1], J. Ferstl[1], H.-A. Krug von Nidda[3], C. Geibel[1], and F. Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — [2]Department of Physics, University of California, Davis, CA 95616 USA — [3]Experimentalphysik V, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The heavy-fermion compound $YbRh_2Si_2$ is located very close to a magnetic field induced quantum critical point. The unexpected observation of electron spin resonance (ESR) of the Kondo-ion Yb^{3+} *below* the Kondo temperature ($T_K \simeq 25$ K) might be a direct verification of the localized moment scenario of quantum criticality [1].

We present the ESR of $Yb_{1-x}R_xRh_2Si_2$, R = La, Lu. The ESR-line observed below ≈ 30 K vanishes with increasing Lu-concentration. Taking advantage of an improved crystal growth process, we found that the crystal quality and the residual linewidth of the ESR signal are closely related. This suggests that the so-called ESR-bottleneck effect is important for the observability of the ESR-line well below the Kondo temperature. We found that the ESR signal intensity also depends on the Yb-concentration.
[1] J. Sichelschmidt et al., Phys. Rev. Lett. 91, 156401 (2003)

TT 25.82 Wed 14:30 P1

Possible critical pressure-induced valence fluctuation in $EuCu_2Ge_2$ — •Gabriel Alejandro Dionicio[1], Heribert Wilhelm[1], Zakir Hossain[2], and Christoph Geibel[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology, Kanpur-208016, India

By means of electrical resistivity measurements under pressure, we investigated the possibility of inducing a valence fluctuating regime in $EuCu_2Ge_2$ at low temperatures. The results are discussed in terms of a possible scenario for unconventional superconductivity driven by virtual exchange fluctuation of the charge density [1]. This mechanism was proposed to explain the high pressure superconducting dome in $CeCu_2(Si_{0.9}Ge_{0.1})_2$ [2]. Our porpuse is to look for further candidates where this model might be apply. Some Eu-compounds with the $ThCr_2Si_2$ structure have shown a thermal activated continuous crossover from a divalent to a trivalent state, due to the degeneracy of the f^7 and f^6 configuration. We would like to address the question whether such a degenerated state can be induced by pressure at very low temperatures in $EuCu_2Ge_2$, taking into account that this situation seems to be achieved

in $EuCu_2(Si_{0.7}Ge_{0.3})_2$. The electrical resistivity measurements were performed up to 10 GPa in the temperature range 100 mK $< T <$ 300 K. A tentative phase diagram is presented and the results are compared with the studies peformed in the alloy $CeCu_2(Si_xGe_{1-x})_2$.
[1] K. Miyake, H. Maebashi; J. Phys. Soc. Jpn. 71 (2002) 1007
[2] H. Q. Yuan *et al*; Science 302 (2003) 2104

TT 25.83 Wed 14:30 P1

Fading of the magnetic order transition in $CePt_3$ Si under pressure — •Johannes Spehling[1], Olaf Zelesnik[1], Andreas Eichler[1], and Ernst Bauer[2] — [1]Inst. f. Angewandte Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Inst. f. Festkörperphysik, TU Wien, A-1040 Wien, Austria

We have carried out specific heat measurements on $CePt_3$ Si at low temperatures from ambient pressure up to 1.5 GPa. A maximum of $\frac{C}{T}$ around 2.2 K is observed which is commonly attributed to an antiferromagnetic transition. From our results it appears to consist of two superimposed anomalies separated by about 0.2 K. The pressure dependence of the lower anomaly can be described by a second order power law $T_1(p)$, which leads to a critical pressure of nearly $p_c = 2.4$ GPa. The second anomaly near the higher temperature T_2 is also weakened under pressure.

TT 25.84 Wed 14:30 P1

The quantum-functional properties of $Pr_{1-x-y}La_xPb_yTe$ — •T. Herrmannsdörfer[1], A. D. Bianchi[1], T. P. Papageorgiou[1], Y. Skourski[2], and J. Wosnitza[1] — [1]Institut Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Rossendorf, D-01314, Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01069 Dresden, Germany

The intermetallic compound $Pr_{1-x-y}La_xPb_yTe$ shows a wide spectrum of physical phenomena. Depending on the metallurgical composition as function of x and y, the compound changes its behavior from nuclear magnetic order to super- or semiconductivity. In addition, there are interesting interplay effects between these ground states. In consequence, $Pr_{1-x-y}La_xPb_yTe$ may serve as an promising material for quantum-computing applications. Here we report our results of the superconducting and magnetic properties investigated in a wide temperature, 0.0001 K $\leq T \leq$ 350 K, and field range, $0 \leq B \leq 50$ T. We present data of the ac susceptibility, magnetization, and electrical conductivity of various compositions x and y, e.g. turning the system from a van Vleck paramagnet, $x = y = 0$ into either a superconductor, $x \geq 0.5$, or a doped semiconductor, $y \geq 0.999$. Recently we have measured the magnetization of $y = 0$, 0.50, and 0.90 in pulsed magnetic fields up to 50 T in order to investigate the influence of doping on the crystalline electrical-field properties.

TT 25.85 Wed 14:30 P1

Fermi Surface of the Half Heusler Compounds $Ce_{1-x}La_xBiPt$ — •A. D. Bianchi[1], J. Wosnitza[1], N. Kozlova[2], D. Eckert[2], L. Schultz[2], I. Opahle[2], S. Elgazzar[2], M. Richter[2], J. Hagel[3], M. Doerr[3], G. Goll[4], H. v. Löhneysen[4,5], G. Zwicknagl[6], T. Yoshino[7], and T. Takabatake[7] — [1]HLD, Forschungszentrum Rossendorf, Postfach 51 01 19, D-01314 Dresden — [2]IFW Dresden, D-01171 Dresden — [3]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden — [4]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — [5]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — [6]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig — [7]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

We report on the Fermi surface in the correlated half-Heusler compound $Ce_{1-x}La_xBiPt$. In CeBiPt we find a field-induced change of the electronic band structure as discovered by electrical-transport measurements in pulsed magnetic fields. For magnetic fields above ∼25 T, the charge-carrier concentration determined from Hall-effect measurements increases nearly 30%, whereas the Shubnikov–de Haas (SdH) signal disappears at the same field. In the non-$4f$ compound LaBiPt the Fermi surface remains unaffected, suggesting that these features are intimately related to the Ce $4f$ electrons. Electronic band-structure calculations point to a $4f$-polarization-induced change of the Fermi-surface topology. In order to test this hypothesis, we have measured the (SdH) signal in a $Ce_{0.95}La_{0.05}BiPt$ sample with a low La concentration.

TT 25.86 Wed 14:30 P1

Electronic structure of Fe_3O_4/MgO — •C. F. Chang[1], J. Schlappa[1], C. Schüssler-Langeheine[1], H. Ott[1], Z. Hu[1], E. Schierle[2], E. Weschke[2], G. Kaindl[2], A. Tanaka[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

Magnetite thin films grown on flat and stepped MgO have been studied using transport and resonant soft x-ray diffraction measurements. Down to a thickness of 38 nm a clear 1st order Verwey transition is observed. Resonant soft x-ray diffraction at the Fe $L_{2,3}$ and O-K resonances was used to study the electronic structure in the low-temperature phase. The broadening of the diffraction peaks along the surface normal in thin films allowed us not only to study the $(00\frac{1}{2})$ superstructure peak at both resonances, but also the tail of the (001) diffraction peak, which cannot be reached at the Fe-$L_{2,3}$ resonance for bulk samples. The electronic origin of both peaks turns out to be clearly different. Possible models for the ordered phase will be discussed.

TT 25.87 Wed 14:30 P1

Tb magnetism in multiferroic $TbMnO_3$ — •Jörg Voigt, Jörg Persson, Michael Prager, Yixi Su, and Thomas Brückel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Recently, there has been a debate on the origin of the ferroelectric transition in the Perowskite $TbMnO_3$ at 28 K. Some authors attribute the spontaneous polarization to a lock-in transition of the Mn^{3+} moments [1]. Kenzelmann et al. [2] observed an ordered Tb^{3+} magnetic moment at the ferroelectric phase transition by a high resolution single crystal neutron study. However, neutron scattering is not element specific and therefore his interpretation could be doubted. We report on X-ray resonance exchange scattering to probe the Tb magnetic order exclusively and time-of-flight neutron spectroscopy to derive the Tb crystal field level scheme above and below the ferroelectric transition.
[1] Kajimoto et al., PRB 70, 012401 (2004)
[2] Kenzelmann et al., PRL 95, 087206 (2005)

TT 25.88 Wed 14:30 P1

Coupling between spin and orbital order in $La_{0.5}Sr_{1.5}MnO_4$? — •C. F. Chang[1], M. Buchholz[1], C. Schüssler-Langeheine[1], M. Benomar[1], E. Schierle[2], E. Weschke[2], G. Kaindl[2], M. Braden[1], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

In $La_{0.5}Sr_{1.5}MnO_4$ spin, orbital and charge order occurs at low temperatures. Resonant soft x-ray diffraction data show an increase in intensity for the superstructure peak related to orbital order below T_N, when the antiferromagnetic spin order sets in [1]. While this results indicates a coupling between antiferromagnetic order and orbital order, a recent study using polarization analysis assigned the gain in intensity to a magnetic scattering contribution to the orbital order peak intensity below T_N [2]. We studied the k-space around the orbital order peak and found a broad diffuse background of magnetic origin, which has considerable intensity at the position of the orbital order peak. The relative intensity of this background varies for different positions on the sample. Sample positions without magnetic background allowed us to study the resonance behavior of the orbital order peak above and below T_N.
[1] S. B. Wilkins et al., Phys. Rev. Lett. 91, 167205 (2003)
[2] U. Staub et al., Phys. Rev. B 71, 214421 (2005)

TT 25.89 Wed 14:30 P1

Electric-field-induced insulator-metal transition in thin films of $Pr_{0.68}Ca_{0.32}MnO_3$ — •Sebastian Schramm, Peter Moschkau, and Christian Jooss — Institut für Materialphysik, Universität Göttingen

Experimental analysis and understanding of electronic phase separation in hole-doped manganites offer a fascinating research area for the fundamental properties of correlated electrons in solids. That is why those manganites are of great interest and their behaviour in electric fields should be understood. In this work $Pr_{0.68}Ca_{0.32}MnO_3$(PCMO)-thin films prepared by Pulsed Laser Deposition on $SrTiO_3$-Substrates are examined concerning their electrical transport properties. In constant-

current-measurements, a resistance collapse of several orders of magnitude is observed while cooling below 175K. The resistivity exhibits a huge temperature hysteresis, which depends on the electric history of the sample. In further research explicit indications will be sought whether this abnormal resistance behaviour is due to a homogeneous or inhomogeneous resistance change in the film. There are a number of experimental evidences in favour of the inhomogeneous model, where a metallic, possibly ferromagnatic filament emerges in an insulating paramagnetic matrix.

TT 25.90 Wed 14:30 P1

Investigation of orbital ordering in $La_{7/8}Sr_{1/8}MnO_3$ by means of x-ray linear dichroism at the Mn L edge — •K. Kuepper[1,2], F. Bondino[3], K. C. Prince[3,4], M. Zangrando[3], M. Zacchigna[3], A. F. Takács[2], M. Matteucci[5], F. Parmigiani[6], A. Winiarski[7], V. R. Galakhov[8], Ya. M. Mukovskii[9], and M. Neumann[2] — [1]Forschungszentrum Rossendorf, D-01328 Dresden, Germany — [2]University of Osnabrück, Department of Physics, D-49069 Osnabrück, Germany — [3]Laboratorio TASC-INFM, I-34012 Basovizza (Trieste), Italy — [4]Sincrotrone Trieste, I-34012 Basovizza (Trieste), Italy — [5]ICGEB, I-34012 Trieste, Italy — [6]Dipartimento di Matematica e Fisica, Università Cattolica, del Sacro Cuore, Brescia, Italy — [7]Silesian Univ., A. Chelkowski Inst. Phys., PL-40007 Katowice, Poland — [8]Institute of Metal Physics, 620219 Yekaterinburg GSP-170, Russia — [9]Moscow State Steel and Alloys Institute, 117936 Moscow, Russia

We have investigated for the first time the orbital ordering in a three dimensional colossal magneto resistance manganite, namely $La_{7/8}Sr_{1/8}MnO_3$, by applying soft x-ray linear dichroism (XLD) to the Mn L edge [1]. We found that the cooperative Jahn Teller distorted orthorhombic phase, which is present at a temperature of 240 K, is probably accompanied by a predominantly cross type $(x^2-z^2)/(y^2-z^2)$ orbital ordering. This result is discussed in the light of previous results obtained by means of resonant x-ray scattering at the Mn K edge and different exchange interaction models.

[1] K. Kuepper *et al.*, J. Phys. Chem. B **109**, 15667 (2005)

TT 25.91 Wed 14:30 P1

Structural properties of Ru-codoped $La_{1-x}Sr_{1+x}MnO_4$ — •O. Schumann[1], D. Senff[1], M. Kriener[1], I. Klassen[1], N. Hollmann[1], T. Lorenz[1], A. Revcolevschi[2], G. Andre[3], F. Bouree[3] und M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]LPCES, Universite Paris Sud XI — [3]Laboratoire Léon Brillouin

We present x-ray and neutron scattering studies on ruthenium codoped $La_{1-x}Sr_{1+x}MnO_4$. This co-doping leads to a suppression of charge, orbital and magnetic order.

$La_{0.5}Sr_{1.5}MnO_4$ is the 2D-analogon of the half-doped 3D-perovskite manganites (Mn^{3+}:Mn^{4+}=1:1). While showing similar charge, orbital and spin order, a CMR effect is only observed in a very high field. As the CMR-effect in the 3D-manganites is due to a competition between antiferromagnetic (insulating) and ferromagnetic (metallic) interactions, this high field indicates a rather stable AF-order in the layered compound. To weaken this order we prepared several single crystals of Ru-codoped $La_{0.5}Sr_{1.5}MnO_4$, with Ru concentrations ranging from 2% up to 30%. Neutron diffraction, magnetization measurements and resistivity measurements shows, that Ruthenium doping rapidly suppress the charge and orbital order. Furthermore we find a ferromagnetic ground-state and an increased magnetoresistivity.

TT 25.92 Wed 14:30 P1

Magnetic excitations in charge and orbital ordered manganites — •D. Senff[1], M. Benomar[1], O. Schumann[1], F. Krüger[2], S. Scheidl[2], Y. Sidis[3], A. Revcolevschi[4] und M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Laboratoire Léon Brillouin, France — [4]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, France

Charge and orbital ordering around half doping is a unique feature in the physics of manganite-oxides and the competition of these insulating phases with FM metallic phases seems to be the origin of the well known colossal magnetoresistance in perovskite manganites. We present the magnetic excitation spectrum within the charge and orbital ordered state of single layered $La_{0.5}Sr_{1.5}MnO_4$, a compound which exhibits a very stable CE-type AFM ordering.

Using inelastic neutron scattering techniques we determined the complete spin-wave dispersion of the CE-phase. At low temperatures the main features of the excitation spectrum is a steep dispersion along the FM exchange pathways of the CE-type structure, while the dispersion in the perpendicular directions exhibits only a very narrow bandwidth. Within linear spin-wave theory we model the observed data and conclude that the FM interaction is the most dominant magnetic energy in the AFM CE-type ordering scheme. This interpretation is confirmed by the excitation spectrum and the quasielastic diffuse magnetic scattering at temperatures well above T_N which both give clear evidence for short-range ferromagnetic correlations.

TT 25.93 Wed 14:30 P1

Anomalies in the excitation spectrum of the spinels $CdCr_2S_4$ and $FeCr_2S_4$ — •P. Scheib[1], V. Gnezdilov[2], K.Y. Choi[3], P. Lemmens[1], J. Hemberger[4], A. Loidl[4], and V. Tsurkan[4,5] — [1]IPKM, TU Braunschweig, D-38106 Braunschweig — [2]B.I. Verkin Inst. for Low Temp. Phys., NASU, 61164 Kharkov — [3]IMR, Tohoku Univ., Sendai — [4]EP V, Univ. Augsburg, 86135 Augsburg — [5]IAP, Acad. Sci. Moldova, MD-2028, Chisinau

Chalcogenide spinels show exceptional dielectric and magnetic properties, as e.g. large magnetoresistance and magnetocapacitive coupling. Using Raman scattering we study the excitations spectrum of these systems. Pronounced phonon and magnetic anomalies are observed that precede the long range ordered phases. Evidence for phase separation is observed. Work supported by ESF-HFM.

TT 25.94 Wed 14:30 P1

Metamagnetism of $(Ca,Sr)_2RuO_4$ studied by thermal expansion and magnetostriction — •J. Baier[1], M. Kriener[1], S. Stark[1], O. Heyer[1], T. Zabel[1], P. Steffens[1], O. Schumann[1], O. Friedt[1], A. Revcolevschi[2], S. Nakatsuji[3], Y. Maeno[3], T. Lorenz[1], M. Braden[1], and J. Mydosh[1] — [1]II. Phys. Institut, University of Cologne,Germany — [2]Lab. de Physico-Chimie de l'État Solide,Université Paris-Sud, France — [3]Dep. of Physics, KyotoUniversity, Japan

We present a study of the thermal expansion $\alpha(T,H)$ and the specific heat $c_P(T,H)$ down to 300 mK near the metamagnetic transition in $Ca_{2-x}Sr_xRuO_4$ with $0.2 \leq x \leq 0.5$. Isovalent substitution of Sr by the smaller Ca drives the spin-triplet superconductor Sr_2RuO_4 to the antiferromagnetic Mott-insulator Ca_2RuO_4. At $0.2 \leq x \leq 0.5$ the compounds are still metallic but close to localization. We find strong and anisotropic anomalies in $\alpha(T)$ which change sign in sufficiently high magnetic fields [1]. Striking similarities with the metamagnets $Sr_3Ru_2O_7$ and $CeRu_2Si_2$ are noticed. At $x = 0.2$, the sign change of the thermal expansion anomaly coincides with the metamagnetic transition (MMT). This MMT is accompanied by a large anisotropic magnetostriction. Furthermore, c_P/T is unusually large and shows a non-monotonic field dependence with a maximum at the MMT which turns into a minimum above 2 K. In contrast, for $x = 0.5$ we observe a strong decrease of c_p/T in a magnetic field similar to the behavior of c_p/T at $x = 0.2$ above the MMT.

[1] Kriener *et al.*, cond-mat 0408015, accepted for publication in PRL

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TT 25.95 Wed 14:30 P1

Magnetic excitations in 214-Ruthenates — •Paul Steffens[1], Olaf Schumann[1], Jörg Baier[1], Markus Kriener[1], Oliver Friedt[1], Yvan Sidis[2], Jiri Kulda[3], Satoru Nakatsuji[4], Yoshiteru Maeno[4], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Kyoto University, Japan

We present investigations of the magnetic excitation spectra of pure and doped Sr_2RuO_4, i.e. $Ca_{2-x}Sr_xRuO_4$ ($0 \leq x \leq 2$) and Ti-doped Sr_2RuO_4.

In the spin-triplet superconductor Sr_2RuO_4, the excitation spectrum is dominated by incommensurate fluctuations, which are caused by Fermi surface nesting. In addition, a weak ferromagnetic component is observed. Upon Ti-doping, the incommensurate component is enhanced and finally condenses into static order.

Substitution of Sr by Ca leads to a complex phase diagram with different magnetic phases. We report studies on samples with $0.2 \leq x \leq 0.6$, i.e. a region where metamagnetism is observed and where the behaviour seems to be controlled by the balance between two different types of magnetic instability: an incommensurate and a ferromagnetic one. Our results reveal how the competition between these two is influenced by temperature, magnetic field and chemical composition.

TT 25.96 Wed 14:30 P1

Valence and spin state in Ca_3FeRhO_6 and Ca_3CoRhO_6 studied by XAS — •Zhiwei Hu[1], Tobias Burnus[1], Seiji Niitaka[2], Chun-Fu Chang[1], Hua Wu[1], Júlio Criginski Ceszar[3], Nicholas B. Brookes[3], Ling-Yun Jang[4], Hong-Ji Lin[4], Hidenori Takagi[2], Keng San Liang[4], Chen Te Chen[4], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Magnetic Material Laboratory, RIKEN (Institute of Physical and Chemical Research), Wako 351-0198, Japan — [3]European Synchrotron Radiation Facility, BP 220, Grenoble 38043, France — [4]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan

The physical properties of triangular-lattice systems has been attracting much interest because the geometrical frustration produces novel types of phase transitions. The triangular lattice in Ca_3CoRhO_6 and Ca_3FeRhO_6 consist of one-dimensional chains with faced-sharing CoO_6 and FeO_6 trigonal prisms and of RhO_6 octahedra. Neutron diffraction experiments indicate ferromagnetic Ising-spin chains in Ca_3CoRhO_6 and a three-dimensional antiferromagnetic transition at 12 K in $CaFeRhO_6$. The valence and spin states in both compounds are a matter of controversy. The combined experimental and theoretical X-ray absorption spectroscopy (XAS) study at the Co-, Fe- and Ru-$L_{2,3}$ edges presents unambiguously Co^{2+}/Rh^{4+} and Fe^{3+}/Rh^{4+} states in Ca_3CoRhO_6 and $CaFeRhO_6$, respectively. The X-ray magnetic circular dichroism at the Co-$L_{2,3}$ edge indicates a large orbital moment of Co^{2+} in Ca_3CoRhO_6.

TT 25.97 Wed 14:30 P1

Dynamical local field corrections — •K. Morawetz — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The finite temperature dynamical response function including the dynamical local field is derived within a quasiparticle picture for interacting one-, two- and three dimensional Fermi systems. The correlations are assumed to be given by a density dependent effective mass, quasiparticle energy and a mean momentum shift as well as a relaxation time. The latter one describes disorder or collisional effects. The mean momentum ensures the zero order frequency sum rule. With a single static local field, the third order frequency sum rule can be fulfilled simultaneously with the compressibility sum rule by relating the effective mass and quasiparticle energy shift to the structure function or pair correlation function. This parameterization of correlations includes local density functionals as a special case and is therefore applicable for density functional theories though the latter ones cannot fullfill both sum rules simultaneously. The comparison to the Monte-Carlo data seems to support such quasiparticle picture.

[1] K. Morawetz, Phys. Rev. B 66 (2002) 07512

TT 25.98 Wed 14:30 P1

Metal-insulator transition in heterojunctions — •K. Morawetz[1,2], C. Olbrich[1], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The conductivity in quasi two-dimensional systems is calculated using the quantum kinetic equation as well as molecular dynamical simulations. The system of quasi two-dimensional electrons in hetero-junctions which interact with charged and neutral impurities and the low temperature correction to the conductivity is calculated analytically. It turns out that the dynamical screening due to charged impurities leads to a linear temperature dependence, while the scattering from neutral impurities leads to the usual Fermi-liquid behavior. The experimental metal-insulator transition at low temperatures are reproduced [1]. The effective mass of quasiparticle excitations in quasi two-dimensional systems is calculated analytically. It is shown that the effective mass increases sharply when the density approaches the critical one of metal-insulator transition. This suggests a Mott-type of transition rather than an Anderson-like transition [2].

[1] K. Morawetz, Phys. Rev. B 67 (2003) 115125
[2] K. Morawetz, Europhys. Lett. 67 (2004) 77–83

TT 25.99 Wed 14:30 P1

Domain Walls in the Hubbard model — •Rolf Helmes, Luis Craco, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Phase separation and the physics of domain walls control the properties of many correlated systems with competing ground states, ranging from the manganites to organic Mott insulators [1]. We therefore study domain walls between different phases of the Hubbard model. The interplay of domain walls and their energetics on the one hand and of long-range Coulomb interaction on the other hand, control for example the physics of phase-separation close to a first-order metal-insulator transition. We use a generalization of dynamical mean field theory (DMFT) to treat inhomogeneous correlated systems such as domain walls of Mott insulators.

[1] Sasaki et al., Phys. Rev. Lett. 92, 227001 (2004)

TT 25.100 Wed 14:30 P1

Properties of the density of states of the three dimensional Bernoulli-Anderson model — •P. Karmann, V. Cerovski, and M. Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The density of states of the Bernoulli-Anderson model, defined as the tight-binding Hamiltonian of non-interacting electrons with disorder introduced by the random distribution of only two on-site energies, is studied using the large scale numerical diagonalization by means of the Lanczos algorithm. In particular, we determine the band structure and the properties of characteristic features for different system sizes and disorder strength of the on-site energies and compare the results with the Anderson model of localization.

TT 25.101 Wed 14:30 P1

Coupled cluster calculation of the ground state of the J_1–J_2 model on the square lattice — •R. Darradi[1], J. Richter[1], Sven E. Krüger[2], R. Zinke[1], and D. J. J. Farnell[3] — [1]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg, P.O.B. 4120, 39016 Magdeburg, Germany — [2]IESK Kognitive Systeme, Universität Magdeburg, PF 4120, 39016 Magdeburg, Germany — [3]Unit Of Ophthalmology, Department of Medicine, University Clinical Departments, Daulby Street, University of Liverpool, Liverpool L69 3GA, United Kingdom

Using the coupled cluster method (CCM) for high orders of approximation we investigate the ground state properties of J_1–J_2 model on the square lattice. By calculation of the sublattice magnetization, the spin stiffness, and the spin gap we determine the quantum critical point J_2^c, where magnetic LRO disappears. We estimate $J_2^c \approx 0.4 J_1$ which is in good agreement with the results obtained by other approximations.

