

TIEFE TEMPERATUREN (TT)

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ÜBERSICHT DER HAUPTVORTRÄGE UND FACHSITZUNGEN

(Hörsäle TU H104, TU H2053, TU H3027)

Hauptvorträge

TT 4.1	Fr	14:00	(TU H104)	Phase Sensitive Tests with Cuprate Superconductors Based on the Josephson Effect and Andreev bound states , Boris Chesca , Dietmar Dönitz, Dieter Kölle, Reinhold Kleiner, A. Tsukada, Michio Naito, Ariando, Hans Hilgenkamp
TT 4.3	Fr	14:45	(TU H104)	Angle-Resolved Photoemission Spectroscopy of High-T_c Superconductors: Identifying the Pairing Boson , Sergey Borisenko
TT 7.1	Fr	16:30	(TU H2053)	Self-Energy Functionals: A New Approach to Strongly Correlated Electron Systems , Michael Potthoff
TT 9.1	Fr	17:00	(TU H3027)	Ultracold Atoms in Optical Lattices: Tunable Quantum Many-Body Systems , Walter Hofstetter
TT 14.1	Sa	13:45	(TU H104)	Flux Qubits , Hans Mooij
TT 14.2	Sa	14:15	(TU H104)	Single-Shot State Measurement of Coupled Phase Qubits , John Martinis
TT 17.1	Mo	10:15	(TU H104)	From Spin to Quantum Order in Coordination Polymer Magnets , Collin Broholm
TT 17.2	Mo	10:50	(TU H104)	Design, Synthesis and Study of Model Quantum Magnets , Andrew Harrison
TT 18.1	Mo	10:00	(TU H2053)	Two-Gap Superconductivity in MgB_2 , Thomas Dahm
TT 18.8	Mo	12:00	(TU H2053)	Point-Contact Spectroscopy on Conventional and Unconventional Superconductors , Gernot Goll
TT 19.5	Mo	11:00	(TU H3027)	Spin Pumping in a Mesoscopic Spin Battery , Bart van Wees
TT 19.6	Mo	11:30	(TU H3027)	Intrinsic Spin Hall Effect , Shuichi Murakami
TT 20.1	Mo	12:30	(TU P270)	Quantum Correlations in Mesoscopic Systems , Wolfgang Belzig
TT 21.2	Mo	14:25	(TU H104)	2D Quantum Antiferromagnets from Néel-Ordered Phases to Spin Liquids , Claire Lhuillier
TT 21.6	Mo	16:20	(TU H104)