TT 25.102 Wed 14:30 P1

T=0-phase diagram of the Kondo-lattice model with quantum localized spins — •Jochen Kienert and Wolfgang Nolting — Humboldt-Universität zu Berlin*Institut für Physik*Theoretische Festkörperphysik*Newtonstraße 15*D-12489 Berlin

The ferromagnetic/non-ferromagnetic phase diagram of the Kondo-lattice model is determined at T=0 in 2D and 3D. Our approach takes into account the quantum character of the localized magnetic moments, which often are treated classically in studies of this model. Consequently, special emphasis is put on the comparison between quantum and classical spins ($S \to \infty$). The maximum region of ferromagnetic stability is reduced for small spins. We compare our findings with results based on different methods by other authors.

TT 25.103 Wed 14:30 P1

Thermodynamics of intermediate-spin Heisenberg-chains — •Simon Grossjohann and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We investigate the crossover from quantum to classical behavior in one-dimensional spin-S chains by a complementary analysis of the thermodynamic properties resulting from quantum Monte-Carlo calculations as well as from the large-S limit. Using the stochastic series expansion, results will be given for the thermodynamic limit of chains with spins ranging from S=1/2 to S=5/2 and for temperatures $0.01 \leq T/J \leq 20$. We find a tendency of the peak-positions T_m of the quantum and classical uniform susceptibilities, χ_q and χ_c, to converge as $S \to 5/2$. However for both, Haldane and non-Haldane systems, substantial quantitative and qualitative differences remain between χ_q and χ_c, regarding the low-temperature behavior even for the larger spin magnitudes. We will compare our results with Bethe-Ansatz calculations and present Padé-approximants for χ_q which improve fit-formulas previously reported in literature.

TT 25.104 Wed 14:30 P1

Series expansion analysis of a tetrahedral cluster spin chain — •Marcelo Arlego and Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

Using series expansion by continuous unitary transformations we study the zero temperature magnetic properties of a frustrated tetrahedral spin-1/2 chain. Starting from the limit of isolated tetrahedra we analyze the evolution of the ground state energy and the elementary triplet dispersion as a function of the inter-tetrahedral coupling. The quantum phase diagram is evaluated and is shown to incorporate a singlet product, a dimer, and a Haldane phase. Comparison of our results with those from several other techniques, such as density matrix renormalization group, exact diagonalization and bond-operator mean field theory are provided and convincing agreement is found.

TT 25.105 Wed 14:30 P1

Theoretical investigation of the magnetic properties of J-alternating chains of monometallic complexes — •Sebastian Fuchs and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Monometallic complexes containing Ni with spin S=1 can be coupled via nitrit bridges to form chains with variable exchange coupling strengths between the Ni spins. We study the magnetic, i.e susceptibility and effective moment with and without external field, and thermodynamic properties of one particular system with three different couplings controlled through the orientation of the nitrit group. We estimate the relative strenghts of the couplings necessary to model the experimental data. Predictions for possible dynamical properties observable in Neutron scattering experiments are also made.

TT 25.106 Wed 14:30 P1

Novel mean-field theory for strongly disordered non-frustrated antiferromagnets — •Heidrun Weber and Matthias Vojta — Institut fuer Theorie der Kondensierten Materie, Universitaet Karlsruhe, 76128 Karlsruhe, Germany

Quantum paramagnets with elementary spin-1 excitations show magnetic ordering upon introducing non-magnetic impurities: the vacancies produce free spins 1/2 which order antiferromagnetically at low temperatures. We have developed a novel mean-field theory for the impurity degrees of freedom, taking into account the random distribution of coupling constants. In particular, we demonstrate that the conventional first-order spin-flop transition is split into two transitions at low temperatures, associated with seperate order parameters along and perpendicular to the easy axis. We apply our results to impurity-induced order in spin-gap magnets like $TlCuCl_3$.

TT 25.107 Wed 14:30 P1

High-order coupled cluster method calculations for the ground-state of quasi-one-dimensional spin systems — •Ronald Zinke[1], Johannes Richter[1], Jörg Schulenburg[2], and Damian J.J. Farnell[3] — [1]Institut für Theoretische Physik, Otto-von-GuerickeUniversität Magdeburg,P.O.B. 4120, 39016 Magdeburg, Germany — [2]Universitätsrechenzentrum, P.O.B. 4120, 39016 Magdeburg, Germany — [3]Unit Of Ophthalmology, Department of Medicine,University Clinical Departments, Daulby Street,University of Liverpool, Liverpool L69 3GA, United Kingdom

We consider ground-state properties of quasi-1-dimensional quantum Heisenberg antiferromagnets for spin quantum numbers $s = \frac{1}{2}$ and $s = 1$. For the investigation of the ground-state long-range order we calculate the sublattice magnetization using the high order coupled cluster method. We find that for the unfrustrated spin-$\frac{1}{2}$ system an infinitesimal inter-chain coupling $J_\perp$ is sufficient to stabilize magnetic long-range order. This result is in agreement with known results obtained by other methods. For $s = 1$ we find that a finite inter-chain coupling is necessary to stabilize magnetic long-range order, which can be interpreted as a result of the gapped ground-state of the spin-1 chain. The estimated value for the critical inter-chain coupling is: $J_\perp^c \approx 0.1$. Furthermore we consider a spin-$\frac{1}{2}$ system were a frustrating next-nearest neighbor in-chain coupling is included. We find for strong frustration that again a finite inter-chain coupling $J_\perp$ is necessary to stabilize long-range order.

TT 25.108 Wed 14:30 P1

An ab-initio correlation treatment for metals — •Beate Paulus[1], Elena Voloshina[1], Nicola Gaston[1], and Krzysztof Rosciszewski[2] — [1]MPI for the Physics of complex Systems, Dresden, Germany — [2]Institute for Physics, Jagellonian University, Krakow, Poland

Up to now wavefunction-based ab-initio correlation treatements are possible for semiconductors and insulators applying the method of increments. This method corresponds to a many-body expansion of the correlation energy of the solid in terms of localized entities. A generalization is possible for metals, where two major problems have to be faced: First, a straight-forward localization of the orbitals is not possible, localized entities have to be generated via an embedding scheme. The influence of the delocalization on the electronic correlation is treated successively with the incremental scheme [1,2] . Second, the quasi-degeneracy at the Fermi level can no longer be described with a single-reference correlation method. To solve this problem the method of increments is extended to multi-reference correlation methods [3]. First applications to the group II metals magnesium, zinc, cadmium and mercury are presented.

[1] B. Paulus and K. Rosciszewski, Chem. Phys. Lett. 394 (2004) 96.
[2] B. Paulus, K. Rosciscewski, N. Gaston, P. Schwerdtfeger and H. Stoll, Phys. Rev. B 70 (2004) 165106.
[3] B. Paulus, Chem. Phys. Lett.371 (2003) 7.

TT 25.109 Wed 14:30 P1

Electron-Phonon Coupling in $Fe_{1-x}Co_xSi$ as derived from Raman-Spectroscopy — •I. Jursic, T. Donig, A.-M. Racu, D. Menzel, and J. Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

FeSi is a paramagnetic semiconductor which is often viewed as Kondo insulator. $Fe_{1-x}Co_xSi$ becomes a ferromagnetic metal with $0.05 < x < 0.8$ whereas CoSi is a diamagnetic metal.

Raman measurements on $Fe_{1-x}Co_xSi$ with different Co content were performed to investigate the effect of Co doping on the vibrational modes. The system crystallizes in the B20 structure which according to a factor group analysis yields 9 raman-active phonons that are all observed in the experiment.

Polarisation resolved measurements allow the identification of the A-mode. For increasing Co content a change in the intensities and distribution of the vibrational modes is observed. The E- and T-modes shift to higher energies contrary to the expectations. The A-mode shifts to lower energies more than expected. The shift of the modes begins with 10% Co content which is approximately at the insulator to metal transition.

Temperature resolved measurements show that the linewidth of one particular E mode strongly depends on the Co content. This is interpretated in terms of a strong electron-phonon coupling which leads to shorter decay times with increasing Co content and a closure of the energy-gap.

TT 25.110 Wed 14:30 P1

Orbital ordering in the two-dimensional ferromagnetic semiconductor Rb_2CrCl_4 — •Udo Schwingenschlögl and Volker Eyert — Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

We present the results of electronic structure calculations for the two-dimensional ferromagnet Rb_2CrCl_4. They are obtained by the augmented spherical wave method as based on density functional theory and the local density approximation. In agreement with experimental data, Rb_2CrCl_4 is found to be semiconducting and displays long-range ferromagnetic order of the localized Cr $3d$ moments. The magnetic properties are almost independent of the structural modifications arising from a Jahn-Teller instability, which leads from the parent body-centered tetragonal K_2NiF_4 structure to a side-centered orthorhombic lattice. In contrast, our calculations give evidence for a strong response of the optical band gap to the corresponding structural changes.

TT 25.111 Wed 14:30 P1

Role of the structural distortions in the phase diagrams of $RE_{1-x}A_xTiO_3$ (A=Ca,...) — •A. C. Komarek[1], M. Cwik[1], W. D. Stein[1], H. Roth[1], H. Hartmann[1], T. Zabel[1], M. Krienер[1], N. Schittner[1], A. El-Filali[1], M. Hölzel[2], F. Bouree[3], T. Lorenz[1], A. Freimuth[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln — [2]Technische Universität Darmstadt, c/o Technische Universität München — [3]Laboratoire Leon Brillouin, CE-Saclay, F-91191 Gif-sur-Yvette, France

Having one electron in the 3d shell, the rare earth (RE) titanates $RETiO_3$ represent interesting systems to study the complex interplay of orbital and magnetic degrees of freedom as well as to investigate metal-insulator (MI) transitions enabled by hole doping due to a partial substitution of the trivalent rare earth by divalent earth alkaline ions. In the series of rare earth titanates we find an anomalous behaviour of the lattice parameter a for the samples with larger rare earth ions showing antiferromagnetic order. However, with decreasing rare-earth ionic radius the anomalous increase of the lattice constant a gets even more pronounced and sets in closer to the magnetic ordering temperature. The hole-doped system $Y_{1-x}Ca_xTiO_3$ shows a complex phase diagram of structural transitions. The structural changes are accompanied by a MI transition and anomalies in the magnetic susceptibility. We ascribe this complex behavior to the coexistence of an insulating monoclinic phase and a metallic low-temperature orthorhombic phase. Our neutron diffraction data give evidence for a charge ordering in the monoclinic phase.

TT 25.112 Wed 14:30 P1

Charge order induced pseudo gap and phonon anomalies in the superconducting cobaltate Na_xCoO_2 yH_2O — •P. Lemmens[1,2], K.-Y. Choi[3], V. Gnezdilov[4], F.C. Chou[5], C.T. Lin[1], and B. Keimer[1] — [1]MPI-FKF, D-70569 Stuttgart, Germany — [2]IPKM, TU Braunschweig, D-38106 Braunschweig — [3]IMR, Tohoku Univ., Sendai — [4]B.I. Verkin Inst. for Low Temp. Phys., NASU, 61164 Kharkov — [5]CMSE, MIT, Cambridge, MA 02139

We report on the observation of an electronic Raman scattering continuum in nonsuperconducting and superconducting cobaltates Na_xCoO_2 yH_2O. Pronounced phonon anomalies are observed in the proximity of the metal-insulator transition and the charge ordering instabilities in $Na_{0.5}CoO_2$. We analyze the scattering rates as function of composition and emphasis an anomalous non-Fermi liquid like regime for x $\geq$0.5. Work supported by DFG SPP1073, ESF-HFM and MRSEC Program of NSF under award number DMR 02-13282.

TT 25.113 Wed 14:30 P1

Probing orbital moment with resonant soft x-ray diffraction: $La_{1.5}Sr_{0.5}CoO_4$ — •C. Schüssler-Langeheine, C. F. Chang, Z. Hu, M. W. Haverkort, T. Burnus, M. Benomar, M. Braden, and L. H. Tjeng — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Magnetic circular dicroism in x-ray absorption (XMCD) is a well-established technique for the investigation of ferromagnetic materials. From the shape of the XMCD signal across resonance the z-component of the orbital and spin moments can be deduced - in many cases by means of a simple sum-rule analysis. We applied this technique to an antiferromagnetic system, which is Sr-doped La_2CoO_4. For an antiferromagnet the MCD effect cannot be observed in the x-ray absorption signal, where it cancels out, but MCD is also one of the contrast mechanisms leading to resonant magnetic x-ray scattering. For $La_{1.5}Sr_{0.5}CoO_4$ we find a vanishing magnetic diffraction signal at the Co-L_2 resonance, which indicates a large z-component of the orbital moment.

TT 25.114 Wed 14:30 P1

Charge, spin and orbital degrees of freedom in $La_{2-x}Sr_xCoO_4$ — •M. Cwik[1], M. Haider[1], M. Benomar[1], M. Reuther[1], A. Hoser[2], Y. Sidis[3], T. Lorenz[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich — [3]Laboratoire Leon Brillouin (CEA-CNRS), CEA-Saclay, 91191 Gif-Sur-Yvette Cedex, France

The layered cobaltate La_2CoO_4 is an orthorhombic distorted antiferromagnetic insulator with $T_N \sim 270$ K and Co^{2+} ($3d^7$) in the S=3/2 high spin state [1]. The substitution of La^{3+} by larger Sr^{2+} ions reduces the orthorhombic distortion, suppresses long range magnetic order and induces a nominal Co^{2+}/Co^{3+} mixed valency. For $La_{1.5}Sr_{0.5}CoO_4$ a checkerboard-like charge order ($T_c \sim 750$ K) and an antiferromagnetic order ($T_s \sim 30$ K) with the propagation vector Q=(0.25 0.25 1) have been found [2]. We present an analysis of the crystal structure, of the spin and charge order and of the magnetic correlations studied on single crystals for $0.1 \leq x \leq 1.0$. For x = 0.4 the magnetic order is incommensurate but we do not find evidence for a stripe-like ordering scheme similar to the observations in cuprates or nickelates. We interpret the different magnetic ordering , the emerging charge order and the structural anomalies in this system in terms of the Co^{3+} spin degree of freedom, several magnetic interaction parameters and geometrical frustration.

[1] K. Yamada et al., Phys. Rev. B 39, 2236 (1989)
[2] I. A. Zaliznyak et al., Phys. Rev. Lett. 85, 4353 (2000)
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TT 25.115 Wed 14:30 P1

Polarized neutron scattering study of the spin-state transition in $LaCoO_3$ — •M. Cwik[1], M. Kriener[1], M. Reuther[1], L.-P. Regnault[2], K. Schmalzl[2], T. Lorenz[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut Laue-Langevin, F-38042 Grenoble Cedex 9, France

$LaCoO_3$ exhibits a spin state transition around 100 K which is associated with the thermal excitation of Co^{3+} ($3d^6$) ions from a nonmagnetic low-spin ($t_{2g}^6e_g^0$, S=0) to a magnetic spin state without long range order [1]. The nature of this magnetic spin state is still discussed controversially. Depending on the crystal-field splitting, the intra-atomic exchange interaction and the hybridization between Co-3d and O-2p orbitals, the so-called intermediate ($t_{2g}^5e_g^1$, S=1) or the high-spin state ($t_{2g}^4e_g^2$, S=2) could be stabilized. We present an analysis of the magnetic fluctuations in $LaCoO_3$ studied by polarized inelastic neutron scattering measurements performed on a co-mounting of six large single crystals. We find evidence for magnetic correlations in the paramagnetic phase. For a quantitative estimation of the magnetic susceptibility one needs to take these correlations into account. However, with the polarized neutrons we do not find the signal reported in reference [2] which was attributed to the LS-IS transition. In addition we present the results of inelastic neutron scattering studies on the phonon dispersion in $LaCoO_3$.
[1] C. Zobel et al., Phys. Rev. B **66**, 020402(R) (2002)
[2] Y. Kobayashi et al., cond-mat/0504351
This work is supported by the DFG through SFB 608.

TT 25.116 Wed 14:30 P1

Thermodynamic and transport properties of doped La_2CoO_4 — •E Rose[1], N Hollmann[1], J Baier[1], M Benomar[1], K Berggold[1], M Cwik[1], M Kriener[1], D Meier[1], A Tanaka[2], T Lorenz[1], and A Freimuth[1] — [1]II.Physikalisches Institut, Universität zu Köln, Germany — [2]Department of Materials Science, Hiroshima University, Japan

Cobaltates are of special interest due to the possibility of spin-state transitions. This has been studied in detail in the insulator $LaCoO_3$. Strontium doping drives $LaCoO_3$ to a metal and induces ferromagnetic order [1,2]. Much less is known about the layered cobaltates $La_{2-x}Sr_xCoO_4$. We prepared single crystals and present a study of magnetic susceptibility, thermal and electric conductivity as well as thermal expansion and thermopower for a strontium doping range of $0.3 \leq x \leq 0.8$. All samples are insulators in the measured temperature range. The magnetic susceptibility is strongly anisotropic and deviates from Curie-Weiss-behaviour. The susceptibility was analyzed via cluster calculation [3]. Thermal transport measurements in a temperature range from 5K to 300K present a small anisotropy. In fields up to 14 Tesla a weak field dependence is found which is related to the magnetic ordering, in particular for $La_{1.5}Sr_{0.5}CoO_4$. Positive Seebeck coefficients observed at room temperature suggest p-type conduction. Furthermore we studied the effect of physical pressure due to calcium doping.
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[3] Tanaka *et al.*, J. Phys. Soc. Jpn. **63**, 2788 (1994)
Supported by the DFG through SFB 608

TT 25.117 Wed 14:30 P1

Temperature- and doping-induced spin-state transitions of $RCoO_3$ — •K. Berggold, N. Hollmann, M. Reuther, M. Kriener, J. Baier, C. Zobel, A. Reichl, and T. Lorenz — II. Physikalisches Institut, University of Cologne, Germany

$LaCoO_3$ attracts a lot of attention, because it undergoes a temperature-induced spin-state transition. There are different ways to tune this spin-state transition, either to stabilize the low-spin state by replacing La with smaller rare earth ions R, or to suppress it by the introduction of charge-carriers[1,2]. For low doping levels so-called high-spin polarons are formed. We studied the thermal conductivity κ on $RCoO_3$ single crystals with R = La, Pr, Nd, and Eu, as well as on $La_{1-x}Sr_xCoO_3$ with $0 \leq x \leq 0.3$ and find that κ is strongly suppressed by the spin-state transition. Particularly we present magnetic-field dependent measurements for low temperatures to investigate the influence of the high-spin polarons to κ. A low thermal conductivity is one pre-condition to reach large values of the thermoelectric figure of merit ZT, which is necessary for thermoelectric applications. We observe a $ZT^{(max)} \approx 0.03$, which is rather

high for oxides[3]. We also present first measurements of $Eu_{1-x}Sr_xCoO_3$. Here, charge-carrier doping should act differently because of the stabilized low-spin state.

[1] Baier et al., PRB **72**, 155116 (2005)
[2] Kriener et al.,PRB **69**, 094417 (2004)
[3] Berggold et al.,PRB **71**, 014443 (2005)

This work was supported by the DFG through SFB 608

TT 25.118 Wed 14:30 P1

Quantum phase transitions in $Nb_{1-y}Fe_{2+y}$ — •Manuel Brando, Dennis Moroni-Klementowicz, Carsten Albrecht, William Duncan, and F. Malte Grosche — Dept. of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK

The C14 Laves phase $NbFe_2$ is a rare example of low temperature spin density wave order (SDW, $T_N \simeq 10$ K) among the d-metal compounds. Magnetic ordering, which is inferred from magnetic, thermodynamic and magnetoresistive signatures, as well as historic NMR and μSR data, emerges out of a nearly ferromagnetic state with a Stoner enhancement factor of about 150, and is easily suppressed by surprisingly low critical fields $\mu_0 H_c \simeq 0.2 - 0.6$ T.

The low temperature state of $NbFe_2$ can be tuned by slightly modifying the stoichiometry within the narrow Nb-Fe homogeneity range. To the Nb-rich side, a quantum critical point is approached for $y \simeq 0.008$, characterised by non-Fermi liquid temperature dependences of heat capacity and resistivity. On the Fe-rich side, however, the SDW state observed in stoichiometric $NbFe_2$ appears to transform continuously into ferromagnetic ordering for $y > 0.01$.

We present low temperature magnetic, thermodynamic and transport measurements at ambient and high hydrostatic pressure, taken on samples across the homogeneity range, in order to elucidate the unusual magnetic phase diagram of $NbFe_2$. The findings are discussed within the working hypothesis that stoichiometric $NbFe_2$ forms low-$\mathbf{Q}$, long wavelength magnetic order, which transforms continuously towards ferromagnetism ($\mathbf{Q} = 0$) on increasing Fe content.

TT 26 Transport - Poster Session

Time: Wednesday 14:30–18:30 Room: P1

TT 26.1 Wed 14:30 P1

Heat transport in ac-driven nanostructures — •Michael Strass[1], Miguel Rey[2], Sigmund Kohler[1], Fernando Sols[3], and Peter Hänggi[1] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Departamento de Física Teórica de Materiales,Universidad Complutense de Madrid, 28040 Madrid, Spain

The charge transport in nanoscale conductors driven by an external, alternating electric field is subject to many recent studies, whereas the mechanisms of heat transfer of nanoconductors far from equilibrium are fairly unknown. In our model calculations, we consider an ac-driven system connected to two leads. The heat current defined by the energy transfer from one metallic lead to the central region is computed with a Floquet theory making use of the time periodicity of the driving. In particular, thermo-electric effects of a ac-driven two-level system induced by a finite temperature difference in the leads are investigated. Open double-quantum dots represent an ideal realization for those kind of systems. The results obtained by the Floquet approach are compared to a different numerical treatment based on a transfer-matrix method.

TT 26.2 Wed 14:30 P1

Conductance Measurements on Ferromagnetic Breakjunctions — •Magdalena Hüfner, Cécile Bacca, Martina Suty, and Elke Scheer — Universität Konstanz

We investigate lithographically fabricated breakjunctions of ferromagnetic metals. With the help of a three-point bending mechanism, the bridges can be opened and stabilized to a single-atom contact, broken to a vacuum-tunnel contact and closed again repeatedly at low temperatures ($T \leq 4.2$K). We observe steps in the conductance that are due to atomic rearrangements in the contact region [1] and calculate the preferred conductance value of a single Co atom with and without magnetic field. In addition we observe very high magnetoconductance effects up to 150% for single-atom or 500% for tunnel contacts in magnetic fields up to 5 T and perpendicular to the sample plane. We analyze the magnetoconductance as a function of the symmetry of the contact and of the free-standing bridge length. We developed a sample preparation method for samples the leads of which are made up of different materials than the contact itself and calculated [2] the magnetization state as a function of the geometry of the contact, the film thickness and its magnetic history. First results are presented.

[1] J.M. Krans et al. Nature 375, 767 (1995)
[2] M.J. Donahue and D.J. Porter, OOMMF's User Guide (see http://math.nist.gov/oommf)

TT 26.3 Wed 14:30 P1

Analytic and numeric Green's functions for a two-dimensional electron gas in an orthogonal magnetic field — •Alessandro Cresti[1,2], Giuseppe Grosso[2], and Giuseppe Pastori Parravicini[3] — [1]NEST-INFM and Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy — [2]NEST-INFM and Dipartimento di Fisica 'E. Fermi', Universita' di Pisa, Largo Pontecorvo 3, I-56127 Pisa, Italy — [3]NEST-INFM and Dipartimento di Fisica 'A. Volta', Universita' di Pavia, Via A. Bassi 6, I-27100 Pavia, Italy

We have derived closed analytic expressions for the Green's function of an electron in a two-dimensional electron gas threaded by a uniform perpendicular magnetic field, also in the presence of a uniform electric field and of a parabolic spatial confinement. A workable and powerful numerical procedure for the calculation of the Green's functions for a large infinitely extended quantum wire is considered exploiting a lattice model for the wire, the tight-binding representation for the corresponding matrix Green's function, and the Peierls phase factor in the Hamiltonian hopping matrix element to account for the magnetic field. The numerical evaluation of the Green's function has been performed by means of the decimation-renormalization method, and quite satisfactorily compared with the analytic results worked out in this paper. As an example of the versatility of the numerical and analytic tools here presented, the peculiar semilocal character of the magnetic Green's function is studied in detail because of its basic importance in determining magneto-transport properties in mesoscopic systems.

TT 26.4 Wed 14:30 P1

A Setup to measure the influence of defects on conductance fluctuations in metallic nanowires — •Michael Wolz, Vojko Kunej, Christian Debuschewitz, and Elke Scheer — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

The goal of the project is to investigate the influence of individual artificial defects on the conductance fluctuation of metallic nanowires. An STM working in a conventional cryostat at 4 K and in magnetic fields up to 1 T has been developed for creating the defects. In order to position the sample with respect to the STM tip the system is equiped with an x-y-table. The nanostructures are fabricated by electron beam lithography and reactive ion etching [1]. The accessibility of the samples by the STM tip is realized by shadow evaporation of the metal (Au) onto the substrate. First low-temperature transport measurements are presented.

[1] T. Hoss et al., Physica E 14 (2002) 341

TT 26.5 Wed 14:30 P1

Electron transport and current fluctuations in short coherent conductors — •Dmitry Golubev, Artem Galaktionov, and Andrei Zaikin — Forschungszentrum Karlsruhe, Institut fuer Nanotechnologie, 76021 Karlsruhe, Germany

Employing a real time effective action formalism we analyze electron transport and current fluctuations in comparatively short coherent conductors in the presence of electron-electron interactions. We demonstrate that, while Coulomb interaction tends to suppress electron transport, it may *strongly enhance* shot noise in scatterers with highly transparent con-

ducting channels. This effect of excess noise is governed by the Coulomb gap observed in the current-voltage characteristics of such scatterers. Our results illustrate a direct relation between electron-electron interaction effects and current fluctuations in disordered mesoscopic conductors.

TT 26.6 Wed 14:30 P1

The role of contacts in transport through Luttinger liquid — •Katharina Janzen, Volker Meden, and Kurt Schönhammer — Friedrich Hund Platz 1 , 37077 Göttingen

We investigate how the linear conductance through a clean Luttinger liquid (quasi one-dimensional quantum wire of correlated electrons) is effected by the contacts. Two models are studied. In the first the inhomogeneous system is described by an effective hydrodynamic model (local Luttinger liquid) obtained from bosonization. Within this approach analytical results can be obtained that generalize earlier findings. In addition, we study a microscopic lattice model applying the functional renormalization group method. This allows a more detailed analysis of problem.

TT 26.7 Wed 14:30 P1

Anomalies in Coupled Quantum Chains as resonances of the bands — •Luca Alloatti[1] and Giuseppe Grosso[2] — [1]Max-Planck Institut fuer Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [2]NEST-INFM and Dipartimento di Fisica "E. Fermi", Universita' di Pisa, Via F. Buonarroti 2, I-56127 Pisa, Italy

We consider the disordered quasi-one-dimensional single particle tight-binding hopping model and we show that the anomalies in the density of states, in the mean conductance and the even-odd effect are related to a resonance of the band structure of the perfect system underlying the disorder and not necessarily to the E=0 point. For the one-dimensional case we calculate the coefficients of the perturbation expansion of the mean conductance up to the twelfth order for both the pure diagonal and real off-diagonal disorder. This calculation evidences a profound difference between the two cases. In the case of two coupled chains we calculate the same expansion to the the fourth order and for general disorder. This is sufficient to make important predictions well verified numerically.

TT 26.8 Wed 14:30 P1

Zeeman Ratchets for Ballistic Spin Currents — •Matthias Scheid, Dario Bercioux, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

We investigate the possiblity of creating directed spin-polarized currents in a two-dimensional electron gas (2DEG) subject to an asymmetric, spatially-periodic magnetic field and an external adiabatic rocking. Thereby we generalize concepts of quantum charge ratchets [1] to the case with spin. Due to the Zeeman term in the Hamiltonian, spin-up and spin-down electrons experience different effective potentials which can be taylored to achieve net spin currents without corresponding charge currents. We consider ballistic, coherent transport in waveguides defined on a 2DEG, where the magnetic field modulation is, e.g., induced from a periodic array of ferromagnetic stripes on top of the 2DEG.

[1] H. Linke, T. E. Humphrey, A. Löfgren, A. O. Sushkov, R. Newbury, R. P. Taylor and P. Omling, Science **286**, 2314 (1999)

TT 26.9 Wed 14:30 P1

Dephasing by transverse gauge field fluctuations — •Thomas Ludwig[1] and Alexander D. Mirlin[1,2] — [1]Institut fuer Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Institut fuer Theorie der Kondensierten Materie, Universitaet Karlsruhe, 76128 Karlsruhe, Germany

We consider the effect of transverse gauge field fluctuations on quantum interference effects in lowdimensional disordered systems. Using a purely diffusive description we reproduce a logarithmic correction to the dephasing rate of the Cooperon in two dimensions first found by Wölfle (2000). In addition, we present new results for the wire geometry where we find a dephasing rate linear in the temperature. Finally, we examine the difference between the dephasing rate due to slow gauge field fluctuations (with frequencies smaller than the dephasing rate) and the dephasing rate due to fast fluctuations (with frequencies larger than the dephasing rate).

TT 26.10 Wed 14:30 P1

Time-dependent Numerical Renormalization Group for Multi-Level Quantum Dots — •David Roosen and Walter Hofstetter — Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Germany

During the last years Kondo phenomena have been realized in a controlled way in quantum dots with odd and even electron number [1]. Recent extensions of the Numerical Renormalization Group (NRG) [2] allow non-perturbative calculations of time-dependent phenomena in the Kondo regime. Here we investigate a two-level lateral quantum dot, taking into account Hund's rule coupling. For this system it has been shown that a singlet-triplet Kondo effect occurs as a function of the level spacing [3]. Applying the time-dependent NRG algorithm of [2], we focus on the evolution of the system after a sudden change in the Hamiltonian, driving the quantum dot from the singlet to a triplet ground state.

[1] D. Goldhaber-Gordon et al., Nature **391**, 156 (1998)
[2] F. Anders and A. Schiller, cond-mat/0505553
[3] W. Hofstetter and H. Schoeller, Phys. Rev. Lett. **88**, 016803 (2002)

TT 26.11 Wed 14:30 P1

Flow equation method for the non-equilibrium Anderson Impurity Model — •Michael Möckel and Stefan Kehrein — LMU München, Lehrstuhl für Theoretische Festkörperphysik,Theresienstraße 37, D-80333 München, Germany

The Anderson impurity model is of central importance in correlated electron physics and is often used as a minimal model for studying quantum dots with Coulomb blockade effects. Steady state non-equilibrium behaviour can be obtained by applying a constant voltage bias across the impurity site. We examine this steady state by means of the flow equation method at zero temperature in the regime of weak to medium correlation strength.

In particular, we study the impurity orbital density of states and the decay of the quasi-particle resonance far away from equilibrium due to current-induced decoherence.

TT 26.12 Wed 14:30 P1

A diagrammatic approach to adiabatic pumping — •Janine Splettstoesser[1,2], Michele Governale[1,2], Jürgen König[2], and Rosario Fazio[1] — [1]Scuola Normale Superiore, Piazza dei Cavalieri, I-56126 Pisa — [2]Institut für Theoretische Physik, Ruhr-Universität Bochum, D-44780 Bochum

We consider adiabatic charge pumping through an interacting single-level quantum dot. We present a general perturbation theory approach for the adiabatic expansion using a diagrammatic technique [1,2] and apply it to the pumped current up to second order Γ contributions in the self energy. It turns out that second leading order contributions of the perturbation expansion of the adiabatically pumped charge are exclusively due to level renormalization effects.

[1] J. König, H. Schoeller, and G. Schön, Phys. Rev. Lett.**76**, 1715 (1996).

[2] J. König, J. Schmid, H. Schoeller, and G. Schön, Phys. Rev. B **54**, 16820 (1996)

TT 26.13 Wed 14:30 P1

Transport properties of a single electron transistor strongly coupled to a nanomechanical resonator — •Charles Doiron[1], Wolfgang Belzig[2], and Christoph Bruder[1] — [1]Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

It is now experimentally possible to create nanometer-sized mechanical resonators and to couple them to quantum point contacts or single electron transistor (SET) to study their behaviour.

Previous theoretical studies of the coupled nanomechanical resonator-SET system have focused on the regime where the coupling between the resonator and the SET is weak. In this regime the electrons tunneling trough the SET act like an effective thermal bath, effectively damping the motion of the oscillator [1]. Until now, the strong coupling regime has not been investigated theoretically.

In this work, we use a master-equation approach to describe the coupled SET-nanomechanical resonator system in the strong coupling regime. We compute the dynamics of the resonator as well as the effect of the coupling on the current and noise characteristics of the SET.

[1]A. D. Armour, M. P. Blencowe, and Y. Zhang, Phys. Rev. B **69**, 125313 (2004)

TT 26.14 Wed 14:30 P1

Rabi spectroscopy in a qubit-oscillator system — •Julian Hauss, Alexander Shnirman, and Carsten Hutter — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

In recent years coherent control of JJ-qubits was demonstrated in many experiments. A promising approach towards efficient non-demolition measurement of a JJ-qubit is the readout via a harmonic oscillator coupled to the qubit. In particular, Rabi spectroscopy experiments in such systems were carried out in Jena.

We analyzed theoretically the Rabi spectroscopy in a qubit-oscillator system. We studied the contributions of one- and two-photon processes to the spectroscopic signal and made a comparison with the experimental results.

TT 26.15 Wed 14:30 P1

Creating microwave photon pairs in superconducting cavity QED — •Florian Marquardt — Sektion Physik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München

With the recent advent of superconducting cavity quantum electrodynamics [1], circuit architectures become possible that process and store quantum information in the form of microwave photons traveling along transmission lines on a chip, interacting with superconducting qubits.

In this talk, I will present and theoretically analyze a setup that may be used to create microwave photon pairs with a very high efficiency. The basic mechanism is parametric down conversion, and the necessary nonlinearity is provided by a charge qubit coupled to a cavity. The main advantage of the scheme is achieved by the fact that the qubit acts as an artificial atom whose parameters are fully tunable and can be optimized. Non-idealities such as non-radiative relaxation and dephasing of the qubit are taken into account employing a Lindblad master equation approach.

[1] A. Wallraff et al., Nature **431**, 162 (2004).

TT 26.16 Wed 14:30 P1

Information transfer in permanently coupled spin chains — •Daniel Burgarth[1], Sougato Bose[1], and Vittorio Giovannetti[2] — [1]Department of Physics & Astronomy, University College London, Gower St., London WC1E 6BT, UK — [2]NEST-INFM & Scuola Normale Superiore, piazza dei Cavalieri 7, I-56126 Pisa, Italy

The transfer of quantum information is a crucial part of any quantum computation. Recently it was suggested to use permanently coupled systems for transferring quantum states. This is especially important in solid state implementations (such as flux qubits) where dynamical control of the couplings is difficult to implement. However, in many cases using permanent couplings leads to dispersion and low fidelity. A proper choice of the coupling strengths overcomes this problem, but may be too difficult to engineer. We suggest a scheme that allows arbitrarily perfect state transfer even in the presence of random fluctuations in the couplings of a quantum chain. Hence our scheme puts minimal demand not only on the control of the chains when using them, but also on the design when building them. No control is required along the transmission line, but the sender and receiver have to be able to perform quantum gates and measurements.

TT 26.17 Wed 14:30 P1

Phase-space theory for nonlinear detectors of superconducting qubits — •Ioana Serban and Frank Wilhelm — Department Physik. Arnold-Sommerfeld-Center for Theoretical Physics, and Center for Nanoscience, Ludwig-Maximilians-Universitaet, Theresienstr. 37 80333 Muenchen, Germany

Superconducting circuits are envisioned as quantum bits and demonstrate quantum-coherent features i.e. Rabi oscillations and Ramsey fringes. The detector (e.g. a superconducting quantum interference device) can itself be described by a Hamiltonian and treated quantum-mechanically.This allows more insights into the measurement process.

Several experimental groups have realized good detectors with strong coupling to the measured system, where nonlinear dynamics plays a significant role.

Motivated by the recent experiment [1], we study a nonlinear detector where the qubit couples to the square amplitude of a driven oscillator, which can be used for dispersive detection. We use a complex-environment approach treating the qubit and the oscillator exactly, expressing their full Floquet-state master equations in phase space. We investigate the backaction of the environment on the measured qubit and explore the resolution of measurement. We emphasize the resulting role of non-Gaussian and non-Markovian effects in the backaction including significant non-exponential shape of the coherence decay.

[1] A. Lupaşcu et al. PRL 93 177006 (2004)

TT 26.18 Wed 14:30 P1

Microwave spectroscopy on single Josephson junctions — •Karl Madek, Sven Beutner, Renke Stolle, Christian Probst, Achim Marx, and Rudolf Gross — Walther-Meißner-Instiut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

In recent years, interest in quantum computing has been continuously growing. Because of the superconducting energy gap, superconducting devices are promising candidates for qubits with sufficiently large decoherence times.

A prerequisite for the investigation of qubits is a suitable low noise experimental set-up. Performing escape rate measurements on single Josephson junctions with and without microwave irradiation is a convenient way to both test the set-up and establish the experimental methods to manipulate qubits.

Our escape temperature measurements on an SIS tunnel junction without microwave irradiation are in good agreement with theory. They show a crossover from the thermal to the quantum regime and thus prove the negligibility of system noise. In spectroscopic measurements, the junction was excited by single and multiple microwave photons, showing the quantization of the energy levels in the tilted washboard potential. From the experimental results, the intrinsic junction parameters (critical current, plasma frequency) could be determined with high accuracy. Currently, we are performing escape rate measurements on "0"- and "π"SIFS junctions.

This work was supported by the DFG through SFB 631.

TT 26.19 Wed 14:30 P1

SIS and SIFS niobium Josephson junctions for superconducting flux qubits — •Georg Wild, Bernhard Huber, Tobias Heimbeck, Karl Madek, Matteo Mariantoni, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Superconducting loops containing Josephson junctions (JJ) are among the most promising candidates for the implementation of quantum computation systems. Unfortunately, the operation point of such a persistent current qubit (PCQB) is around half an applied flux quantum, which is hard to be applied stably and uniformly for systems consisting of a large number of PCQBs. A possibility to circumvent this problem is to insert π-phase-shift elements into the qubit loop. These may be implemented by superconductor/ferromagnet/superconductor (SFS) JJ, where the correlated electron-hole-pairs created by Andreev reflection are modified by the magnetic exchange interaction.

The quality of niobium based Josephson junctions depends crucially on the properties of the relevant interfaces. Therefore, we have developed an in-situ multilayer process to prepare $Nb/AlO_x/Ni_{0.18}Pd_{0.82}/Nb$ stacks. A mesa is defined in the top layers using optical lithography and RIE. After deposing an isolating SiO_2 layer the top niobium electrode is contacted. Transport measurements on SIS and SIFS junctions have been performed to characterize Josephson coupling.

This work was supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft.

TT 26.20 Wed 14:30 P1

Experimental Realization and Testing of Microwave Beam Splitters — •Andreas Emmert[1], Matteo Mariantoni[1], Henning Christ[2], Enrique Solano[2,3], Markus J. Storcz[4], Frank K. Wilhelm[4], Achim Marx[1], and Rudolf Gross[1] — [1]Walther-Meissner-Institut, Walther-Meissner-Str. 8, D-85748 Garching, Germany — [2]Department Physik, ASC and CeNS, Ludwig-Maximilians-Universität, Theresienstr. 37, D-80333 München, Germany — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany — [4]Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado 1761, Lima, Peru.

Balanced quantum homodyne detection and tomography are powerful techniques which allow for the entire Wigner function reconstruction of weak quantum signal in the optical and microwave domains. In both domains, the central device of these schemes is a balanced and lossless

beam splitter. As recently proposed [1] (see also presentation TT 19, E. Solano), at microwave frequencies a beam splitter can be implemented on a chip by means of a so-called hybrid ring.

We report on the realization and measurement of the characteristic S-parameters of microwave beam splitters made of Niobium thin films, in a coplanar wave guide design. In particular, the coupling and isolation properties of this device have been experimentally tested. The simple design architecture is suitable for a large scale production. This work was supported by the SFB 631 of the DFG.

[1] M. Mariantoni *et al.*, cond-mat/0509737.

TT 26.21 Wed 14:30 P1

Coupled Josephson Phase Qubits — •T. Wirth[1], J. Lisenfeld[1], A. Lukashenko[1], S. Shitov[2], and A.V. Ustinov[1] — [1]Physikalisches Institut III, Universität Erlangen, Germany — [2]Institute of Radio Engineering and Electronics, Moscow, Russia

Solid-state quantum bits based on current-biased Josephson junctions have recently been shown as very promising. They require appropriate isolation from the bias leads which can be achieved by the use of superconducting transformers. The resulting rf-SQUID has a double-well potential, where the discrete quantum levels in one well can be used as qubit states. State-dependent tunneling to the other well changes the magnetic flux in the qubit, which is measured by a dc-SQUID. We experimentally demonstrate the preparation of an arbitrary quantum state using nanosecond long microwave pulses and observe Rabi oscillations using samples fabricated by a standard foundry. Another crucial point is the coupling of qubits, which we currently study in a system of two capacitively coupled flux-biased phase qubits. Our ongoing experiments are focused on spectroscopic measurements of the coupling strength and the demonstration of coherent interaction in the time domain by observing antiphase oscillation of the two-qubit states at the degeneracy point.

TT 26.22 Wed 14:30 P1

Implementation of two-cell flux qubits — •A. K. Feofanov, A. A. Abdumalikov, and A. V. Ustinov — Physikalisches Institut III, UniversitätErlangen-Nürnberg, Erlangen, Germany

The standard flux qubit implemented at Delft [1] consists of a superconducting loop with three Josephson junctions and features a double well potential at half frustration. Its limitation is that the barrier height cannot be changed without breaking the symmetry. An alternative device proposed by Yukon [2] is a two-cell flux qubit containing four junctions. One of the useful properties of Yukon's qubit is that the barrier height can be controlled without violating the symmetry of the potential, which in turn permits implementation of geometric quantum computation using a Cirac-Zoller [3] type of bus. We have established a technological process for fabricating two-cell qubits based on sub-micron Al-AlO_x-Al Josephson tunnel junctions with a critical current density around 500 A/cm^2. We have also developed a design for reading out such qubits using inductive coupling. Results reflecting actual progress in this experiment will be presented.

[1] I. Chiorescu et al., Science **299**, 1869 (2003)
[2] S.P. Yukon, Physica C **368**, 320 (2002)
[3] J.I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995)

TT 26.23 Wed 14:30 P1

Long Josephson junction filters for qubit control — •H. H. Eglmeier[1], A. Kemp[1], V.S. Kaplunenko[2], and A. V. Ustinov[1] — [1]University of Erlangen-Nuremberg — [2]Stanford linear accelerator, metrol magnetic measurement

Josephson junctions have been demonstrated to perform as macroscopic quantum systems with a well-controlled Hamiltonian. Most superconducting qubits require magnetic flux control for their operation. One choice is to use rapid single flux quantum (RSFQ) logic for qubit control and interfacing with room temperature electronics.

Decoherence due to 1/f noise in the RSFQ circuitry leads to the need for efficient low-frequency isolation between the control circuitry and the qubit. We present characterization measurements and simulations of a novel low-pass filter based on a long Josephson junction.

An input signal fed into the long junction is transmitted only if its frequency exceeds the plasma frequency of the junction, otherwise it is attenuated as an exponentially vanishing (evanescent) wave. For qubit control one can use low frequency signals which are only transmitted as multiples of the flux quantum. The transmission properties of the filter in the GHz range are currently investigated experimentally.

TT 26.24 Wed 14:30 P1

Preparation and readout of bistable vortex states in a long annular Josephson junction containing a lithographic microshort. — •Alexander Kemp, Astria Price, and Alexey V. Ustinov — Physikalisches Institut III, Universitaet Erlangen-Nuernberg, Erlangen D-91058, Germany

We demonstrate classical state preparation and readout for a novel type of vortex qubit, in which a short section of the insulating barrier of a long annular Josephson junction is made slightly wider. This section of the junction acts like a microshort, where the height of the potential barrier so created can be tuned during experiment by varying the strength of an applied in-plane magnetic field. We develop a model for the double well potential, based on the one-dimensional sine-Gordon equation, in which the change in vortex rest mass energy due to the wider section of the junction is explicitly considered, and find the magnetic field dependence of the barrier height. Good agreement with measured vortex depinning currents from each well is obtained. The vortex was prepared in a given well by applying a series of "shaker" bias current pulses to the junction.

TT 26.25 Wed 14:30 P1

Frequency dependence of full counting statistics in AC-biased mesoscopic conductors — •Dmitry Bagrets[1] and Fabio Pistolesi[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128, Karlsruhe, Germany — [2]Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS-UJF B.P. 166, F-38042 Grenoble, France

We develop a theory to obtain the current noise and the full counting statistics of charge transfer for AC biased mesoscopic conductors. We illustrate the theory by considering two specific examples: a diffusive wire and a chaotic quantum dot. We find that all cumulants of current fluctuations depend on the frequency Ω of the external AC field on the scale of the inverse diffusion time through the structure. This dependence stems from the multiple photon absorption processes and disappears when the AC voltage amplitude V is much smaller than $\hbar\Omega/e$ (e being the electron charge). The detection of the frequency dependence of the second cumulant, the current noise, is within reach of present experimental technology.

TT 26.26 Wed 14:30 P1

Full Counting Statistics of an Aharonov-Bohm Interferometer with an embedded Quantum Dot — •Daniel Urban and Jürgen König — Ruhr-Universität Bochum, 44780 Bochum, Germany

The electron's wave nature becomes apparent in Aharonov-Bohm interferometers, where constructive and destructive interference between two electron paths can be observed. The visivility of the Aharonov-Bohm signal provides information on the coherence of transport channels.

Correlations of electron transport are reflected in shot noise and higher moments of the current distribution. These reveal infomation not contained in the average current. All moments can be conveniently extracted from the Cumulant Generating Function, whose calculation is the aim of Full Counting Statistics (FCS).

Originally developed for situations without interaction FCS has recently been extended to strongly interacting systems such as quantum dots. Treating the coupling to the leads perturbatively, it was found that non-Markovian effects cannot be neglected [1]. We expand this scheme to describe a quantum dot embedded in an Aharonov-Bohm geometry.

[1] A. Braggio, J. König, and R. Fazio, cond-mat/0507527, submitted to Phys. Rev. Lett.

TT 26.27 Wed 14:30 P1

Revealing entanglement of spin qubits with counting statistics — •Holger Schaefers and Walter T. Strunz — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

We investigate two electron spin qubits in quantum dots. The spins are measured by separate currents through the dots. Our approach is based on quantum trajectories, widely used in quantum optics, here adapted to describe conditional quantum dot dynamics in a fermionic environment. We use the quantum trajectory approach to simulate the quantum dynamics conditioned on the continuous measurement outcome, here the electron currents through the dots. We propose a simple experiment and give a sufficient criterion for revealing entanglement with the help of counting statistics.

TT 26.28 Wed 14:30 P1

Molecular conductance from ab initio calculations: self energies and absorbing boundary conditions — •Andreas Arnold[1] and Ferdinand Evers[2] — [1]Institut für Theorie der kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Calculating an exact self energy for ab initio transport calculations relevant to *Molecular Electronics* can be troublesome. Errors or insufficient approximations made at this step are a frequent reason why many molecular transport studies become inconclusive. We propose a simple and efficient approximation scheme, that follows from interpreting the self energy as an absorbing boundary condition of an effective Schroedinger equation. Our approximation is controlled by a small parameter, which essentially is the inverse number of electrode atoms, that are kept in the ab initio calculation.

The method is illustrated using a tight binding wire as a toy model, for which an analytical solution is available, against which we can check our numerical results. Also more realistic applications for transport calculations based on the density functional theory have been performed. They yield results in very good agreement with the conventional way to set up the electronic self energy.

TT 26.29 Wed 14:30 P1

Structure and conductance histogram of atomic-sized Au contacts — •Markus Dreher[1], Fabian Pauly[2], Jan Heurich[2], Carlos Cuevas[2,3], Elke Scheer[1], and Peter Nielaba[1] — [1]Physics Department, University of Konstanz, 78457 Konstanz, Germany — [2]Institut für Theoretische Festkörperphysik, University of Karlsruhe,76128 Karlsruhe, Germany — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic for the corresponding material. The origin of these peaks still remains as an open problem. In order to shed some light on this issue, we present a theoretical analysis of the conductance histograms of Au atomic contacts. We have combined classical molecular dynamics simulations of the breaking of nanocontacts with conductance calculations based on a tight-binding model. This combination gives us access to crucial information such as contact geometries, forces, minimum cross section, total conductance and transmission coefficients of the individual conduction channels.

The ensemble of our results suggests that the low temperature Au conductance histograms are a consequence of a subtle interplay between mechanical and electrical properties of these nanocontacts. At variance with other suggestions in the literature, our results indicate that the Au conductance histograms are not a simple consequence of conductance quantization or of existence of exceptionally stable radii.

TT 26.30 Wed 14:30 P1

Absence of fractional conductance quantization in ferromagnetic atomic contacts — •Michael Häfner[1], Juan-Carlos Cuevas[1,2,3], Janne Viljas[1], Diego Frustaglia[3], and Fabian Pauly[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Quantum Transport and Information, Scuola Normale Superiore, 56126 Pisa, Italy

In this work we present a theoretical analysis of the current through atomic contacts of ferromagnetic materials (Co and Ni). Several experimental groups have recently reported the observation of half-integer conductance quantization in nanowires of these materials. This suggests that the current in these contacts is completely spin polarized and all the contributing channels are perfectly transmissive. In order to analyze these surprising observations, we have performed conductance calculations of Ni and Co atomic junctions based on a tight-binding model. Contrary to these experiments, we find that the conductance is in general neither quantized nor spin polarized. We show that the transport is mainly dominated by both the s and d bands close to the Fermi energy. These bands give rise to several conduction channels that are partially open. Typically, both spin bands give a significant contribution to the transport suggesting that the fractional conductance quantization should not appear in ferromagnetic atomic contacts.

TT 26.31 Wed 14:30 P1

Influence of vibrations on electronic transport through DNA — •Benjamin Schmidt[1,2], Matthias Hettler[2], Gerd Schön[1,2], E.B. Starikov[2], and Wolfgang Wenzel[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Conductance measurements on DNA 'wires' display various types of behavior ranging from insulating over semi-conducting to quasi-metallic, depending on the measurement setup and the measured DNA molecule. The variance of the experimental results as well as ab-initio calculations suggest that the environment and vibrational modes of DNA have a dominating influence on the transport properties of DNA wires. In this work we study transport through simple models of homogeneous DNA wires (poly-DNA) using standard Green function technique and Landauer-Buettiker formalism. In particular, we address the influence of specific DNA vibrational modes (with parameters determined by ab-initio methods) on transport in the presence of an environment described by a general bosonic bath. We can describe the crossover from semi-conducting to quasi-metallic behavior in dependence of temperature and the electronic coupling to the vibrational modes and bath.

TT 26.32 Wed 14:30 P1

Influence of Adsorbates on the Structure and Electronic Properties of Molecular-size Junctions — •Sören Wohlthat[1], Fabian Pauly[1], Janne Viljas[1], Juan-Carlos Cuevas[2,1,3], and Gerd Schön[1,3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe

During the last few years, the conduction properties of molecuar-size contacts between two metallic leads have attracted a great deal of attention. Motivated by recent experiments concerning the effect of hydrogen [1] and oxygen [2] on metallic nanocontacts, we investigate theoretically the influence of adsorbates on this type of junctions. We analyse the stability of different geometries and determine their electronic transport properties. The calculations are based on density functional theory (DFT) using the quantum chemistry package TURBOMOLE. The electronic transport properties are obtained by non-equilibrium Green's function (NEGF) techniques. Our simulations show that adsorbates have a significant influence on the properties of our molecular-size junctions and that they could serve as design tools for future atomic and molecular circuits.

[1] R.H.M. Smit et al., Nature 419, 906, (2002).
[2] W.H.A. Thijssen et al., cond-mat/0509376.

TT 26.33 Wed 14:30 P1

First-principles study of single row Al and Pt wires — •Thomas Gnielka[1,2], Klaus-Peter Bohnen[1], and Rolf Heid[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — [2]Universität Karlsruhe, Fakultät für Physik, D-76128 Karlsruhe

Over the past several years there has been a great deal of interest in the physical properties of atomic wires. Although there have been some studies of the structural and electronic properties of nanowires so far lattice dynamics of these systems has been hardly studied. This is in strong contrast to the importance of lattice dynamics for structural stability (Peierls transition) and superconductivity. Thus we have investigated the lattice dynamics, the atomic and electronic structures and the relation between them for single-row Al and Pt wires using density-functional theory. The calculations reveal that the wires transform from planar zigzag structure to linear and further to dimerized wires during elongation. Phonon dispersions have been calculated and anomalies nicely correlate with Fermi surface nesting effects. Dimerization effects as seen for Pt wires on Ge(100) seem to be qualitatively in agreement with these findings, however the substrate influence has still to be studied. Prelimenary results seem to indicate the importance of substrate effects.

TT 26.34 Wed 14:30 P1

Transport properties of carbon nanotubes synthesized by chemical vapor deposition — •T. Pietsch, I. Mönch, J. Schumann, K. Biedermann, H. Vinzelberg, and B. Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The electrical properties of multiwalled carbon nanotubes (MWCNT) synthesized by chemical vapor deposition (CVD) depend on the used CVD method. In this work we investigate MWCNT with outer diameters from 30 to 60 nm and length over 6 μm grown by a thermal-catalytic CVD method. TEM images show that the concentric layers of the nanotubes are not perfect. The MWCNT devices for the transport measurement with low ohmic contacts were prepared by using an ac-electrophoresis deposition either on Ti-microfinger structures followed by a HV annealing at 800°C or on oxidized silicon wafers with prestructured leads, electron beam lithography, oxygen plasma treatment and evaporated Cr/Au contacts on the nanotubes. The contact resistance are for the Ti contacts about 50 kΩ and for the Cr/Au contacts smaller than 1 kΩ. The average intrinsic room temperature resistance of the MWCNT measured in four-point configuration is 1500 $\mu\Omega$cm and comparable to that of natural graphite of 1350 $\mu\Omega$cm. At room temperature the current-voltage characteristics are linear but at low temperatures not linear. The temperature coefficient of the zero-bias resistance in the temperature range between 300K and 4.2K is negative. Positive magnetoresistances at 4.2K of about 2 % at 8T were measured. The results show that - caused by the defect structure of the MWCNT walls - the conduction is diffusive.

TT 26.35 Wed 14:30 P1

Transport through molecules — •Bernd Briechle, Simon Verleger, and Artur Erbe — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

The aim of our studies is the characterisation of electronic transport through a single or a few molecules. It is important that the coupling of the molecules to the electrodes is mechanically and electronically stable throughout the experiment. As a first step two different structures allowing for the change of the mechanical coupling will be analysed to find an optimal configuration. On the one hand a mechanically controllable break-junction (MCB) technique will be studied, on the other a shadow evaporation technique based on a silicon structure will be tested. Transport through the molecules can be investigated at different temperatures. Additionally the integration of a gate electrode for detailed characterisation of the charge transport is in preparation.

TT 26.36 Wed 14:30 P1

Hofstadter butterfly of carbon nanotubes — •Norbert Nemec and Gianaurelio Cuniberti — Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg

The electronic spectrum of a two dimensional square lattice in a perpendicular magnetic field, known as Hofstadter butterfly, was discovered in Regensburg thirty years ago [1]. We have calculated the Hofstadter butterfly for carbon nanotubes (CNTs) in the tight-binding approximation. For the case of single wall CNTs, it is straightforward to implement magnetic fields parallel to the tube axis by means of zone-folding in the graphene reciprocal lattice. We have also studied perpendicular magnetic fields which, in contrast to the parallel case, lead to a much richer, non-periodic spectrum. Moreover, we have investigated magnetic fields piercing double-wall CNTs and found strong signatures of intershell interaction in the resulting butterfly-spectrum. Ubiquitous to all perpendicular magnetic field spectra is the presence cusp-catastrophes at specific values of energy and magnetic field. At these particular points, the electronic wave function can be correspondingly visualized.
[1] D. Hofstadter, Phys. Rev. B 14, 2239 (1976)

TT 26.37 Wed 14:30 P1

Signatures of vibron-assisted transport in DNA molecular wires — •Rafael Gutierrez[1], Sudeep Mandal[1], Soumya Mohapatra[1], Danny Porath[2], and Gianaurelio Cuniberti[1] — [1]Molecular Computing Group, University of Regensburg, D-93040 Regensburg, Germany — [2]Physical Chemistry Department, The Hebrew University, 91904, Jerusalem, Israel

We investigate the coupling of tunneling charges to intrinsic or extrinsic vibrational degrees of freedom in model Hamiltonians which effectively mimic the low-energy electronic structure of DNA molecular wires. We especially discuss two cases: (i) interaction with an external dissipative bosonic bath, and (ii) coupling to intrinsic vibrational modes. The first case can be relevant to experiments in aqueous solution, see e.g. B. Xu et al., Nano Lett. 4, 1105 (2004). The second case takes into account the influence of intrinsic dynamical fluctuations of the double helix on a propagating charge. Our results suggest that in the recent experiments of H. Cohen et al., Proc. Natl. Acad. Sci. (USA) 102, 11589 (2005) on short suspended DNA wires, vibrational modes might give a non-negligible contribution in determining the measured high currents.

TT 26.38 Wed 14:30 P1

Effects of chemical substitution on quantum transport through single aromatic molecules — •Florian Pump[1], Alessandro Pecchia[2], Aldo Di Carlo[2], and Gianaurelio Cuniberti[1] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]INFM and Department of Electronic Engineering, University of Rome "Tor Vergata"I-00133 Rome, Italy

Recent experimental investigations show that the measurement of unimolecular transport is possible. Still, signatures of truly molecule-mediated quantum transport have to be selectively identified in experiments and their theoretical mechanisms need to be understood. Such signatures can be obtained by separating an aromatic molecule into two electronically different parts. This can be attained by the substitution of certain H-atoms asymmetrically on one side of phenylene ethynylene based molecules by atoms with larger electronegativity (e.g. F). Then, the π-conjugation can be broken by means of steric repulsion groups like NO_2 and/or CH_3. Depending on the position of these groups on the molecule, it is possible to further engineer electrical dipoles able to incrementally break the π-conjugation in response to an external electric field. We have thus investigated nonlinear quantum transport through phenylene ethynylene based molecules as a function of a gatable intramolecular coupling to understand the role of chemical substitution on the observable nonequilibrium electrical current. Contacts to the recent experiments by Elbing *et al.* [1] are also provided.
[1] M. Elbing *et al.*, Proc. Natl. Acad. Sci. USA **102**, 8815 (2005).

TT 26.39 Wed 14:30 P1

Quantum transport through single azobenzene molecules: contact effects — •Miriam del Valle[1,2], Rafael Gutiérrez-Laliga[2], Carlos Tejedor[1], and Gianaurelio Cuniberti[2] — [1]Dpto. Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]Institute of Theoretical Physics, Universität Regensburg, Germany

We investigate the transport properties of azobenzene, a photosensitive molecule which could provide a light-driven switch. The I–V characteristics are studied in the linear response regime using first-principle methods and Green function techniques. Focus is made on the effect of contacts such as gold leads or carbon nanotubes. The trans configuration of this molecule proves to be a better conducting element than its metastable cis configuration. Remarkable is that zigzag carbon nanotubes have a strong effect of enhancement in the current features up to four orders of magnitude.

TT 26.40 Wed 14:30 P1

STM spectroscopy and STM imaging of linear molecules — •Dmitry Ryndyk and Gianaurelio Cuniberti — Molecular Computing Group, Institute for Theoretical Physics, University of Regensburg, Germany

Inelastic tunneling spectroscopy (IETS) in combination with scanning tunneling microscopy (STM) is a powerful method to investigate electronic spectrum and transport properties of large molecules. We consider theoretically nonequilibrium electronic transport through a single molecule placed between a conducting substrate and an STM tip at finite voltages. A semi-empirical tight-binding model is used to describe linear molecules (as DNA). The STM based molecular junction is considered as a strongly asymmetric double tunnel junction. The molecule is weakly coupled to the substrate and to the STM tip. The coupling of the different parts of the molecule to the STM tip is a function of the distance, which results in a tunneling current dependence on the position of the STM tip (STM image of the molecule). In the limit of small voltages the conductance of nonmetallic molecules is very small and determined by environ-mentally induced states. At finite voltages resonant transport through molecular orbitals gives peaks in the differential conductance as a function of the voltage. The nonequilibrium Green function method is applied to calculate the contribution of different molecular orbitals at finite voltages. It is shown that molecular spectra are modified by charging and vibrational effects.

TT 26.41 Wed 14:30 P1

Influence of laser irradiation on the transport in molecular wires — •U. Kleinekathöfer, S. Welack, and M. Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The electron transport through a molecular wire under the influence of an external laser field is studied using a reduced density matrix formalism [1]. The full system is partitioned into the relevant part, i.e. the wire, electronic reservoirs and a thermal phonon bath. An earlier second-order perturbation theory approach of Meier and Tannor for bosonic environments which employs a numerical decomposition of the spectral density is used to describe the coupling to the phonon bath and is extended to deal with the electron transfer between the reservoirs and the molecular wire. Furthermore, from the resulting time-nonlocal (TNL) scheme a time-local (TL) approach can be derived. Both are employed to propagate the reduced density operator in time for a time-dependent system Hamiltonian which incorporates the laser field non-perturbatively. In addition, an optimal control algorithm designed for open quantum systems is employed in order to compute optimal laser control fields to control the current through the wire.

[1] S. Welack, M. Schreiber and U. Kleinekathöfer, cond-mat/0509442.

TT 26.42 Wed 14:30 P1

Nanometer spaced electrodes of different metals on cleaved surfaces for molecular electronics applications — •Simone Lingitz, Sebastian Luber, Fan Zhang, Allan Hansen, Max Bichler, and Marc Tornow — Walter Schottky Institut, TU München, 85748 Garching, Germany

Current efforts in molecular electronics both aim for novel devices as well as the understanding of the electronic transport in molecules. Here one of the major challenges is the preparation of defined electrodes which allow reliably contacting and electrically investigating molecules of a given size. We pursue a novel strategy to fabricate nanometer spaced metal electrodes which is based on the cleavage plane of a GaAs-AlGaAs heterostructure.

Using Molecular Beam Epitaxy (MBE) we embedded a 5nm-GaAs layer in between two AlGaAs layers. By cleaving the substrate and selectively etching the GaAs layer, the remaining AlGaAs layers act as a support for deposited metal electrodes. We also used an inverse template structure (AlGaAs layer within GaAs) to profit from the unsurpassed selectivity of HF based etchants. In both approaches the electrode distance is precisely predetermined and various electrode metals can be used. This provides a platform to investigate the alignment of molecular and metal energy levels. In our contribution we will report on electrical investigations on thiolated @\pi@-conjugated aromatic molecules assembled on 5nm spaced gold electrodes. Here the current-voltage characteristics show an exponential like increase in current at voltages above approx. 0.3V. We compare this to similar investigations on platinum electrodes.

TT 27 Symposium Twenty Years High-T_c Cuprates - Recent Progress

Time: Thursday 09:30–13:00 Room: HSZ 02

Invited Talk

TT 27.1 Thu 09:30 HSZ 02

Vorticity in the phase diagram of cuprates: evidence from Nernst effect and torque magnetometry — •N. P. Ong — Department of Physics, Princeton University, Princeton, New Jersey 08544, U.S.A.

A key question in cuprates is whether the critical transition at T_c corresponds to the BCS gap-closing scenario or the loss of long-range phase coherence. The observation in LSCO of a large Nernst signal that extends from above the T_c "dome" to a temperature T_{onset} with a peak value of 130 K has provided strong evidence for the phase-disordering scenario[1]. The vortex-Nernst signal implies that the pair condensate remains finite above T_c. Similar evidence for a large vortex Nernst signal has been reported in the hole-doped cuprates Bi 2201, Bi 2212, Bi 2223, YBCO, but not in the electron-doped cuprate NdCeCuO. The existence of vorticity in turn implies that significant 2D diamagnetism must exist above T_c. Recently, the diamagnetic signal has been confirmed using torque magnetometry. The signal remains robust in fields up to 45 T and scales closely with the vortex-Nernst signal over a broad range of T. I will review the evidence and discuss implications for the phase diagram and the pseudogap state.

1. Yayu Wang, Lu Li and N. P. Ong, cond-mat/0510470.

Invited Talk

TT 27.2 Thu 10:00 HSZ 02

Recent Photoemission Data from Layered Manganites and Cuprates — •Zhi-xun Shen — Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University

We present recent angle-resolved photoemission data from manganites and cuprates. Despite the difference in their ground state properties, superconductivity versus ferromagnetism, these materials exhibit interesting similarity in their electronic structure. In particular, the pseudogap state in deeply underdoped curpates finds a counterpart in manganites. We will also report recent data from a new cuprate with four CuO$_2$ planes per unit cell, where we discovered a strong Fermi surface dependence of the superconducting gap.

Keynote Talk

TT 27.3 Thu 10:30 HSZ 02

"Kinks", Nodal Bilayer Splitting and Interband Scattering in YBCO — •Sergey Borisenko — IFW Dresden, Institute for Solid State Research, P.O.Box 270116, D-01171 Dresden

We apply the new-generation ARPES methodology to the most widely studied cuprate superconductor YBCO. Considering the nodal direction, we found noticeable renormalization effects known as "kinks" both in the quasiparticle dispersion and scattering rate, the bilayer splitting and evidence for strong interband scattering - all the characteristic features of the nodal quasiparticles detected earlier in BSCCO. Typical energy scale and the doping dependence of the "kinks" clearly point to their intimate relation with the spin-1 resonance seen in the neutron scattering experiments performed on the same samples. Our findings strongly suggest a universality of the electron dynamics in the bilayer superconducting cuprates and a dominating role of the spin-fluctuations in formation of the quasiparticles along the nodal direction.

This work is supported by the Deutsche Forschungsgemeinschaft (Research unit 538).

— 30 min. break —

Keynote Talk

TT 27.4 Thu 11:30 HSZ 02

Universal magnetic spectrum in high-temperature superconductors — •Bernhard Keimer — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

We outline recent experimental evidence for a magnetic excitation spectrum of the cuprate high-temperature superconductors whose main features are independent of materials-specific details. The spectrum consists of upward- and downward-dispersing branches that merge at the wave vector characteristic of antiferromagnetism in the undoped parent compounds. We will argue that information about the in-plane anisotropy of the spectrum is crucial for its microscopic interpretation. In order to determine this anisotropy, we have use neutron scattering to collect an extensive data set on untwinned $YBa_2Cu_3O_{6+x}$ single crystals with different doping levels x. The results will be compared to calculations based on Fermi-liquid states and states with static and dynamic "stripe" order. Combined with complementary photoemission data on the same single samples, these data provide a detailed, microscopic picture of the interaction between spin and charge excitations in the copper oxide superconductors.

Collaborators: V. Hinkov, S. Pailhès, P. Bourges, Y. Sidis, A. Ivanov, A. Kulakov, C.T. Lin, D.P. Chen, C. Bernhard

This work is supported by the Deutsche Forschungsgemeinschaft (Research unit 538).

Recent publications: B. Keimer, Nature 430, 650 (2004); S. Pailhès, Y. Sidis, P. Bourges, V. Hinkov, A. Ivanov, C. Ulrich, L.P. Regnault, and B. Keimer, Phys. Rev. Lett. 93, 167001 (2004).

Keynote Talk

TT 27.5 Thu 12:00 HSZ 02

Spin-fluctuation mechanism of high-temperature superconductivity — •Andrey Chubukov — Physics, UW-Madison, 1150 University ave, Madison, WI 53706, USA

I will review the spin-fluctuation approach to high-temperature superconductivity. The key idea behind the approach is to depart from

relatively high dopings, where fermions form Landau Fermi liquid, and consider how the 2D system behavior evolves as the system approaches an antiferromagnetic instability. I show that in the normal state, spin fluctuations are overdamped. The interaction with overdamped spin fluctuations gives rise to the fermionic self-energy which mimics marginal Fermi-liquid behavior over a wide range of frequencies. I next consider the pairing and show that there exists two regimes on the phase diagram: the low-T regime, in which the pairing involves Fermi-liquid quasiparticles, and the high -T regime, in which the pairing involves incoherent fermions. I argue that Fermi-liquid pairing leads to a $d-$wave superconductivity, while the pairing of incoherent fermions produces spin-singlet pairs, which still remain incoherent and do not carry a supercurrent. I discuss various feedbacks from the pairing on both electronic and magnetic properties (including the emergence of the resonance peak), and link spin-fluctuation approach to theories that depart from a Mott insulator at half-filling.

Keynote Talk TT 27.6 Thu 12:30 HSZ 02

The origin of anomalous transport in a high-temperature superconductor — •Nigel Hussey — H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, UK

The metallic state of high-temperature superconductors is anomalous in that the Hall coefficient is strongly temperature dependent while the resistivity varies linearly in temperature over a wide temperature range. Although this T-linear resistivity gradually weakens with doping, crucially it survives until superconductivity is destroyed. Both the superconducting pairing interaction and the origin of this anomalous transport have yet to be determined, though most theoretical approaches consider them to be intrinsically linked. Through analysis of polar angular magnetoresistance oscillations, we have succeeded to determine the full temperature and momentum dependence of the mean free path of the charge carriers in highly doped Tl_2 Ba_2 $CuO_{6+\delta}$ (T_c = 15K) up to 60K. From this, we have been able to identify the origin of the T-linear resistivity and the temperature dependence of the Hall coefficient for this particular compound. Given the correlation between the appearance of the T-linear resistivity and the onset of superconductivity, this new scattering mechanism is also a prime candidate for the pairing mechanism for high temperature superconductivity itself.

TT 28 Correlated Electrons: General Theory

Time: Thursday 10:00–13:00 Room: HSZ 301

TT 28.1 Thu 10:00 HSZ 301

Transport and optical properties of the Kondo lattice model — •Theo Costi — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Dynamical mean field theory is used to investigate transport and optical properties of the Kondo lattice model as a function of increasing hole doping around the Kondo insulating state. The two low energy scales of the model [1,2,3], the lattice coherence scale or single-ion Kondo scale, and the Fermi liquid coherence scale, are identified in spectral, transport, and optical properties. The gaps in transport and optics for Kondo insulators are identified and compared with those found by other approaches. The temperature dependence of the resistivity and frequency dependent optical conductivity is described. Close to the Kondo insulating state we find an incoherent metallic behaviour. Dynamical mean field theory is shown to provide a straightforward interpretation of the resistivity of such prototypical paramagnetic heavy fermion systems as $CeAl_3$.

[1] Pruschke, Th., R. Bulla, and M. Jarrell, 2000, Phys. Rev. B **61**, 12799.
[2] S. Burdin, A. Georges, D. R. Grempel, Phys. Rev. Lett. **85**, 1048-1051 (2000).
[3] T. A. Costi and N. Manini, J. Low Temp. Phys. **126**, 835 (2002).

TT 28.2 Thu 10:15 HSZ 301

Symmetry projection schemes for Gaussian Monte Carlo methods. — •F. F. Assaad[1], P. Werner[2], P. Corboz[2], E. Gull[2], and M. Troyer[2] — [1]Universität Würzburg — [2]ETH-Zürich

A novel sign-free Monte Carlo method for the Hubbard model has recently been proposed by Corney and Drummond. High precision measurements on small clusters show that ground state correlation functions are not correctly reproduced. We argue that the origin of this mismatch lies in the fact that the low temperature density matrix does not have the symmetries of the Hamiltonian. Here we show that supplementing the algorithm with symmetry projection schemes provides reliable and accurate estimates of ground state properties.

Preprint: http://arxiv.org/abs/cond-mat/0509149. Accepted for publication in PRB

TT 28.3 Thu 10:30 HSZ 301

Single hole dynamics in the bilayer Heisenberg model — •Christian Brünger and Fakher Assaad — Universität Würzburg

We consider a bilayer Heisenberg model exhibiting a quantum phase transition between ordered and disordered magnetic phases as a function of the interplanar coupling. Our aim is to study the following points: i) The evolution of the single particle spectral function from the disordered to ordered phase. ii) The coupling of the hole to critical magnetic fluctuations and the related fate of the quasiparticle residue in the vicinity of the critical point. As a function of decreasing interplanar coupling, the spectral function deforms continuously from its strong coupling behavior with band maximum at $\vec{k} = (\pi, \pi)$ to that of the planar t-J model with maximum at $\vec{k} = (\pi/2, \pi/2)$. Surprisingly, and on lattices up to 20×20, both for static and dynamic holes, the quasiparticle residue does not seem to be affected by critical magnetic fluctuations.

TT 28.4 Thu 10:45 HSZ 301

Static and dynamic properties of the spinless Falicov-Kimball model — •Steffen Sykora[1], Klaus W. Becker[1], and Veliko Zlatic[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Physics, Bijenika c. 46, P.O.B 304, 10000 Zagreb, Croatia

The spinless Falicov-Kimball model in one dimension is studied by use of a recently developed projector-based renormalization method (PRM) for many-particle Hamiltonians. The method is used to evaluate static and dynamic quantities of the system at half-filling. To these belong the quasiparticle excitation energy $\tilde{\varepsilon}_{\mathbf{k}}$ and the momentum distribution $n_{\mathbf{k}}$ of the conduction electrons and spatial correlation functions of the localized electrons. One of the most remarkable results is the appearance of a gap in $\tilde{\varepsilon}_{\mathbf{k}}$ at the Fermi level of the order of the Coulomb repulsion U which is accompanied by a smooth behavior for $n_{\mathbf{k}}$. The density of states for the conduction electrons and the one-particle spectral functions for the localized electrons are also discussed. In both quantities a gap opens with increasing U.

TT 28.5 Thu 11:00 HSZ 301

Correlated hybridization in transition metal complexes — •Arnd Hübsch[1], Jong-Chin Lin[2], Jianping Pan[2], and Daniel L. Cox[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [2]Department of Physics, University of California, Davis, CA 95616, USA

We apply local orbital basis density functional theory (using SIESTA) coupled with a mapping to the Anderson impurity model to estimate the Coulomb assisted or correlated hybridization between transition metal d-orbitals and ligand sp-orbitals for a number of molecular complexes. We find remarkably high values which can have several physical implications including: (i) renormalization of effective single band or multiband Hubbard model parameters for the cuprates and, potentially, elemental iron, and (ii) spin polarizing molecular transistors.

TT 28.6 Thu 11:15 HSZ 301

Momentum-resolved spectral functions of $SrVO_3$ calculated by LDA+DMFT — •M. Kollar[1], I. A. Nekrasov[2,1], K. Held[3], G. Keller[1], D. E. Kondakov[4], Th. Pruschke[5], O. K. Andersen[3], V. I. Anisimov[4], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute for Electrophysics, Ekaterinburg, Russia — [3]MPI for Solid State Research, Stuttgart — [4]Institute of Metal Physics, Ekaterinburg, Russia — [5]Institute for Theoretical Physics, University of Göttingen

We have calculated momentum-resolved spectral functions of $SrVO_3$ using LDA+DMFT [1]. To this end, we have employed Nth order muffin-tin (NMTO) downfolding to set up an effective low-energy Hamiltonian with three t_{2g} orbitals. This effective Hamiltonian was solved by DMFT. Our results for momentum-dependent spectra show renormalized quasi-particle bands over a broad energy range from -0.7 eV to +0.9 eV with small "kinks" discernible in the dispersion below the Fermi energy. A similar feature was also found recently in angle-resolved photoemission experiments [2].

[1] I. A. Nekrasov *et al.*, cond-mat/0508313.
[2] T. Yoshida *et al.*, cond-mat/0504075.

— 15 min. break —

TT 28.7 Thu 11:45 HSZ 301

Self-energy-functional approach (SFA) as a scheme for reduction of finite size effects — •Krunoslav Požgajčić — Institut für Physik, KOMET 337, Universität Mainz, 55099 Mainz, Germany

Self-energy-functional approach (Michael Potthoff, Eur. Phys. J. B 32, 429(2003)) and its extensions (Ning-Hua Tong, Phys. Rev. B 72, 115104(2005)) have been proposed as a general framework for embedded cluster methods. We will use SFA for different models in regimes which are characterized by strong finite size effects, like is the case with metallic states. It will be demonstrated that SFA can be regarded as a prescription for reduction of those effects. Other schemes devised for reduction of finite size effects will also be discussed.

TT 28.8 Thu 12:00 HSZ 301

Static vs. Dynamical Mean Field Theory of Mott Antiferromagnets — •Giorgio Sangiovanni[1], Alessandro Toschi[1], Erik Koch[2], Karsten Held[1], Massimo Capone[3,4], Claudio Castellani[4], and Olle Gunnarsson[1] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart — [2]Institut für Festkörperforschung, Forschungszentrum, Jülich — [3]Istituto dei Sistemi Complessi del CNR, Rom — [4]Dipartimento di Fisica Università di Roma "La Sapienza", Rom

In recent years, our ability to calculate strongly correlated materials has substantially improved. For instance, local density approximation supplemented by a local Coulomb interaction U treated in the static Hartree-Fock (HF) mean field theory (LDA+U), gives extremely accurate results for ground-state properties at large U, especially in the presence of magnetic or orbital ordering. On the other hand, dynamic properties are not well described by LDA+U, due to the too poor treatment of excited states given by HF. To go beyond this approximation, the more sophisticated LDA+DMFT has been recently developed. Considering the antiferromagnetic phase of a simple model, the single-band Hubbard model, we explicitely analyze the differences between static and dynamical mean field theory. In DMFT the HF band is strongly renormalized and spectral weight is trasferred to spin-polaron side bands. Already for intermediate U the overall bandwidth is larger than in HF and the gap is considerably smaller. Such differences survive any renormalization of U. We compare our results with photoemission experiments for Cr-doped V_2O_3 obtaining extremely good qualitative agreement.

TT 28.9 Thu 12:15 HSZ 301

Non-local corrections to DMFT: magnetic correlation effects on the spectral function — •Alessandro Toschi, Andrey Katanin, and Karsten Held — Max-Planck Institut für Festkörperforschung, Heisenbergstr. 1,*D-70569 Stuttgart, Germany

We consider non-local corrections to the dynamical mean-field theory (DMFT) self-energy and spectral functions in the presence of strong magnetic fluctuations. Specifically, we evaluate the momentum-dependent self-energy starting from the one- and two-particle DMFT Green functions. Contrary to previous studies (e.g., the GW+DMFT approach) the local three-frequency vertex corrections are taken into account. Unlike the dynamical cluster approximation or the cellular DMFT approach, our method allows to study the effect of magnetic fluctuations with large correlation length. The effect of antiferromagnetic fluctuations is studied for the single-band Hubbard model at half filling. Going beyond DMFT we find precursor effects of the antiferromagnetic order already in the paramagnetic phase: the momentum dependence of the self-energy becomes particularly strong in the vicinity of the antiferromagnetic transition.

TT 28.10 Thu 12:30 HSZ 301

Thermodynamics of a Fermi liquid in a magnetic field. — •Dmitri Efremov[1], Joseph Betouras[2], and Andrey Chubukov[3] — [1]Technical University of Dresden — [2]University of Leiden — [3]University of Wisconsin

We present calculations of the non-analytic terms in the spin susceptibility $\chi_s(T)$ and the specific heat $C(T)$ to systems in a magnetic field. Without a field, $\chi_s(T)$ and $C(T)/T$ are linear in T in 2D, while in 3D, $\chi_s(T)$ is proportional to T^2 and $C(T)/T$ proportional to $T^2 \log T$. We show that in a magnetic field, the linear in T terms in 2D become scaling functions of $\mu_B H/T$. We present explicit expressions for these functions and show that at high fields, $\mu_B H \gg T$, $\chi_s(T,H)$ scales as $|H|$. We also show that in 3D, $\chi_s(T,H)$ becomes non-analytic in a field and at high fields scales as $H^2 \log |H|$

TT 28.11 Thu 12:45 HSZ 301

Exotic excitations with fractional charges on frustrated lattices — •Frank Pollmann[1], Peter Fulde[1], and Erich Runge[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau, Germany

Geometrical frustration of lattices can lead to a macroscopic degeneracy in the classical limit and thus to many interesting physical effects. In spin systems these are e.g. translational invariant spin liquid ground states and deconfined spinons. In contrast to magnetic properties, one began only recently to explore the charge degrees of freedom on frustrated lattices.

For the systematic study of charge degrees of freedom, we consider a model of spinless fermions with nearest-neighbor hopping t and Coulomb repulsion V. Quantum fluctuations reduce the classical ($t = 0$) macroscopic degeneracy. For the strongly correlated limit $V \gg |t|$, it has been predicted that an added electron can decay into two mobile quasiparticles, leading to fractional charges of $e/2$ in 2D and 3D systems.

For a deeper understanding of these charge degrees of freedom we calculated numerically the properties of static and dynamic charges on the 2D checkerboard lattice. Evidence for a weak mutual confinement of two fractional charges is found, leading to excitations with very large spatial extend. We argue that the fractional charges should be deconfined on the 3D pyrochlore lattice.

TT 29 Transport: Quantum Coherence and Quantum Information Systems - Part 1

Time: Thursday 09:30–12:45 Room: HSZ 304

Invited Talk TT 29.1 Thu 09:30 HSZ 304

Decoherence of fermions subject to a quantum bath — •Florian Marquardt — Sektion Physik, Arnold Sommerfeld Center for Theoretical Physics, und Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München

The destruction of quantum-mechanical phase coherence by a fluctuating environment is both of fundamental interest and essential for applications of quantum dynamics. While the theory of decoherence is well developed for a two-level system or a single particle, the case of many fermions is less understood, despite its relevance for nanoelectronics.

After giving a general introduction, I will focus on the analysis of decoherence in the most basic interferometer, the Mach-Zehnder setup, whose electronic version has been been realized only recently [1]. Based on our earlier work on the influence of classical noise [2], we have studied the case of a fully quantum-mechanical environment [3]. Using a novel equations-of-motion approach, we have calculated the dephasing rate, including many-body effects like Pauli blocking. I will give a transparent physical interpretation of the results, describe related work on weak localization [4], and discuss the shot noise in the output current.

[1] Y. Ji et al., Nature **422**, 415 (2003); I. Neder et al., cond-mat/0508024.
[2] F. Marquardt and C. Bruder, Phys. Rev. Lett. **92**, 056805 (2004); Phys. Rev. B **70**, 125305 (2004).
[3] F. Marquardt, cond-mat/0410333, to appear in Europhys. Lett. (Dec. 2005).
[4] F. Marquardt, J. v. Delft, R. Smith, and V. Ambegaokar, cond-mat/0510556.

TT 29.2 Thu 10:00 HSZ 304

Landau-Zener transitions in qubits and qubit-oscillator systems — •Martijn Wubs[1], Keiji Saito[2], Sigmund Kohler[1], Yosuke Kayanuma[3], and Peter Hänggi[1] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg — [2]Department of Physics, Graduate School of Science, University of Tokyo, Bunkyo-Ku, Tokyo 113-0033, Japan — [3]Department of Mathematical Science, Graduate School of Engineering, Osaka Prefecture University, Sakai 599-8531, Japan

In recent years, several solid-state systems have been identified as effective two-level systems, flux qubits and phase qubits for example. An advantage of these 'artificial atoms' is that they can be driven by gate voltages and external radiation fields. These systems are well suited for manipulation via Landau-Zener transitions. In this talk, we first discuss Landau-Zener transitions in a semiclassical model where both the energy difference and the interaction strength between the levels are controlled by external fields [1]. This model is a combination of the classic Landau-Zener and the Rabi problem. The probability of Landau-Zener transitions now depends sensitively on the amplitude, the frequency and the phase of the interaction. Secondly, motivated by recent advances in circuit QED, we studied Landau-Zener transitions in qubits that are strongly coupled to one or several quantum harmonic oscillators. We present exact calculations of some Landau-Zener transition probabilities also for these more complicated quantum systems. Moreover, we discuss the mapping of the quantum model onto the semiclassical model.
[1] M. Wubs, K. Saito, S. Kohler, Y. Kayanuma, P. Hänggi, New J. Phys. **7**, 218 (2005).

TT 29.3 Thu 10:15 HSZ 304

Excitation and Entanglement Transfer and Quantum Critical Points — •Michael J. Hartmann[1,2], Moritz E. Reuter[1,2], and Martin B. Plenio[1,2] — [1]Institute for Mathematical Sciences, Imperial College London, SW7 2PE, UK. — [2]QOLS, The Blackett Laboratory, Imperial College London, SW7 2BW, UK.

We consider analytically and numerically quantum many body systems as quantum channels in the vicinity of their quantum critical point. In our setup two ancillas are weakly coupled to the quantum many body system at different sites and we study the propagation of an excitation and quantum information from one ancilla to the other. We observe two different scenarios: A slow but perfect transfer if the gap between the ground state and the first excited state of the system is large and a fast but un-complete transfer otherwise. We provide a simplified physical model explaining our findings and suggest ways in which they may be employed to detect quantum critical points experimentally.

TT 29.4 Thu 10:30 HSZ 304

Decoherence of spatially separated qubits — •Roland Doll, Sigmund Kohler, Martijn Wubs, and Peter Hänggi — Institut für Physik, Universität Augsburg, 86135 Augsburg

We consider spatially separated qubits coupled to a phonon field which acts as a heat bath and, thus, causes decoherence. For a theoretical description, it is frequently assumed that depending on the spatial separation, either each qubit couples to a separate bath or that all qubits couple via a collective coordinate to one common bath. For weak qubit-bath coupling it is in both cases possible to describe the dissipative dynamics within a Born-Markov approximation, i.e. one neglects memory effects induced by the bath.

In many experimental situations, however, the bath correlation length and the distances between the qubits are comparable such that neither limit is justified. Then it is necessary to take the spatial dependence of the phonon field explicitely into account. We developed a generalized master equation formalism for the dissipative dynamics which becomes intrinsically non-Markovian. The resulting memory effects and the limitations of a Markovian approximation are discussed.

This work is supported by the DFG through SFB631.

TT 29.5 Thu 10:45 HSZ 304

Analytic solution for the multiphoton resonances in the mono- and bichromatically driven quantum Duffing oscillator — •Michael Thorwart and Vittorio Peano — Institut für Theoretische Physik IV, Universität Düsseldorf

We investigate the nonlinear response of an anharmonic monostable quantum mechanical resonator to external periodic mono- and bichromatic driving in presence of a harmonic bath. We therefore apply a Floquet-Born-Markovian master equation for the reduced density operator. The quasienergies of the pure system show multiple avoided level crossings corresponding to multiphoton transitions in the resonator. Around the resonances, the master equation can be solved analytically using Van-Vleck perturbation theory. Studying the oscillator position, the lineshape of the resonances will be calculated resulting in simple expressions. For the monochromatic case, we find the general solution for the multiple multiphoton resonances and, most interestingly, a bath-induced transition from a resonant to an antiresonant behavior. In the bichromatic case, the harmonic mixing signals are calculated. Our model finds applications in a suspended nanomechanical beam excited to transverse vibrations as well as for the inductive measurement of a superconducting qubit by a driven Josephson junction.

TT 29.6 Thu 11:00 HSZ 304

Full read and write access to sets of permanently coupled qubits by local control only — •Daniel Burgarth[1] and Vittorio Giovannetti[2] — [1]Department of Physics & Astronomy, University College London, UK — [2]NEST-INFM & Scuola Normale Superiore, Pisa, Italy

We propose a protocol that transfers arbitrary quantum states from a quantum memory to a set of permanently coupled qubits and vice versa by controlling a local subset of qubits only. We give a sufficient condition for the convergence of the protocol and provide some numerical examples. In particular, we demonstrate that perfect state transfer and state preparation is possible on 1d Heisenberg spin chains with random coupling strengths.

— 15 min. break —

TT 29.7 Thu 11:30 HSZ 304

Optimal spin-entangled electron-hole pair pump — •Mikhail Titov[1], Carlo Beenakker[2], and Bjorn Trauzettel[2] — [1]University of Konstanz, Department of Physics, Germany — [2]Instituut Lorentz, Universiteit Leiden, The Netherlands

A nonperturbative theory is presented for the creation by an oscillating potential of spin-entangled electron-hole pairs in the Fermi sea. In the weak potential limit, considered earlier by Samuelsson and Buttiker, the entanglement production is much less than one bit per cycle. We demonstrate that a strong potential oscillation can produce an average of one Bell pair per two cycles, making it an efficient source of entangled flying qubits.

TT 29.8 Thu 11:45 HSZ 304

Spin Decay in a Quantum Dot Coupled to a Quantum Point Contact — •Massoud Borhani, Vitaly Golovach, and Daniel Loss — Department of Physics - University of Basel - Basel - Switzerland

We consider a mechanism of spin decay for an electron spin in a quantum dot due to coupling to a nearby quantum point contact (QPC) with and without an applied bias voltage. The coupling of spin to charge is induced by the spin-orbit interaction in the presence of a magnetic field. We perform a microscopic calculation of the effective Hamiltonian coupling constants to obtain the QPC-induced spin relaxation and decoherence rates in a realistic system. This rate is shown to be proportional to the shot noise of the QPC in the regime of large bias voltage and scales as "a^(-6)" where "a" is the distance between the quantum dot and the QPC. We find that, for some specific orientations of the setup with respect to the crystallographic axes, the QPC-induced spin relaxation and decoherence rates vanish, while the charge sensitivity of the QPC is not changed. This result can be used in experiments to minimize QPC-induced spin decay in read-out schemes.

TT 29.9 Thu 12:00 HSZ 304

Nuclear spin state narrowing via gate–controlled Rabi oscillations in a double quantum dot — •Daniel Klauser, W.A. Coish, and Daniel Loss — Departement of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

We study spin dynamics for two electrons confined to a double quantum dot under the influence of an oscillating exchange interaction. This leads to driven Rabi oscillations between the $|\uparrow\downarrow\rangle$–state and the $|\downarrow\uparrow\rangle$–state of the two–electron system. The width of the Rabi resonance is proportional to the amplitude of the oscillating exchange. A measurement of the Rabi resonance allows one to narrow the distribution of nuclear spin states and thereby to prolong the spin decoherence time. Further, we study decoherence of the two-electron states due to the hyperfine interaction and give requirements on the parameters of the system in order to initialize in the $|\uparrow\downarrow\rangle$–state and to perform a $\sqrt{\text{SWAP}}$ operation with unit fidelity.

TT 29.10 Thu 12:15 HSZ 304

How does a spin decay? A novel time dependent numerical renormalization group approach — •Frithjof B Anders — Theoretische Physik, Universität des Saarlandes, Saarbrücken, Germany

In contrast to equilibrium conditions, the understanding of real-time evolution of many-particle quantum systems is still at its infancy. A novel approach to time dependent non-equilibrium quantum impurity systems based on the numerical renormalization group is presented [1]. As a first application, a spin coupled either a bosonic or a fermionic bath is considered. While the spin-boson model is often used in context of decoherence of qubits as well as for charge transfer reactions in chemistry, the latter describes spin- and charge-relaxation processes in ultra-small quantum dots. I will discuss how the environment governs the time scales of the spin decay in both cases. I will present an outlook to the application of our method to charge transfer dynamics in large functional bio-molecules as well as to DC-currents though ultra-small quantum dots.

[1] F. B. Anders and A. Schiller, Phys. Rev. Lett. 95, 196801 (2005)

TT 29.11 Thu 12:30 HSZ 304

Entanglement scaling in critical two-dimensional fermionic and bosonic systems — •Ming-Chiang Chung — Institut für Theoretische Physik C RWTH Aachen D-52074 Aachen Germany

We study the scaling of entanglement in critical two-dimensional (2D) fermionic and bosonic systems at zero temperature. Our method, which uses coherent states and Green function matrices, is introduced in detail. Examining exactly solvable models, we find that the entanglement entropy for critical 2D systems scales with the linear system size L like $S \sim L \ln L$ for fermions and $S \sim L$ for bosons. For fermions the coefficient of the leading divergence is a function of the chemical potential. We also confirm previous results for noncritical systems.

TT 30 Superconductivity: Twenty Years High-T_c Cuprates - Recent Progress

Time: Thursday 14:00–18:45 Room: HSZ 02

TT 30.1 Thu 14:00 HSZ 02

Electron-phonon coupling reflecting dynamic charge inhomogeneity in copper-oxide superconductors — •Dmitri Reznik[1], L. Pintschovious[1], M Ito[2], S. Iikubo[2], M. Sato[2], H. Goka[3], M. Fujita[3], K. Yamada[3], G. Gu[4], and J.M. Tranquada[4] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe, Germany — [2]Department of Physics, Division of Materials Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan — [3]Institute for Material Research, Tohoku University, Katahira, Aoba-ku, Sendai, 980-8577, Japan — [4]Physics Department, Brookhaven National Laboratory, Upton, New York 11973

The attempt to understand cuprate superconductors is complicated by the presence of multiple strong interactions. While many believe that antiferromagnetism is important for the superconductivity, there has been resurgent interest in electron-lattice coupling. The conventional superconductor MgB2 has a very strong electron-lattice coupling predicted by standard theory. We show that there is a similarly strong anomaly in the Cu-O bond-stretching phonon in cuprate superconductors however, this behavior is completely absent in conventional calculations. Instead, the anomaly is strongest in compounds that exhibit static stripe order.It occurs at a wave vector corresponding to the charge order. The results suggest that this giant electron-phonon anomaly, which is absent in undoped and over-doped non-superconductors, is associated with charge inhomogeneity. It follows that electron-phonon coupling may be important to understanding superconductivity although its contribution to the mechanism is likely indirect.

TT 30.2 Thu 14:15 HSZ 02

Origin of dynamic stripe correlations in the charge response of cuprates — •Peter Horsch and Giniyat Khaliullin — Max-Planck-Institut FKF, 70569 Stuttgart, Germany

We discuss the dynamical density fluctuation spectra of cuprates starting from the $t-J$ model in the slave-boson $1/N$ framework [1]. Our theory provides the generic density response of a doped Mott-insulator and reveals novel low-energy structure on the energy scale $J+\delta t$ due to the correlated motion of holes in a RVB spin liquid. This low-energy response implies an anomalous renormalization of several phonon modes [2,3]. In particular our approach explains the peculiar doping dependence of breathing and bond-stretching phonons as observed by neutron scattering [4]. Here we further extend the discussion and analyse the connection between incommensurabilities in the spin-response and dynamic stripe correlations in the charge response of cuprates. Finally we address the question why collinear charge stripes are favored in LSCO compounds.

[1] G. Khaliullin and P. Horsch, Phys. Rev. B 54, R9600 (1996).
[2] G. Khaliullin and P. Horsch, Physica C 282-287, 1751 (1997).
[3] P. Horsch and G. Khaliullin, Physica B 359-361, 620 (2005).
[4] L. Pintschovius, phys. stat. sol. (b) 242, 30 (2005).

TT 30.3 Thu 14:30 HSZ 02

Charge and spin ordering phenomena in HTSC — •Leonardo Tassini, Wolfgang Prestel, Rudi Hackl, Michael Lambacher, and Andreas Erb — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

We present a detailed study of the underdoped range of the phase diagram of various single crystals of $La_{2-x}Sr_xCuO_4$ (LSCO) and of $Y_{1-x}Ca_xBa_2Cu_3O_6$ (YBCO) using electronic Raman scattering. We conclude from the experimental data that there is a clear indication of a charge and/or spin modulation (stripes) in the two-dimensional CuO_2 planes manifesting themselves as additional Drude-like peaks at low energies and temperatures. The additional response in LSCO is in the B_{2g} and B_{1g} symmetry at doping levels of x = 0.02 and x = 0.10, respectively, and in the B_{2g} symmetry for all YBCO samples studied. The selection rules allow us to determine the orientation of the stripes to be along the diagonal of the CuO_2 plane in YBCO and in LSCO at x = 0.02, and along the principle axes in LSCO at x = 0.10. The stripes fluctuate, and the correlation length is of the order of the electronic mean free path. In LSCO temperature is the only scale of the response at different doping levels demonstrating the importance of quantum critical behaviour.

This work is supported by the Deutsche Forschungsgemeinschaft (Research unit 538).

TT 30.4 Thu 14:45 HSZ 02

Dispersion and geometry of spin excitations in the normal and superconducting state of twin-free YBCO(6.6) — •Vladimir Hinkov[1], Bernhard Keimer[1], P. Bourges[2], S. Pailhes[2], Y. Sidis[2], A. Ivanov[3], and CT. Lin[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Laboratoire Leon Brillouin, CEA-CNRS, France — [3]Institut Laue-Langevin, Grenoble, France

There is a strong debate about the normal state (NS) and the *pseudogap* (PG) state in the high-Tc cuprates. For now, our understanding of their magnetism suffers from the lack of information about the regimes above Tc. We present an inelastic neutron scattering study (see also V. Hinkov et al, Nature 430, 650 (2004)), of the in-plane (a-b) anisotropy of spin-excitations between 26meV and 60meV in twin-free, underdoped YBCO(6.6), T_c =61 K. We identify three fundamentally different temperature regimes: the superconducting regime exhibits incommensurate peaks both along a and b with a X-shaped dispersion. Intensity shows a-b-anisotropy below the resonance peak and no anisotropy above. Heating to 70 K (PG-state), the dispersion changes to Y-shape, with a flat top, steeply dispersing signal below the resonance, which is 50% broader along a. Finally, at 290 K (NS), intensity is depleted below the resonance and is only visible at higher energies. We discuss the implication of our findings on different theoretical models proposed for the PG-regime: the stripe-model, spin-ladder models, preformed Cooper-pairs, competing order parameter. We compare our results with other tech-

niques such as ARPES and STM, and with other systems such as the Haldane-compound YBaNiO(5).

This work is supported by the Deutsche Forschungsgemeinschaft (Research unit 538).

TT 30.5 Thu 15:00 HSZ 02

Theory for Inelastic Neutron Scattering in Orthorhombic High-T_c Superconductors — •Andreas Schnyder[1], Dirk Manske[2], Christopher Mudry[1], and Manfred Sigrist[2] — [1]Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [2]Institut für Theoretische Physik, ETH Zürich, Hönggerberg, CH-8093 Zürich, Switzerland

Extending our earlier fermiology-based studies on the magnetic susceptibility we analyze the in-plane anisotropy of the spin response in hole-doped high-T_c cuprates [1]. Employing the two-dimensional one-band Hubbard model and a generalized RPA-type theory we consider anisotropic hopping matrix elements ($t_x \neq t_y$) and a mixing of d- and s-wave symmetry of the superconducting order parameter in order to describe orthorhombic superconductors. We compare our calculations with available inelastic neutron scattering data on untwinned YBCO and find good agreement [2]. Furthermore, we predict a strongly anisotropic in-plane dispersion of the resonance peak and contrast our results to theories based on stripe formation.

[1] A. P. Schnyder, D. Manske, C. Mudry, and M. Sigrist, cond-mat/0510790.
[2] V. Hinkov, S. Pailhes, P. Bourges, Y. Sidis, A. Ivanov, A. Kulakov, C. T. Lin, D. P. Chen, C. Bernhard, and B. Keimer, Nature **430**, 650 (2004).

TT 30.6 Thu 15:15 HSZ 02

Spin excitations in fluctuating stripe phases — •Matthias Vojta[1], Thomas Vojta[2], and Ribhu Kaul[1,3] — [1]Universität Karlsruhe, Germany — [2]University of Missouri, Rolla, USA — [3]Duke University, Durham, USA

Using a phenomenological lattice model of coupled spin and charge modes, we determine the spin susceptibility in the presence of fluctuating stripe charge order. We assume the charge fluctuations to be slow compared to those of the spins, and combine Monte Carlo simulations for the charge order parameter with exact diagonalization of the spin sector. Our calculations unify the spin dynamics of both static and fluctuating stripe phases and support the notion of a universal spin excitation spectrum in doped cuprate superconductors.

TT 30.7 Thu 15:30 HSZ 02

Resonant spin excitations in the id-density wave state: probe for the pseudogap scenario in underdoped cuprates — •Jan-Peter Ismer[1], Ilya Eremin[1,2], and Dirk K. Morr[3] — [1]Max-Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institut für Mathematische und Theoretische Physik, Technische Universität Carolo-Wilhelmina zu Braunschweig, D-38106 Braunschweig, Germany — [3]Department of Physics, University of Illinois at Chicago, Chicago, IL 60607, USA

Inelastic neutron scattering (INS) experiments probing dynamical spin susceptibility in the pseudogap phase of the high-T_c cuprates are addressed in the framework of the ordered d-density wave(DDW) state. In particular, we analyze the formation of the resonance peak at the antiferromagnetic wave vector $\mathbf{Q}_{AF} = (\pi, \pi)$ and its dispersion in three different ordered states: d-wave superconductor (DSC), DDW state, and coexisting DDW and DSC states. In particular, we find that the resonance excitations in the DDW-state exists in a narrow region around (π, π) forming nearly no dispersion due to peculiar structure of the Fermi surface. At the same time, in the combined DDW+DSC-state the resonance peak dispersion is determined mainly by the superconducting gap, although both phases interfere around (π, π) yielding a non-monotonic intensity cusp of the resonance peak dispersion. A comparison with existing INS experiments shows certain constraints on the application of the DDW-scenario for the pseudogap in underdoped cuprates.

TT 30.8 Thu 15:45 HSZ 02

Nuclear Magnetic Resonance Studies of Rare Earth co-doped Lanthanum Cuprates — •Hans-Joachim Grafe[1,2], Nicholas J. Curro[2], Markus Hücker[3], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]Los Alamos National Laboratory, NM , USA — [3]Physics Department, Brookhaven National Laboratory, Upton NY, USA

^{17}O and ^{63}Cu Nuclear Magnetic Resonance (NMR) results in stripe ordered $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ will be presented. At low temperatures the local electric field gradient (EFG) as well as the absolute intensity of the NMR signal of the planar O site exhibit a dramatic decrease. We interpret these results as microscopic evidence for a spatially inhomogeneous charge distribution, where the NMR signal from O sites in the domain walls of the spin density modulation are wiped out due to large hyperfine fields, and the remaining signal arises from the intervening Mott insulating regions. At similar temperatures the Cu NMR signal experiences a complete wipe out, suggesting that the oxygens are wiped out by the same mechanism that renders the Cu invisible, namely slowly fluctuating Cu electronic spins. Despite of this static magnetic and charge order, the Knight shift exhibits the same pseudogap-like temperature dependence as in superconducting $La_{2-x}Sr_xCuO_4$.

TT 30.9 Thu 16:00 HSZ 02

Exploring the phase diagram of $Bi_{2-y}Pb_ySr_{2-x}La_xCuO_{6+\delta}$ — •L. Dudy[1], B. Müller[1], A. Krapf[1], H. Dwelk[1], C. Janowitz[1], R. Manzke[1], and H. Höchst[2] — [1]Institut f. Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin — [2]Synchrotron Radiation Center, Stoughton, WI, U.S.A

Using angular resolved photoemission we are able to study the temperature dependence of the electronic structure of $Bi_{2-y}Pb_ySr_{2-x}La_xCuO_{6+\delta}$ (Pb-Bi2201) with high accuracy. The lead- ($0 \leq y \leq 0.4$) and lanthanum- ($0.2 \leq x \leq 0.8$) content was varied continously over a large range by controlling the crystal growth parameters. While lead doping raises the superconducting critical temperature (T_c) from $T_c^{max} \simeq 29K$ in lead-free samples to $T_c^{max} \simeq 35K$, the pseudogap temperature is slightly lowered in the hole-underdoped regime with increasing lead-content. We discuss the superconducting transition temperature and the pseudogap temperature in dependence of x and y. In agreement with Sato et al. [1] we find that the maximum gap magnitude near the antinodal point (Δ_{max}) for y=0.4 is much smaller (about four times) than in the two-layer compound of $Bi_2Sr_2CaCu_2O_8$ (Bi2212) at the same doping level. When measuring $\Delta_{max}(T)$ no significant change in this gap function was found within the experimental resolution when lowering the temperature through T_c .

[1] T. Sato et al. , Journal of Physics and Chemistry of Solids 62 (2001) 157-161

— 15 min. break —

TT 30.10 Thu 16:30 HSZ 02

Temperature dependent hole distribution in $Sr_{14-x}Ca_xCu_{24}O_{41}$ — •C. Hess[1], T. Kim[1], M. Knupfer[1], G. Behr[1], B. Büchner[1], N. Nücker[2], S. Schuppler[2], P. Nagel[2], U. Ammerahl[3], and A. Revcolevschi[3] — [1]IFW Dresden, Institute for Solid State Research, Germany — [2]FZ Karlsruhe, Institut für Festkörperphysik — [3]Laboratoire de Physico-Chimie des Solides, Université Paris-Sud, France

We studied the effect of charge order in the spin ladder material $Sr_{14-x}Ca_xCu_{24}O_{41}$ by means of polarization dependent Near-edge x-ray absorption fine structure measurements at the oxygen K-edge (O1s-NEXAFS). Stoichiometry gives a total hole count per formula unit of 6, and the holes are located mainly in the chains although some fraction does dope the ladders as well. At low doping levels a charge ordering transition, which affects the physical properties of both the doped spin chains and spin ladders, is present. We therefore investigated the temperature dependence of the spectra in order to look for a possible redistribution of holes between the different sites (chains and ladders) in the structure, especially at the charge-order transition. From the low temperature spectra we can clearly exclude that the ladder-doping becomes zero as suggested by other experiments. Nevertheless we observe a strong temperature dependence of the spectra.

TT 30.11 Thu 16:45 HSZ 02

Dopant-modulated pair interaction in cuprate superconductors — •Tamara Nunner[1], Brian Andersen[2], Ashot Melikyan[2], and Peter Hirschfeld[2] — [1]Institut fuer theoretische Physik, FU Berlin, Arnimallee 14, 14195 Berlin — [2]Department of Physics, University of Florida, Gainesville, FL 32611 (USA)

High-resolution STM experiments on superconducting BSCCO-2212 have revealed the existence of nanoscale inhomogeneities in the electronic structure at biases near the superconducting energy gap. Very recently, a strong correlation between this nanoscale electronic disorder and the locations of the oxygen dopant atoms has been identified by McElroy *et*

al. [1]. We suggest that the primary effect of the oxygen dopant atoms is to modulate the pair interaction locally [2]. Based on single impurity T-matrix and many-impurity Bogoliubov-de Gennes calculations we show that a dopant modulated pair interaction can reproduce most of the correlations observed in recent STM experiments: nanoscale inhomogeneity of the coherence peak position, homogeneity of the local density of states at low bias, low charge disorder, negative correlation between the height of the coherence peaks and the gap magnitude and a positive correlation between the gap magnitude and the locations of the oxygen dopant atoms.

[1] K. McElroy, J. Lee, J. A. Slezak, D.-H. Lee, H. Eisaki, S. Uchida, and J.C. Davis, Science **309**, 1048 (2005).
[2] T.S. Nunner, B.M. Andersen, A. Melikyan, and P.J. Hirschfeld, Phys. Rev. Lett. **95**, 177003 (2005).

TT 30.12 Thu 17:00 HSZ 02

Optical spectral weight shifts and sum rules in cuprates: role of strong correlation — •Alessandro Toschi[1], Massimo Capone[2,3], and Claudio Castellani[3] — [1]Max-Planck Institut für Festkörperforschung, Heisenbergstr. 1,*D-70569 Stuttgart, Germany — [2]Istituto dei Sistemi Complessi del CNR, Via dei Taurini 19, I-00185*Roma, Italy — [3]Dipartimento di Fisica Università di Roma "La Sapienza"piazzale Aldo Moro 5,*I-00185 Roma, Italy

We show that many unusual features recently observed in the optical spectroscopy experiments on the high-temperature superconducting cuprates can be simply understood as arising from the vicinity to the Mott transition, without invoking more involved and exotic mechanisms. More specifically we compare calculations based on the Dynamical Mean Field Theory of the Hubbard model with the infrared spectral weight $W(\Omega, T)$ of $La_{2-x}Sr_xCuO_4$ and other cuprates. We find that most of the anomalies observed in the T- and the doping dependence of $W(\Omega, T)$ with respect to normal metals can be ascribed to strong correlation effects. Moreover the variation of weight at the superconducting transition in optimally and underdoped cuprates, that can be interpreted as a gain in kinetic energy, is accounted for by a strong-coupling (almost bosonic) superconductivity, while the overdoped materials behave more like standard superconductors.

[1] A.T., M. Capone, M. Ortolani, P. Calvani, S. Lupi, and C. Castellani, Phys. Rev. Lett. **95**, 097002 (2005)
[2] A.T., M. Capone and C. Castellani, cond-mat/0509188, to appear on Phys. Rev. B

TT 30.13 Thu 17:15 HSZ 02

Doping dependent tunneling behavior in electron-doped cuprates — •Yoshiharu Krockenberger[1], Andreas Winkler[1], Akio Tsukada[2], Michio Naito[3], Dirk Manske[4], and Lambert Alff[1] — [1]TU Darmstadt — [2]NTT, Atsugi, Japan — [3]TUAT, Tokyo, Japan — [4]MPI-FKF Stuttgart

Recently in the electron doped cuprates a pseudogap of the order of the superconducting gap has been observed by tunneling experiments [1]. In order to investigate the phase diagram in more detail, we have studied a series of $Pr_{2-x}Ce_xCuO_{4+y}$ thin film junctions within the whole doping region between $0 < x < 0.2$. Our results support the idea that the phase diagram of the electron doped cuprates is governed by a competition of superconductivity and other types of order. It is an open question how an ordered state at low doping can coexist with antiferromagnetic order.

This work is supported by the Deutsche Forschungsgemeinschaft (Research unit 538).

[1] L. Alff *et al.*, Nature **422**, 698 (2003).

TT 30.14 Thu 17:30 HSZ 02

Quasiparticle transport characteristics of thin film $La_{2-x}Ce_xCuO_4$ bicrystal junction SQUIDs — •Michael Wagenknecht[1], Boris Chesca[1], Martin Mueller[1], Dieter Koelle[1], Reinhold Kleiner[1], Akio Tsukada[2], and Michio Naito[3] — [1]Physikalisches Institut - Experimentalphysik II, Universitaet Tuebingen, Auf der Morgenstelle 14, 72076 Tuebingen — [2]NTT Basic Research Laboratories, 3-1 Morinosato Wakamiya, Atsugi-shi, Kanagawa 243, Japan — [3]Department of Applied Physics, Tokyo University of Agriculture and Technology (TUAT) 2-24-16 Naka-cho, Koganei, Tokyo 184-8588, Japan

While it is widely recognized that hole doped cuprates have predominantly d-wave symmetry of the superconducting order parameter, for electron doped cuprates the issue remains controversial. Here we present quasiparticle transport measurements of electron doped $La_{2-x}Ce_xCuO_4$ thin film bicrystal Josephson junction SQUIDs. The 900 nm thin films were deposited by molecular beam epitaxy on $SrTiO_3$ 24° and 30° [001]-tilt bicrystal substrates and have a Ce doping of $x \sim 0.08$ and a $T_c \sim 30$ K. At 4.2 K we observe in some SQUIDs a pronounced zero-bias anomaly in the quasiparticle differential conductance in magnetic fields up to 7 T, consistent with the formation of Andreev bound states at the junction interface. These results are strongly supportive of a d-wave symmetry, in accordance with previous work [1]. In addition we will discuss the subgap structures as well as some resonances at energies above the superconducting gap, which we repeatedly observed in quasiparticle transport measurements.

[1] B. Chesca et al., Phys. Rev. B **71**, 104504 (2005).

TT 30.15 Thu 17:45 HSZ 02

Symmetry and shape of the gap function in the hole- and electron-doped superconductors: the functional renormalization-group analysis — •Andrey Katanin[1,2] and Arno Kampf[3] — [1]Max-Planck-Institut für Festkörperforschung, D-70569, Stuttgart, Germany — [2]Institute of Metal Physics, 620219 Ekaterinburg, Russia — [3]Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

The problem of symmetry of superconducting pairing and the form of the gap function in the hole- and electron-doped superconductors are considered within the temperature-cutoff functional renormalization group approach combined with the Bethe-Salpeter equations. The momentum dependence of the order parameter for antiferromagnetic and superconducting instabilities in these compounds is analyzed. In the superconducting channel we find significant deviations from the conventional d-wave form of the gap functions. For hole-doped case a higher angular momentum component arises besides the standard $d_{x^2-y^2}$-wave component, which flattens the angular dependence of the gap. In the electron-doped case the gap function in the antiferromagnetic (particle-hole) channel has its maxima at the hot spots, or at the diagonal of the Brillouin zone in their absence. The wavefunction in the singlet superconducting channel is non-monotonic in the vicinity of the $(\pi, 0)$ and $(0, \pi)$ points in striking similarity with recent experimental data. The instability in the triplet superconducting channel is much weaker than in the singlet one and has f-wave like form of the gap function.

TT 30.16 Thu 18:00 HSZ 02

From d- to p-wave pairing in the t-t' Hubbard model at zero temperature — •K. Held and R. Arita — Max-Planck Institut für Festkörperphysik, Stuttgart

The Hubbard model is commonly considered to be relevant for unconventional superconductors like cuprates and ruthenates. For a more thorough insight into the physics of this model (is it explaining superconductivity?), the dynamical cluster approximation (DCA) combined with quantum Monte Carlo (QMC) [1] is a promising approach. DCA(QMC) is however restricted to rather high temperatures T. A prediction of superconducting phases at low-T is hence problematic. As a new path to low T, a projective QMC algorithm for impurity problems was recently developed [2], allowing for the solution of the dynamical mean field approximation (DMFT) equations in the $T \to 0$ limit.

We extend this projective QMC algorithm to DCA [3], and apply it for studying pair susceptibilities of the two-dimensional Hubbard-model with next-nearest neighbor hopping. In particular, we identify which pairing symmetry is dominant in the U-n parameter space (U: repulsive Coulomb interaction; n: electron density). We find that p_{x+y}- ($d_{x^2-y^2}$-) wave is dominant among triplet (singlet) pairings -at least for $0.3 < n < 0.8$ and $U <= 4t$. The crossover between $d_{x^2-y^2}$-wave and p_{x+y}-wave occurs around $n \sim 0.4$.

[1] M.H. Hettler *et al.*, Phys. Rev. B **58** R7475 (1998).
[2] M. Feldbacher, K. Held, and F. F. Assaad, Phys. Rev. Lett. **93**, 136405 (2004).
[3] K. Held and R. Arita, cond-mat/0508639.

TT 30.17 Thu 18:15 HSZ 02

Superconductivity and Antiferromagnetism in the 2d-Hubbard model – An RG and MF approach — •Julius Reiss, Daniel Rohe, and Walter Metzner — MPI-FKF,Heisenbergstrasse 1, 70569 Stuttgart

The functional renormalisation technique in the wick-ordered scheme is used to derive an low energy model, which is treated with an extended mean-field calculation to get insight into the symmetry-broken phase of

the 2–dimensional Hubbard model. d-wave superconductivity (SC) and s-wave antiferromagnetism (AF) and coexistence of both is found. The issue of the reliability of low energy models for order parameters, which show first order transitions, like the AF, is discussed.

TT 30.18 Thu 18:30 HSZ 02

Kondo screening in unconventional superconductors: The role of anomalous propagators — •Lars Fritz and Matthias Vojta — Theorie der Kondensierten Materie, Universitaet Karlsruhe

The Kondo effect in superconductors is frequently investigated using the local quasiparticle density of states as sole bath characteristics, i.e., the presence of anomalous propagators is ignored. We show that this is exact for a number of experimentally relevant situations, including point-like impurities in d-wave superconductors.

TT 31 Correlated Electrons: Metal Insulator Transition - Part 2

Time: Thursday 14:00–18:30 Room: HSZ 301

TT 31.1 Thu 14:00 HSZ 301

The spin states of $LaCoO_3$; a revision revised — •M. W. Haverkort[1], Z. Hu[1], J. C. Cezar[2], H. Wu[1], J. Gegner[1], T. Burnus[1], T. Koethe[1], H. Hartmann[1], M. Reuther[1], T. Lorenz[1], A. Tanaka[3], N. B. Brookes[2], H. H. Hsieh[4], H.-J. Lin[5], C. T. Chen[5], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]European Synchrotron Radiation Facility, Boîte Postale 220, 38043 Grenoble Cédex, France — [3]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [4]Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — [5]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan

Using soft x-ray absorption spectroscopy and magnetic circular dichroism at the Co-$L_{2,3}$ edge we show that the spin state transition in $LaCoO_3$ can be well described by a low-spin ground state and a high-spin first excited state which becomes populated at elevated temperatures. Sum rules used on the magnetic circular dichroism signal reveal a large orbital momentum, in good agreement with a low-/high-spin scenario, but hard to reconcile with a low-/intermediate-spin picture. We discuss why the original prediction of the intermediate-spin state from band theory may be questionable.

TT 31.2 Thu 14:15 HSZ 301

Electronic structure of $LaTiO_3$ and $YTiO_3$ — •A. Gössling[1], R. Rückamp[1], H. Roth[1], T. Lorenz[1], A. Freimuth[1], and M. Grüninger[2] — [1]II. Phys. Institute, University of Cologne, Germany — [2]II. Phys. Institute, University of Aachen, Germany

In Mott-Hubbard insulators, excitations from the lower to the upper Hubbard bands give rise to an interesting multi-peak structure in the optical conductivity. The spectral weight of these features is very sensitive to magnetic and orbital correlations.

Using spectroscopic ellipsometry, we determined the optical conductivity σ between 0.8 and 6 eV of the Mott-Hubbard insulators $YTiO_3$ and $LaTiO_3$ as function of temperature. While the spectra of $YTiO_3$ show a sizeable redistribution of spectral weight with temperature, those of $LaTiO_3$ are almost temperature independent. In $YTiO_3$ a strong anisotropy between $\sigma_{a,b}$ and σ_c is observed, which we trace back to an orbitally-ordered ground state.

Supported by the DFG in SFB 608

TT 31.3 Thu 14:30 HSZ 301

Raman light-scattering in the Mott-insulators $LaTiO_3$ and $YTiO_3$: Evidence for orbital excitations — •C. Ulrich[1], A. Gössling[2], M. Grüninger[3], M. Guennou[1], H. Roth[2], M. Cwik[2], T. Lorenz[2], G. Khaliullin[1], and B. Keimer[1] — [1]Max-Planck-Institut FKF, Stuttgart — [2]Universität zu Köln — [3]RWTH Universität Aachen

Collective excitations of the valence electrons between different atomic orbitals (termed "orbitons") contain a wealth of information about the different types of interactions between the spin, charge and orbital arrangement of the electrons. Experiments introducing Raman scattering as a direct probe of orbitons in $LaMnO_3$ [1] have hence opened up new perspectives. However, the results have proven to be quite controversial [2,3]. In order to identify orbital excitations in the titanates $LaTiO_3$ and $YTiO_3$ we have used the Raman light scattering technique. The Raman spectrum of these Mott-insulators exhibits pronounced electronic excitations around 230 meV, i.e. well above the energy range of two-phonon excitations. Based on the temperature, polarization, and photon energy dependence, this mode is identified as orbital excitation. The observed profiles bear a striking resemblance to magnetic Raman modes in the insulating parent compounds of the superconducting cuprates, indicating an unanticipated universality of the electronic excitations in transition metal oxides. [1] E. Saitoh et al., Nature 410, 180 (2001). [2] M. Grüninger et al., Nature 418, 39 (2002). [3] E. Saitoh et al., Nature 418, 40 (2002).

TT 31.4 Thu 14:45 HSZ 301

Surface acoustic wave investigations of the metal-to-insulator transition of V_2O_3 thin films — •Claus Müller, Alexei A. Nateprov, Günter Obermeier, Matthias Klemm, Reinhard Tidecks, Achim Wixforth, and Siegfried Horn — Institut für Physik, Universität Augsburg, D-86159, Augsburg, Germany

A sensitive tool to study the lattice and electronic system of thin solid films are surface acoustic waves (SAW) generated on a piezoelectric substrate on which the material of interest is attached. By electron-beam evaporation a V_2O_3 film was deposited onto piezoelectric $LiNbO_3$. To investigate the metal-to-insulator (MI) transition surface acoustic wave studies were performed in a temperature range from 260K to 10K. The attenuation becomes maximal at the MI-transition and shows a hysteresis not only of electronic nature. The sound velocity change reveals a precursor of the MI-transition of V_2O_3 [1], which can also be detected in the attenuation using a self-retuning SAW delay line.

[1] C. Müller, A. A. Nateprov, G. Obermeier, M. Klemm, R. Tidecks, A. Wixforth, and S. Horn, J. Appl. Phys. **98**, 084111 (2005)

TT 31.5 Thu 15:00 HSZ 301

Evidence for dimer formation in XPS investigation of VO_2 — •T.C. Koethe[1], Jan Gegner[1], Z. Hu[1], F. Venturini[2], N.B. Brookes[2], W. Reichelt[3], and L.H. Tjeng[1] — [1]II. Physikalisches Institut der Universität zu Köln — [2]ESRF, Grenoble, France — [3]Institut für Anorganische Chemie, TU Dresden

VO_2 is a non-magnetic d^1-system that undergoes a metal-to-insulator transition (MIT) at 340K. Above this temperature VO_2 is metallic and has a rutile structure (R-phase). At low temperatures it is an insulator with a monoclinic structure (M_1-phase) in which V-V pairs are formed.

The long standing debate about this compound concerns the nature of the MIT. The issue is whether it can be regarded as a Peierls-transition with the character of a band insulator (one electron picture) or whether it should be viewed as a Mott-insulator (many-body-picture). Recently the scenario of an orbital assisted MIT has been proposed on the basis of the dramatic change of the orbital occupation across the MIT as observed by soft-X-ray absorption spectroscopy measurements.[1]

We present the results of our photoemission investigation of the MIT in VO_2 using high quality single crystals and 700eV photon energy. We observe a huge transfer of spectral weight across the MIT and a pronounced two peak structure in the R-phase, supporting recent LDA+DMFT cluster calculations.[2] Similar features are also observed in the insulating phase of the d^1-system Ti_2O_3. The origin of this double peak structure in the insulating phase can be related to the formation of dimers.

[1] M.W. Haverkort *et al.*, Phys. Rev. Lett. **95**, 196404 (2005)
[2] S. Biermann *et al.*, Phys. Rev. Lett. **94**, 026404 (2005)

TT 31.6 Thu 15:15 HSZ 301

Orbital fluctuations and Mott gap in $LaVO_3$ and YVO_3 — •E. Pavarini[1], M. Raychaudhury[2], and O.K. Andersen[2] — [1]IFF-Forschungzentrum Juelich, D-52425 Germany — [2]MPI-FKF, Heisenbergstrasse 1, D-70569 Stuttgart

The Mott insulators $LaVO_3$ and YVO_3 have attracted a lot of attention because of their anomalous magnetic and electronic properties, which are

ascribed to the interplay bewteen orbital (t_{2g}) degrees of freedom, lattice and Coulomb repulsion. Here, by using the Nth-order Muffin Tin Orbital (NMTO)-based downfolding procedure, we construct a low energy Hubbard Hamiltonian for the partially filled t_{2g} bands; we than solve this Hamiltonian by means of LDA+DMFT, and obtain the full self-energy matrix in orbital space; we have already applied successfully this approacht to the series of $3d^1$ perovskites [1]. We will show that, in the case of $LaVO_3$ and YVO_3, orbital fluctuations are strong (more for $LaVO_3$ than for YVO_3) in the high temperature paramagnetic phase, and that they play an important role also in the low temperature magnetic phases. The interplay between filling, Coulomb repulsion, crystal field splitting and band widths is discussed, and their role in determining the size of the Mott gap in $LaVO_3$ and YVO_3 clarified.
[1] E. Pavarini, S. Biermann, A. Poteryaev, A.I. Lichtenstein, A. Georges, and OK Andersen, PRL **92** 176403 (2004).

TT 31.7 Thu 15:30 HSZ 301

Polarization- and temperature-dependent Ru-$L_{2,3}$ XAS study of Ca_2RuO_4 — •T. Burnus[1], Z. Hu[1], T. T. Tran[2], T. Mizokawa[2], H. H. Hsieh[3], L.-Y. Jang[4], S. Nakatsuji[5], Y. Maeno[5,6], M. Braden[1], K. S. Liang[4], and L. H. Tjeng[1] — [1]II. Phys. Inst., Univ. zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Dep. of Physics, Univ. of Tokyo, Bunkyo-ku, Tokyo 113, Japan — [3]Chung Cheng Inst. of Tech., National Defense Univ., Taoyuan 335, Taiwan — [4]Nat. Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30077, Taiwan — [5]Dep. of Physics, Kyoto Univ., Kyoto 606-8501, Japan — [6]Intern. Innov. Center, Kyoto Univ., Kyoto 606-8501, Japan

In the quasi-two-dimensional $Ca_{1-x}Sr_xRuO_4$, the strong correlations due to narrow electron bands and the active orbital degree of freedom yield a wide range of interesting properties. Ca_2RuO_4 has a transition at 350 K from a paramagnetic metal to a paramagnetic insulator and, cooling further down, it turns at 110 K into an antiferromagnetic insulator. We carried out polarization- and temperature-dependent X-ray absorption spectroscopy (XAS) at the Ru-$L_{2,3}$ edges in order to determine the occupation of the Ru 4*d* orbitals and their changes crossing the phase transitions; until now the occupation has been only obtained from O-*K* XAS, which contrary to the Ru-$L_{2,3}$ XAS only indirectly contains this information via the hybridization of the oxygen 2*p* with the ruthenium 4*d* orbitals. We observed the hysteretic change of the orbital occupation crossing the phase transitions. Furthermore, we confirmed the recently found additional phase transition around 260 K (Zegkkinglou *et al.* PRL, 2005).

TT 31.8 Thu 15:45 HSZ 301

New perspectives on charge ordering phenomena in complex transition-metal oxides — •Y. Su[1], H.F. Li[1], A. Nefedov[2], J. Persson[1], P. Meuffels[1], J. Grabis[2], H. Zabel[2], D. Wermeille[3], V. Kaiser[4], D. Schrupp[5], R. Claessen[5], V.A.M. Brabers[6], D. Prabhakaran[7], A.T. Boothroyd[7], P.D. Hatton[8], and Th. Brueckel[1] — [1]Institut für Festköperforschung, Forschungszentrum Juelich, D-52425 Juelich — [2]Inst. für Experimentalphysik IV, Ruhr-Universität Bochum — [3]MuCAT, Advanced Photon Source, Argonne National Laboratories — [4]Inst. für Kristallographie, RWTH — [5]Experimental Physik IV, Universität Wüzburg — [6]Dept. of Phys., Eindhoven University of Technology — [7]Dept. of Phys., Univ. of Oxford — [8]Dept. of Phys., Univ.of Durham

New insights on the nature of charge ordering in transition-metal oxides (TMO) have been gained via the latest resonant scattering experiments carried out in both soft (< 1 KeV) and hard (~ 8 KeV) X-ray regimes on high-quality single crystals of lightly hole-doped La7/8Sr1/8MnO3 and mixed-valence Fe3O4. A giant resonance at the oxygen K absorption edge has been observed from the charge ordering superstructure reflections of both compounds, suggesting that the charge ordering is strongly associated with a spatial modulation of ligand-hole states near the Fermi surface. Comprehensive data obtained at the corresponding L3/L2 and K-edges also strongly supports this scenario. These investigations not only allow us to resolve the long-standing puzzles concerning the nature of the Verway transition, but also indicate that the localized ligand holes might be a key ingredient for many charge-transfer type TMO.

TT 31.9 Thu 16:00 HSZ 301

Bandwidth-controlled Mott transition in κ-phase BEDT-TTF salts — •Martin Dressel[1], N. Drichko[1], M. Dumm[1], D. Faltermeier[1], C. Meziere[2], and P. Batail[2] — [1]1. Phys. Inst., Univ. Stuttgart, Germany — [2]Lab. CIMI, CNRS-Univ. d'Angers, France

Infrared reflection measurements of the half-filled two-dimensional organic conductors κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_x$Cl$_{1-x}$ are performed as a function of temperature and Br-substitution ($x = 0\%$, 40%, 73%, 85%, and 90%) in order to study the metal-insulator transition. The mid-infrared band centered around 3400 cm^{-1} for $E \parallel c$ is assigned to localized charge transfer within the dimers which is barely visible along the *a* direction. As the charge becomes delocalized for increasing Br content and low temperatures, the band shifts to higher frequencies. In a similar way, intramolecular vibrations which are observed via electron-molecular vibration coupling change in frequency. As the temperature drops below 50 K an energy gap develop in the Cl-rich samples which increase for $T \to 0$. With increasing Br concentration spectral weight shifts into the gap region and eventually fills it up completely. As these samples ($x = 85\%$ and 90%) become metallic at low temperatures, a Drude-like component develops due to the coherent quasiparticles. We perform a detailed analysis of the spectral weight transfer which gives us insight into the influence of electronic correlations on the dynamical properties. The observed behavior of the Drude spectral weight at the critical value of U/t (which is reached for $x \approx 70\%$) agrees with the abrupt jump to a finite value predicted by theory. The series of alloys is a good model of a bandwidth-controlled Mott insulator.

— 15 min. break —

TT 31.10 Thu 16:30 HSZ 301

Signature of collective excitations close to the metal-to-insulator transition — •Götz Uhrig[1], Carsten Raas[1], and Michal Karski[2] — [1]FR 7.1, Geb. E2.6, Universität des Saarlandes, D-66123 Saarbrücken — [2]Insitut für Angewandte Physik, Universität Bonn, D-53115 Bonn

A high-resolution calculation of the dynamical mean-field equations for the half-filled Hubbard model reveals a clear signature of collective excitations close to the metal-to-insulator transition. This calculation has become possible by current advances in dynamical density-matrix renormalization. The effect of collective excitations is seen as sharp peaks at the inner edges of the Hubbard bands. These peaks evidence a strong interaction between charge and collective degrees of freedom. The corresponding susceptibilities display signatures of the involved collective modes.

TT 31.11 Thu 16:45 HSZ 301

Orbital-selective Mott transitions in Hubbard models with orbital-dependent hopping — •Nils Blümer, Carsten Knecht, Krunoslav Požgajčić, and Peter van Dongen — Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz

The anisotropic degenerate two-orbital Hubbard model is studied within dynamical mean-field theory at low temperatures. High-precision calculations on the basis of a refined quantum Monte Carlo (QMC) method reveal that two distinct orbital-selective Mott transitions occur for a bandwidth ratio of 2 even in the absence of spin-flip contributions to the Hund exchange. The second transition – not seen in earlier studies using QMC, iterative perturbation theory, and exact diagonalization – is clearly exposed in a low-frequency analysis of the self-energy and in local spectra. These published [1] results are complemented with recent studies using QMC and Potthoff's self-energy functional method.
[1] C. Knecht, N. Blümer, and P.G.J. van Dongen, Phys. Rev. B **72**, 081103(R) (2005).

TT 31.12 Thu 17:00 HSZ 301

Continuous-time quantum Monte Carlo Scheme for Multi-orbital Impurity Problems — •Evgeny Gorelov[1], Alexey Rubtsov[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia

A determinantal continuous-time quantum Monte Carlo (CTQMC) algorithm has been applied for the numerically exact calculation of the fermionic multiorbital impurity path-integral. The five-band model for realistic transition metal atoms with full Coulomb interaction vertex as Kondo impurities in a metal matrix is calculated. The metal-insulator phase transition for two and three anisotropic orbitals on the Bethe lattice with spin-flip interactions is considered. The obtained results are in good agreement with available previous studies. Application to a cobalt impurity in the copper matrix shows the formation of a many-body Abrikosov-Suhl-Kondo resonance near the Fermi level.

TT 31.13 Thu 17:15 HSZ 301

Spectral properties of correlated materials — •Jan M. Tomczak — Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France

Strong Coulomb interactions in solids can give rise to phenomena in the electronic excitation spectrum that lie beyond the one-particle picture, and are thus not accessible by density functional theory in the local density approximation (LDA), or any static treatment of the correlations (as in LDA+U). Among these are large transfers of spectral weight, the appearance of satellite structures and non-negligeable lifetime effects. By means of analytical continuation of Quantum Monte-Carlo data obtained within the framework of LDA + Dynamical Mean-Field Theory, we determine the real-frequency selfenergy for realistic materials. Therewith interesting quantities, such as k-resolved spectral functions, quasi-particle bands and optical conductivities become accessible. We discuss technical aspects of the scheme, and, as an application, we make predictions for angle resolved photoemission spectra of vanadium dioxide.

TT 31.14 Thu 17:30 HSZ 301

Gapped and gapless phases of the Hubbard model with disorder — •Krzysztof Byczuk[1], Walter Hofstetter[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institut of Theoretical Physic A, RWTH Aachen, Templergraben 55, 52056 Aachen, Germany

The ground state phase diagram of correlated electrons with disorder is calculated within dynamical mean-field theory using the geometrically averaged ("typical") local density of states. The transitions between different gapped and gapless phases (paramagnetic, antiferromagnetic, Anderson localized) are described. In particular, the metal-insulator transition due to electronic correlations ("Mott-Hubbard transition") and disorder ("Anderson localization"), respectively, and the transition between a Slater and a Heisenberg antiferromagnet are discussed. The staggered magnetization is calculated as a function of disorder strength and interaction.

K. Byczuk, W. Hofstetter, and D. Vollhardt, Phys. Rev. Lett. 94, 056404 (2005); Physica B 359-361, 651 (2005).

TT 31.15 Thu 17:45 HSZ 301

Stochastic Green's function approach to disordered systems — •Andreas Alvermann and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17487 Greifswald, Germany

We adopt a stochastic approach based on distributions of Green's functions to study the electronic structure of disordered systems. Exemplarily, we address Anderson localisation as well as cluster effects in binary alloys. Combining this stochastic Green's function approach with dynamical mean field theory, we investigate the competition between polaron formation and Anderson localisation in a generic model for a disordered electron-phonon system.

TT 31.16 Thu 18:00 HSZ 301

Effective model for $E \otimes \beta$-coupling and electron-electron interaction — •Daniela Schneider, Klaus Ziegler, and Karl-Heinz Höck — Institut für Physik, Universität Augsburg, 86135 Augsburg

We investigate the effect and interplay of orbital and spin degrees of freedom. The model takes electron-electron interaction and electron-phonon coupling of the $E \otimes \beta$-type into account. The hopping is considered as orbital conserving. We derive an effective spin-orbital Hamiltonian at quarter filling through projection on singly occupied sites, treating the phonons quantummechanically, and discuss the symmetry of the initial and the effective model. Furthermore we identify the similarities and differences to the purely electronic and the adiabatic effective Hamiltonian. The anisotropy in the orbital part reflects the difference of spin and orbital exchange. The groundstate properties are studied for small clusters and the influence of the electron-phonon interaction and the spin and orbital occupancy are investigated. For dimers we compare the results obtained by exact diagonalisation with those achieved with the effective Hamiltonian.

This work is supported by DFG (SFB 484).

TT 31.17 Thu 18:15 HSZ 301

Transport properties of polaronic systems at finite temperature — •Alexander Weisse[1], Andreas Alvermann[1], Gerald Schubert[1], Gerhard Wellein[2], and Holger Fehske[1] — [1]Theoretische Physik II, Universität Greifswald, 17487 Greifswald — [2]RRZ Erlangen, Universität Erlangen, 91058 Erlangen

We review recent developments of Chebyshev expansion based algorithms for the calculation of dynamical correlation functions and apply these techniques to the one-dimensional Holstein model. Focussing on the case of finite temperatures, we present exact numerical results for the optical response in this prototypical model for electron-lattice interaction. In addition, we analyze deviations from the standard small polaron theory in the intermediate coupling regime and discuss non-adiabaticity effects in detail. [Phys. Rev. B 72, 104304 (2005)]

TT 32 Transport: Quantum Coherence and Quantum Information Systems - Part 2

Time: Thursday 14:00–17:45 Room: HSZ 304

TT 32.1 Thu 14:00 HSZ 304

Voltage control in a three-junction flux qubit — •Luca Chirolli and Guido Burkard — Department of Physics-University of Basel-Basel-Switzerland

By means of a general circuit analysis, we study a superconducting flux qubit with three Josephson junction in which enhanced control is achieved by introducing electrostatic gates. We discuss the additional terms in the single-qubit Hamiltonian due to an applied gate voltage.

[1] G.Burkard, Phys.Rev.B 71, 144511 (2005)
[2] J.E.Mooij et al., Science 285, 1036 (1999)

TT 32.2 Thu 14:15 HSZ 304

Inductive effects in tunable capacitive coupling of charge qubits — •Carsten Hutter and Alexander Shnirman — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D–76128 Karlsruhe, Germany

Recently, tunable capacitive [1] and inductive [2] coupling of Josephson charge and flux qubits have been proposed. Here, we concentrate on coupling of charge qubits via a Josephson junction, which provides a tunable effective capacitance. For this situation, it was suggested [3], that the capacitive coupling could be accompanied by an inductive one. We clarify the situation by considering the limits where the Josephson energy of the coupling junction is much greater (much smaller) than its charging energy, $E_J \gg E_c$ ($E_J \ll E_c$). In the limit $E_J \ll E_c$, the inductive coupling appears as a small correction to the capacitive one. It will however play a role at the point, where the capacitive coupling vanishes. In the limit $E_J \gg E_c$, we find that the inductive coupling dominates over the capacitive one.

[1] D. V. Averin and C. Bruder, Phys. Rev. Lett. 91, 057003 (2003).
[2] B. L. T. Plourde *et al.*, Phys. Rev. B 70, 140501(R) (2004).
[3] A. Zorin, cond-mat/0510435 (2005)

TT 32.3 Thu 14:30 HSZ 304

Readout of a Flux Qubit Using a Capacitive Bias — •Frank Deppe[1,2,3], Shiro Saito[2,3], Kosuke Kakuyanagi[2,3], Takayoshi Meno[4], Kouichi Semba[2,3], Hideaki Takayanagi[2,3], and Rudolf Gross[1] — [1]Walther-Meissner-Institut, Garching, Germany — [2]NTT Basich Research Laboratories, NTT Corporation, Atsugi, Japan — [3]CREST JST, Saitama, Japan — [4]NTT AT, Atsugi, Japan

A promising candidate for the basic information unit for (future) scalable solid state based quantum computing is the Mooij flux qubit [1]. It consists of a superconducting loop with 3 Josephson junctions. The flux signal of the qubit states ((anti-)clockwise circulating current) can be detected with a superconducting quantum interference device (SQUID). We successfully implemented a novel variant of the pulse&hold switching method. Creating the SQUID bias current via a coupling capacitor instead of the usual coupling resistor allows faster switching pulses while keeping proper filtering conditions for the bias line. The bias capacitor also reduces external low frequency noise. Our setup allows a direct comparison between resistive and capacitive environment on the *same* qubit. We present the results of measurements on a SQUID/flux qubit system based on nanoscale Al/AlO_x/Al junctions. In time domain experiments near the qubit magic point we find a slighly reduced dephasing time

$T_2 \approx 150$ ns for the capacitive bias compared to 250 ns for the resistive bias. The reults indicate that the impact of external low frequency on qubit phase coherence is small in our system.
Supported by: SFB 631 of the Deutsche Forschungsgemeinschaft
[1] J. E. Mooij et al., *Science* **285**, 1036 (1999)

TT 32.4 Thu 14:45 HSZ 304

On-chip Quantum Information Processing in Circuit QED — •Henning Christ[1], Matteo Mariantoni[2], and Enrique Solano[1,3] — [1]Max-Planck Institute for Quantum Optics, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, D-85748 Garching, Germany — [3]Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado 1761, Lima, Peru

We consider an on-chip linear array of flux-based qubits inside individual quasi-1D superconductive resonators and introduce, in the context of quantum information theory, different possibilities of realizing quantum computation with suitably designed long-lived qubits. In particular, we present in a comparative manner the advantages and disadvantages of establishing on-chip quantum communication protocols via single photon exchange or via novel continuous-variable schemes. For the purpose, the latter turn out to be the most promising avenue given that single-photon detectors are still unavailable in the microwave domain. Finally, we propose a deterministic single-qubit teleportation protocol based on unitary generation of qubit-cavity Schrödinger cats, where no single-photon detector is needed.

TT 32.5 Thu 15:00 HSZ 304

Theory of Microwave Homodyne Tomography of Quantum Signals — •Matteo Mariantoni[1], Markus J. Storcz[2], Frank K. Wilhelm[2], William D. Oliver[3], Andreas Emmert[1], Achim Marx[1], Rudolf Gross[1], Henning Christ[4], and Enrique Solano[4,5] — [1]Walther-Meissner-Institut, Walther-Meissner-Str. 8, D-85748 Garching, Germany — [2]Department Physik, ASC and CeNS, Ludwig-Maximilians-Universität, Theresienstr. 37, D-80333 München, Germany — [3]MIT Lincoln Laboratory, 244 Wood Street, Lexington, Massachussets 02420, USA — [4]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany — [5]Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado 1761, Lima, Peru.

Weak quantum signals cannot be detected using standard ultra-low-noise cryogenic amplifiers or the state-of-the-art available classical methods. As a consequence, the measurement of nonclassical states of microwave electromagnetic radiation is a fundamental problem and necessity in the novel field of circuit QED [1] (see TT 19, E. Solano).

We propose a microwave quantum homodyne detection technique that enables the measurement of quantum states at the level of single photons and allows the reconstruction of their Wigner function through microwave quantum homodyne tomography. Our method is based on a superconducting hybrid ring acting as an on-chip microwave beam splitter (see also presentation TT 19, A. Emmert). This work was supported by the SFB 631 of the DFG.
[1] M. Mariantoni *et al.*, cond-mat/0509737.

TT 32.6 Thu 15:15 HSZ 304

Mesoscopic Superpositions, Nonclassical States, and their Measurement in Circuit QED — •Markus J. Storcz[1], Matteo Mariantoni[2], Andreas Emmert[2], Rudolf Gross[2], Frank K. Wilhelm[1], Henning Christ[3], and Enrique Solano[3,4] — [1]Department Physik, ASC and CeNS, Ludwig-Maximilians-Universität, Theresienstr. 37, 80333 München, Germany — [2]Walther-Meissner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, 85748 Garching, Germany — [4]Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado 1761, Lima, Peru

We propose a novel scheme consisting of a superconducting qubit coupled to a microwave cavity with an additional transverse control line. We show that an orthogonal and strong classical driving allows for the simultaneous implementation of Jaynes-Cummings and anti-Jaynes-Cummings dynamics, opening new avenues in the generation of nonclassical states and mesoscopic superpositions (Schrödinger cats). Moreover, the proposed set-up can also be used for implementing a projective qubit measurement and for reconstructing the associated field Wigner function. Relevant decoherence aspects and specific design parameters for a superconducting charge qubit inside a coplanar waveguide resonator are presented.

This work was supported by the SFB 631 of the DFG.

TT 32.7 Thu 15:30 HSZ 304

Microshort induced pinning potential for a Josephson vortex, probed in the quantum limit with microwave spectroscopy. — •Astria Price, Alexander Kemp, and Alexey V. Ustinov — Physikalisches Institut III, Universitaet Erlangen-Nuernberg, Erlangen D-91058, Germany

A long annular Josephson junction with a lithographic microshort, produced by widening a short section of the junction, constitutes a vortex qubit candidate in which the height of the microshort induced potential barrier seen by a Josephson vortex is tuned via an applied magnetic field. We investigate the energy level structure of the vortex potential in this type of junction by means of microwave spectroscopy, and compare the results to a model based on the one-dimensional sine-Gordon equation. Applying bias current creates a metastable state for the vortex, in which it is pinned by either the magnetic field or the microshort, and escapes via thermal activation or quantum tunnelling. We measure the energy level separation between the ground and first excited states of the vortex in both types of metastable potential well, and extract the cross-over temperature from thermal activation to quantum tunnelling as a function of bias current and magnetic field strength.

— 15 min. break —

TT 32.8 Thu 16:00 HSZ 304

Observation of Rabi oscillations in a phase qubit — •J. Lisenfeld[1], A. Lukashenko[1], S. Shitov[2], and A.V. Ustinov[1] — [1]Physikalisches Institut III, Universität Erlangen, Germany — [2]Institute of Radio Engineering and Electronics, Moscow, Russia

Quantum bits based on superconducting tunnel junction circuits are promising candidates to realize solid-state quantum computation. A phase qubit is formed from an rf-SQUID, whose Josephson phase eigenstates are used as logical states [1]. Those are mapped to macroscopically distinct flux states in the readout process, which is based on quantum tunneling stimulated by a short pulse of magnetic flux.

We experimentally demonstrate the preparation of an arbitrary quantum state in such a system, which has been fabricated using our design at a standard foundry. Rabi oscillation, a spectroscopic measurement of the dephasing time and evidence of qubit coupling to parasitic resonators are presented. From upcoming data on the temperature dependence of decoherence processes we hope to clarify whether the observed Rabi-type oscillations, alternatively, originate from a classical junction dynamics in the microwave field [2].
[1] R.W. Simmonds et al., Phys. Rev. Lett. 93, 077003 (2004)
[2] N. Grønbech-Jensen and M. Cirillo, Phys. Rev. Lett. 95, 067001 (2005)

TT 32.9 Thu 16:15 HSZ 304

Adiabatic passage in superconducting nanocircuits — •Jens Siewert[1,2], Tobias Brandes[3], and Giuseppe Falci[1] — [1]MATIS-INFM, CNR and DMFCI, University of Catania, I-95125 Catania, Italy — [2]Institut fuer Theoretische Physik, University of Regensburg, D-93040 Regensburg, Germany — [3]Department of Physics, The University of Manchester, Manchester M60 1QD, United Kingdom

With the rapid technological progress in quantum-state engineering in superconducting devices there is an increasing demand for techniques of quantum control. Stimulated Raman adiabatic passage (STIRAP) is a powerful method in quantum optics which has remained largely unknown to solid-state physicists. It is used to achieve highly efficient and controlled population transfer in (discrete) multilevel quantum systems. Apart from other potential applications in solid-state physics, adiabatic passage offers interesting possibilities to manipulate qubit circuits, in particular for the generation of nonclassical states in nanomechanical or electromagnetic resonators. In this contribution, we explain the idea of the method and describe examples of controlled quantum dynamics in superconducting nanocircuits by applying adiabatic passage.

TT 32.10 Thu 16:30 HSZ 304

Macroscopic quantum dynamics in one-dimensional Josephson junction arrays — •Mikhail V. Fistul — Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum Germany

I present a theoretical study of the current-voltage characteristics (I-V curves) of one-dimensional Josephson junction arrays containing small Josephson junctions. The transport properties of such a system are determined by the dynamics of both "classical"degrees of freedom, i.e. the phases of superconducting order parameter in leads, and the macroscopic quantum degrees of freedom, i.e. the Josephson phases of intrinsic junctions. I will show that at low temperature and in a particular regime characterizing by a large damping in leads and a small damping in an internal part of the system, the I-V curves are determined by the quantum correlations of Josephson phases, and therefore, it allows to obtain a direct information on the macroscopic quantum dynamics, i.e. macroscopic quantum tunneling of vortices or Coulomb blockade of Cooper pairs. In the framework of this analysis the Cooper pair cotunneling regime [1] and the superconductor-insulator transition [2] in Josephson junction arrays will be discussed.

[1] S. V. Lotkhov, S. A. Bogoslovsky, A. B. Zorin, and J. Niemeyer, Phys. Rev. Lett. 91, 197002 (2003)
[2] E. Chow, P. Delsing, and D. B. Haviland, Phys. Rev. Lett. 81, 204 (1998)

TT 32.11 Thu 16:45 HSZ 304

Quantum tunneling of semifluxons in 0-π-0 long Josephson junction: Theory — •Edward Goldobin[1], Karl Vogel[2], Oliver Crasser[2], Reinhold Walser[2], Wolfgang Schleich[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Universität Tübingen, Physikalisches Institut - Experimentalphysik II, Auf der Morgenstelle 14, D-72076, Tübingen, Germany — [2]Universität Ulm, Abteilung Quantenphysik, D-89069 Ulm, Germany

We consider a system of two semifluxons of opposite polarity in a 0-π-0 long Josephson junction, which classically can be in one of two degenerate states: $\uparrow\downarrow$ or $\downarrow\uparrow$. When the distance a between the 0-π boundaries (semifluxon's centers) is a bit larger than the crossover distance a_c, the system can switch from one state to the other due to thermal fluctuations or due to quantum tunneling. We map this problem to the dynamics of a single particle in a double well potential and estimate parameters for which quantum effects emerge. We also determine the classical-to-quantum crossover temperature as well as the tunneling rate (energy level splitting) between the states $\uparrow\downarrow$ and $\downarrow\uparrow$. This system may be a promising candidate for realization of qubits since semifluxons represent the ground state of the system. See [1] for details.

[1] Phys. Rev. B. **72**, 054527 (2005).

TT 32.12 Thu 17:00 HSZ 304

Non-Markovian dynamics of double quantum dot charge qubits due to a phonon bath — •Jens Eckel, Stephan Weiss, and Michael Thorwart — Institut fuer Theoretische Physik IV, Universitaetsstrasse 1, 40225 Duesseldorf

We investigate the decoherent dynamics of charge qubits in two particular setups: (i) GaAs double quantum dots and (ii) two single P donor ions in a Si host lattice. In both cases, one excess electron is shared and a single charge qubit is formed. In particular, we study the charge qubit coupled to acoustic phonons which induce a non-Markovian dynamical behavior of the oscillations between the two charge states. Upon applying the numerically exact quasiadiabatic propagator path-integral scheme for both setups, the reduced density matrix is calculated, thereby avoiding the Born-Markov approximation. The damped coherent oscillations of the electron between the two dots determine a quality factor whose dependence on the lattice temperature, on the size of the quantum dots, as well as on the interdot coupling is studied systematically [1]. The comparison with the recent experimental result by Hayashi and coworkers [2] for double quantum dots will be discussed.

[1] M. Thorwart, J. Eckel and E. R. Mucciolo, Phys. Rev. B, in press.
[2] T. Hayashi et al., Phys. Rev. Lett. 91, 226804 (2003).

TT 32.13 Thu 17:15 HSZ 304

How fat is Schrödinger's cat? — •Benjamin Abel, Florian Marquardt, and Jan von Delft — Ludwig-Maximilians-Universität, Arnold Sommerfeld Center for Theoretical Physics and Center for Nanoscience,Theresienstr. 37, 80333 München

Recent experiments have tried to produce superpositions of "macroscopically distinct"quantum states, e.g. in small superconducting quantum interference devices (SQUIDs) or in microwave cavities. These superpositions are commonly referred to as "Schrödinger cat states"(1). In this work, we provide an answer to the following important question: "How 'macroscopic' is such a superposition?". We present a general measure of the distance between two arbitrary many-body states forming such a superposition, going beyond previous works that only considered a special class of possible states (2). After illustrating its general features, we apply our measure to experiments employing three-junction SQUIDs (Mooij), where the ground state at half a flux quantum is a superposition of clockwise and counterclockwise flowing supercurrents: $|\Psi\rangle = (|\text{left}\rangle + |\text{right}\rangle)/\sqrt{2}$.

[1] E. Schrödinger, *"Die gegenwärtige Situation in der Quantenmechanik"*, Naturwissenschaften, **48**, 807, **49**, 823, **50**,844 (1935).
[2] W. Dürr, C. Simon, and J. I. Cirac, Phys. Rev. Lett. **89**, 210402 (2002).
[3] J. E. Mooij, *et al.*, Science **285**, 1036 (1999).

TT 32.14 Thu 17:30 HSZ 304

Investigation of the ground state of Nb charge-phase qubits — •Hermann Zangerle, J. Könemann, B. Mackrodt, R. Dolata, S. A. Bogoslovsky, M. Götz, and A. B. Zorin — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

There are several implementations of qubits built of small Josephson junctions. The Bloch transistor included in a superconducting loop can serve as a so-called charge-phase qubit with both electrostatic and magnetic control of its quantum state. For readout the device is inductively coupled to a rf-driven tank circuit. Applying chemical-mechanical polishing technique we have fabricated from Nb/Al/AlO_x/Nb sandwich the charge-phase qubits with junction size of 60 nm by 60 nm and nominal critical current of the single junction of about 50 nA. Our all-Nb samples of gradiometer design include the transistor in the loop and the tank circuit inductance on the same chip. The high critical temperature of Nb and our circuit layout make it possible to precharacterize the samples at 4.2 K. We report the radio-frequency measurements of Nb qubit circuits with characteristic ratio of the Josephson to charging energy E_J/E_c between 1 and 2 carried out at 20 mK. Due to appreciable charging energy E_c of about 50 μeV the transistor critical current was remarkably modulated by the gate. We investigated the ground state of our qubit samples as a function of two control parameters: flux Φ and charge Q. The sample with the energy ratio $E_J/E_c \sim 1$ allowed to map the complete ground state energy surface $E(\Phi, Q)$.

TT 33 Superconductivity: Vortex Dynamics, Vortex Phases, Pinning

Time: Friday 10:15–12:30 Room: HSZ 304

TT 33.1 Fri 10:15 HSZ 304

Fluxoid quantization effect on the specific heat of mesoscopic superconductors — •Florian Ong[1], Olivier Bourgeois[1], Sergey Skipetrov[2], and Jacques Chaussy[1] — [1]CRTBT-CNRS 25 Avenue des Martyrs BP 166 38042 GRENOBLE cédex 9 France — [2]LP2MC-CNRS *(same address)*

Up to now, despite their deep fundamental relevance, thermal properties of matter stuctured at the nanoscale have not received much attention. Here we present highly sensitive specific heat measurements of mesoscopic superconductors, at low temperature (down to 0.5 K) and under a tunable magnetic field (up to 1 T).

Our calorimeter is a thin suspended silicon membrane, containing a heater and a thermometer, on which nanostructures are deposited after an e-beam lithography. Using a temperature oscillation method and ultra low noise electronics, the resolution $\frac{\Delta C}{C}$ can reach 5.10^{-5}.

We investigated thin Aluminium loops [1] and disks of 1 to 2.5 μm in diameter, a size closed to the superconducting coherence length $\xi(T)$ at 1 K. When sweeping the magnetic field H at a fixed temperature the behavior of the specific heat C is strongly governed by the fluxoid quantization. Indeed $C(H)$ exhibits a periodicity of $n \times \Phi_0$ (n is an integer depending on the temperature, and on the sample topology and size ;

$\Phi_0 = h/2e$ is the superconducting flux quantum). These oscillations are the signatures of phase transitions between different vortex states, and can be described within the framework of the Ginzburg-Landau theory.
[1] O. Bourgeois, S. Skipetrov, F. Ong, J. Chaussy, Phys. Rev. Lett. 94, 0557007 (2005)

TT 33.2 Fri 10:30 HSZ 304

Temperature Dependent Matching in a Periodic Pinning Lattice with Disorder — •J. Eisenmenger[1], M. Oettinger[1], C. Steiner[1], C. Pfahler[1], A. Plettl[1], H.-G. Boyen[1], A. Ethirajan[1], P. Walther[2], and P. Ziemann[1] — [1]Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Zentrale Einheit Elektronenmikroskopie, Universität Ulm, D-89069 Ulm, Germany

We prepared a lattice of nanoscaled artificial pinning centers (APCs) into a Nb film. The patterning technique is based on self-organization of inverse micelles of diblock-copolymers on a substrate. The resulting lattice of APCs mirrors the order of the micellar array which is triangular on the short range, but loses its directional order for larger distances. A unique feature of such prepared samples is that, in contrast to perfectly ordered pinning arrays, the matching field, as defined by the field where the critical current I_c has a maximum, depends on temperature. At the first glance any temperature dependence is unexpected, since the value of matching field for a triangular lattice $B_1 = (2\Phi_0)/(\sqrt{(}3)a^2)$ only depends on the lattice constant a of the APCs and the flux quantum Φ_0, which both are temperature independent. Several possible interpretation of this unusual behavior are discussed. In particular it is considered that a is not a fixed value for the entire self-assembled APC lattice but varies over a certain range.

TT 33.3 Fri 10:45 HSZ 304

Nonlocal Vortex Dynamics in Narrow Superconducting Channels — •Andreas Helzel[1], Ivan Kokanović[2], Dinko Babić[2], and Christoph Strunk[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, HR-10000 Zagreb, Croatia

We investigated superconducting microstructures composed of a vertical wire crossed by two horizontal wires. In presence of an external magnetic field, a supercurrent in the upper horizontal wire drives a flow of vortices in the vertical wire. This results in a nonlocal voltage response in the lower wire [1]. We use very low pinning amorphous NbGe as superconductor, resulting in a 100 times larger nonlocal response compared to [1] and a moderate decrease when varying the channel length between 2 and 5 μm. Comparing with the local flux flow properties, we observe that the nonlocal flux flow is maximal around the irreversibility line of plain NbGe wires and extends up to B_{c2}. In the regime of very few vortex rows in the channel reproducible fluctuations occur in the nonlocal signal, which can be understood as jamming effects near the detector cross.
[1] Grigorieva et. al., Phys. Rev. Lett. 92, 237001 (2004)

TT 33.4 Fri 11:00 HSZ 304

Bending of magnetic avalanches in MgB_2 thin films — •J. Albrecht[1,2], A. T. Matveev[1,2], M. Djupmyr[1], H.-U. Habermeier[2], and G. Schütz[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

The penetration of magnetic flux lines into a superconductor above the lower critical field happens not necessarily in a regular way. It is found that under particular conditions a chaotic penetration in form of magnetic avalanches occurs. These avalanches are closely related to the so called thermomagnetic instability, which identifies local heating due to flux line movement as the origin of the effect. In case of MgB_2 thin films these avalanches are found only below $T = 10$ K and are suppressed by a covering metallic layer with high thermal conductivity and sufficient thickness. These avalanches are observed in case of partly gold covered MgB_2 films by the magnetooptical Faraday-effect. The investigation of avalanches propagating into a gold covered region revealed a change of the propagation direction depending on the incident angle of these avalanches.

TT 33.5 Fri 11:15 HSZ 304

Overcritical currents across grain boundaries in YBaCuO thin films — •Christian Jooss[1], Eva Brinkmeier[1], and Harald Heese[2] — [1]Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Numerische Mathematik, University of Göttingen, Germany

The current distribution in thin superconducting films can be strongly modified by the presence of soft magnetic environments. A soft magnet put parallel to a thin film edge can reduce or completely prevent flux entry and therefore stabilize Meissner screening currents in the film. This effect is of particular importance for the modification of the current distributions across grain boundaries in high-Tc superconductors, where the intergranular critical current density strongly depends on the flux which penetrates into the grain boundary. Furthermore, using special magnetic arrangements, asymmetric flux and current distributions can be obtained. An increase of the grain boundary critical current is obtained in the Meissner state, compared to the flux penetrated states [1]. The experimental studies via quantitative magneto-optical imaging are combined with theoretical calculations of the flux and current density distributions of superconducting strips in magnetic environments of arbitrary shape. The theoretical simulations are obtained by considering a boundary value problem for the Laplace equation as a mathematical model, which is then treated via integral equation methods.
[1] Ch. Jooss, E. Brinkmeier and H. Heese, Phys. Rev. B **72** (2005) 144516.

TT 33.6 Fri 11:30 HSZ 304

Anisotropic temperature-dependent current densities in vicinal YBCO — •Märit Djupmyr and Joachim Albrecht — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Thin epitaxial films of $YBa_2Cu_3O_{7-\delta}$ grown on vicinal cut substrates exhibit a substantial anisotropy of the critical current density j_c in the film plane. By means of quantitative magneto-optical analysis it is possible to independently investigate the current densities along the two occurring current directions. A detailed analysis of the temperature dependence of the critical currents in the range of $T = 5 - 90$ K will be shown. Completely different behavior of $j_c(T)$ along the different directions were found. Describing the data by a step-wise power-law ansatz allows to distinguish between different current limiting mechanisms like thermal depinning and depairing which are important in different temperature ranges.
[1] S. Brück and J. Albrecht, Phys. Rev. B **71**, 174508 (2005)
[2] M. Djupmyr, G. Cristiani, H.-U. Habermeier and J. Albrecht, Phys. Rev. B, submitted

TT 33.7 Fri 11:45 HSZ 304

Defect Melting of Vortices in High-T_c Superconductors — •Jürgen Dietel and Hagen Kleinert — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We set up a melting model for vortex lattices in high-temperature superconductors based on the continuum elasticity theory. The model is Gaussian and includes defect fluctuations by means of a discrete-valued vortex gauge field. We derive the melting temperature of the lattice and predict the size of the Lindemann number. Our result agrees well with experiments for $YBa_2Cu_3O_{7-\delta}$, and with modifications also for $Bi_2Sr_2CaCu_2O_8$. We calculate the jumps in the entropy and the magnetic induction at the melting transition.

TT 33.8 Fri 12:00 HSZ 304

Microscopic Study of Pinning Mechanisms in YBCO HTSC Films — •Tetyana Shapoval, Volker Neu, Ulrike Wolff, Ruben Hühne, Jens Hänisch, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

The direct microscopic imaging of flux lines is a powerful tool for the understanding of vortex pinning mechanism at natural and artificial defects and can help to increase the critical current density. For these investigations a low-temperature scanning probe microscope (Omicron Cryogenic SFM) is used, which allows AFM, MFM and STM/STS measurements in UHV combined with magnetic fields of 7 T (vertical) and 3 T (transversal) at low temperatures (9 K - 300 K). Flux lines of an YBCO film have been successfully imaged by measuring their stray field in MFM modus. The 300 nm thick film with mean roughness less than 10 nm has been prepared by off-axis PLD and has been cooled down in the microscope to 7.7 K in a magnetic field of 3 mT prior to imaging. The number

of vortices that we observed corresponds to the theoretically expected one. Whereas a constant current leads to the unacceptable heating of the sample, the use of current pulses allows transport measurements, avoiding thermal movement of vortices. The depinning mechanism is studied on a structured YBCO film by in situ imaging of flux lines under the influence of increasingly larger current pulses.

TT 33.9 Fri 12:15 HSZ 304

How the Flux Line Lattice in the Anisotropic High-T_c Superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ Melts: A Magnetic Force Microscopy study — •Alexander Schwarz[1], Marcus Liebmann[2], Ung Hwan Pi[1], and Roland Wiesendanger[1] — [1]University of Hamburg, IAP, Jungiusstr. 11, 20355 Hamburg — [2]Present Address: RWTH Aachen, Department of Physics, 52056 Aachen

The behavior of a trigonal flux line lattice corresponding to a flux density of about 3.5 mT was investigated in a $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal upon increasing the temperature stepwise from 5.1 K towards T_c. In this highly anisotropic material flux lines consist of relative weakly bound pancake vortices confined to the copper oxide planes. Magnetic force microscopy images recorded with single flux line resolution revealed a temperature dependence of the regularity of the long-range order and the apparent flux-line size. Both observations can be explained by the interplay between the temperature dependence of the London penetration depth, collective pinning and subsequent depinning above 30 K, thermal motion of the vortices and lateral dragging by the force sensor itself. At the highest temperature the typical flux line contrast composed of a coherent alignment of pancake vortices along the crystal c-axis disappeared. Instead, a liquid-like behavior of individual pancakes can be observed.

TT 34 Correlated Electrons: Spin Systems and Itinerant Magnets

Time: Friday 10:15–12:30 Room: HSZ 301

TT 34.1 Fri 10:15 HSZ 301

Nonmagnetic Impurities in the Two-Dimensional Kondo-Necklace — •Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

The effects of nonmagnetic impurities on the two-dimensional spin-1/2 Kondo-necklace model are investigated. In its undoped state this spin-model displays a quantum-critical point at a Kondo-exchange coupling of $J \approx 1.4$ which separates a dimerized singlet-phase from an antiferromagnetically ordered ground state. Using quantum Monte-Carlo calculations based on the stochastic series expansion, results will be presented for the uniform susceptibility and the staggered structure factor as a function of temperature, impurity concentration, and Kondo exchange. It will be shown, that on dilution of the Kondo sites the systems develops quasi-free moments with a renormalized Curie-constant. Moreover, the quantum critical point is suppressed, with a disorder induced long-range antiferromagnetic order to appear also in the singlet phase, which amounts to an order-from-disorder phenomenon.

TT 34.2 Fri 10:30 HSZ 301

Phase diagram of the two-dimensional quantum Heisenberg antiferromagnet with an easy-axis anisotropy — •Martin Holtschneider[1], Stefan Wessel[2], and Walter Selke[1] — [1]Institut für Theoretische Physik, RWTH Aachen — [2]Institut für Theoretische Physik, Universität Stuttgart

The square lattice spin-1/2 Heisenberg antiferromagnet with an easy-axis anisotropy is studied in an external magnetic field, using Quantum Monte Carlo simulations based on the stochastic series expansions with a directed loop update. The model displays long range ordered antiferromagnetic, algebraically ordered spin-flop, and paramagnetic phases. The low-temperature phase diagram is determined by studying both thermodynamic quantities such as the (staggered) suszeptibility and the staggered magnetization as well as histograms of e.g. the order parameter distribution. The numerical results are compared to previous findings on this model (being equivalent to a hard core boson Hubbard model), in particular G. Schmid et al., Phys. Rev. Lett. 88, 167208 (2002), and the results on the corresponding classical model in M. Holtschneider et al., Phys. Rev. B 72, 064443 (2005).

TT 34.3 Fri 10:45 HSZ 301

Reduction of surface coverage of finite systems due to geometrical steps — •C. Olbrich[1], K. Morawetz[1,2], S. Gemming[3], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Institute of Physical Chemistry, Technical University Dresden, Germany

The coverage of surfaces interrupted by a step with molecules is simulated by a two-dimensional Ising model. An analytical mean-field model is developed which is capable to describe main properties of this frustrated Ising model due to the surface geometry. We find a reduction of coverage (magnetization) at low temperatures due to the presence of the surface step for certain bonding strengths. This represents a second transition besides the usual phase transition and is characterized by a diverging susceptibility and magnetization as a finite-size effect. The specific heat diverges with a power law due to the surface step.

TT 34.4 Fri 11:00 HSZ 301

Evidence for collective orbital excitations in YVO_3 — •E. Benckiser[1,2], R. Rückamp[1], M. Grüninger[2], A.A. Nugroho[3], and T.T.M. Palstra[3] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]II. Physikalisches Institut, RWTH Aachen, Germany — [3]Materials Science Centre, Rijksuniversiteit Groningen, The Netherlands

The compound YVO_3 recently has attracted a lot of interest because of its unusual structural, orbital and magnetic properties [1,2]. The compound undergoes a series of temperature-induced phase transitions accompanied by a change of orbital and magnetic order. Furthermore it has been proposed that YVO_3 represents the first realization of a one-dimensional orbital liquid and an orbital Peierls phase, with a transition to an orbitally ordered phase at lower temperatures [3].

We present the optical conductivity $\sigma(\omega)$ of YVO_3 single crystals for energies from 0.1 eV to 1.6 eV and temperatures from 15 K to 300 K. The data have been collected by performing measurements using linearly polarized light with the electric field vector parallel to the crystallographic axes (σ_a,σ_b,σ_c). The results give clear evidence for orbital excitations. In particular the strong polarization and temperature dependence of two peaks observed at 0.3 eV in σ_c and 0.5 eV in σ_a are hard to reconcile with an interpretation in terms of local crystal-field excitations. We propose an interpretation in terms of orbitons and discuss a simple model describing a two-orbiton absorption process. [1] Ren *et al.*, Nature **396**, 441(1998); [2] Blake *et al.*, PRB **65**, 174112 (2002); [3] Ulrich *et al.*, PRL **91**, 257202 (2003). *Supported by the DFG through SFB 608.*

TT 34.5 Fri 11:15 HSZ 301

Helimagnetism and Weak Ferromagnetism in the Edge-Shared Chain Cuprate $NaCu_2O_2$ — •S.-L. Drechsler[1], J. Richter[2], A.A. Gippius[3], A.N. Vasiliev[3], A.A. Bush[4], A.S. Moskvin[5], J. Malek[6], Yu. Prots[7], W. Schnelle[7], and H. Rosner[7] — [1]IFW-Dresden, 01171 Dresden, PF 270116, Germany — [2]Universität Magdeburg, Germany — [3]Moscow State University, Russia — [4]Moscow Inst. of Radiotechnics, Electronics and Automation, Russia — [5]Ural State University Ekaterinburg, Russia — [6]FZU AVCR, Praha, Czech Rep. — [7]MPI-cPfS Dresden, Germany

We report on susceptibility, magnetization, ^{23}Na NMR, and specific heat data of the spin-chain material $NaCu_2O_2$ in the paramagnetic and ordered phases. Below 13 K, where a sharp field-dependent specific heat peak appears, the NMR lineshape points to an incommensurate static modulation of the local magnetic field consistent with a spiral arrangement of the Cu magnetic moments. At 2 K weak ferromagnetism with a small ordered moment of about $4{\cdot}10^{-3}\mu_B$ has been observed. LDA based estimates of exchange integrals reveal a large inchain frustration leading to a magnetic spiral.

TT 34.6 Fri 11:30 HSZ 301

Itinerant iron magnetism and high spin polarization in filled skutterudites — •Helge Rosner, Andreas Leithe-Jasper, Walter Schnelle, Joerg Sichelschmidt, Steffen Wirth, John Mydosh, and Yuri Grin — MPI CPfS Dresden

Compounds with the filled skutterudite structure are currently under intensive investigation due to their wide spectrum of ground state

properties. Here, we report a combined theoretical and experimental study of the electronic and magnetic properties of the compound family AFe_4Sb_{12} (A=Na,K,Ca,Ba,Yb) by means of band structure calculations and measurements of point-contact Andreev reflections, optical spectra and thermodynamic properties (χ, C_P, ρ). Whereas the compounds with A=Na,K order ferromagnetically [1] with a high transport spin polarisation $P_t \sim 67\%$ [2], the magnetic order for A=Ca,Ba,Yb is suppressed by strong spin fluctuations. The latter compounds show a metamagnetic transition in high magnetic fields as suggested by fixed spin moment calculations. The Yb compound, formerly considered as a heavy fermion system, is proven to be in a stable divalent state by band structure calculations and optical and thermodynamic data [3].

[1] A. Leithe Jasper *et al.* Phys. Rev. Lett. **91**, 037208 (2003).
[2] G. Sheet *et al.* Phys. Rev. B **72**, in print (2005).
[3] W. Schnelle *et al.* Phys. Rev. B **72**, 020402(R) (2005).

TT 34.7 Fri 11:45 HSZ 301

Orbital Ordering and Spin-Ladder Formation in La_2RuO_5 — •Volker Eyert, Stefan G. Ebbinghaus, and Thilo Kopp — Institut für Physik, Universität Augsburg

The semiconductor-semiconductor transition of La_2RuO_5 is studied by means of augmented spherical wave (ASW) electronic structure calculations as based on density functional theory and the local density approximation. This transition has lately been reported to lead to orbital ordering and a quenching of the local spin magnetic moment. Our results give strong hints for a different orbital ordering scenario than the one previously proposed. In our type of ordering, the local $S = 1$ moment at the Ru sites is preserved in the low-temperature phase. The unusual magnetic behaviour is interpreted by the formation of spin-ladders, which result from the structural changes occurring at the transition and are characterized by antiferromagnetic coupling along the rungs.

TT 34.8 Fri 12:00 HSZ 301

Investigation of Orbital and Magnetic Order in Ruthenates with Resonant X-ray Diffraction — •Ioannis Zegkinoglou[1], J. Strempfer[1], B. Bohnenbuck[1], C.S. Nelson[2], C. Bernhard[1], and B. Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, USA

Resonant x-ray diffraction at the L_{II} and L_{III}-absorption edges of ruthenium has been used to investigate orbital and magnetic order in $4d$ transition metal oxide single crystals. A large resonance enhancement of the magnetic scattering cross-section due to electric dipole transitions directly into the $4d$ band is observed. In the single-layered Mott transition system Ca_2RuO_4, a new phase transition between two paramagnetic phases is observed around 260 K, at the wave-vector characterizing the low-temperature antiferromagnetic order [1]. Based on the polarization and azimuthal angle dependence of the diffracted intensity, the new phase transition is attributed to the ordering of the Ru t_{2g} orbitals. In $RuSr_2GdCu_2O_8$, the antiferromagnetic order of Ru ions and the possible effect of the onset of superconductivity on it below $T_c \approx 40$ K are investigated. Due to the sensitivity of resonant x-ray diffraction to the azimuthal angle, a precise determination of the direction of the magnetic moment in the system is possible.

[1] I. Zegkinoglou, J. Strempfer et al., Phys. Rev. Lett. 95, 136401 (2005)

TT 34.9 Fri 12:15 HSZ 301

Spin-Orbital Model for Layered Manganites — •Maria Daghofer[1] and Andrzej Oleś[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Jagellonian University Kraków, Poland

We present a spin-orbital t-J model for undoped and doped manganites at $T = 0$ and at finite temperature. The model fully takes into account onsite Coulomb repulsion of these strongly correlated materials. We investigate it by use of Exact Diagonalization and Monte Carlo techniques.

With inclusion of a crystal field term, we obtain a realistic model for $La_{1-x}Sr_{1+x}MnO_4$, showing a gradual change from predominantly out-of-plane ($3z^2 - r^2$) to more in-plane ($x^2 - y^2$) orbital occupation both with doping and with rising temperature. At higher doping, we obtain the CE-AF phase for $x = 0.5$ as well as the C-AF phase observed in $Nd_{1-x}Sr_{1+x}MnO_4$ at $x > 0.75$.

For undoped bilayer clusters, we obtain for realistic parameter values the A-AF phase observed in three-dimensional compounds, with orbital correlations in accordance with experiment. At high doping, the model predicts the C-AF and G-phases as they are found in strongly doped $La_{2-2x}Sr_{1+2x}Mn_2O_7$.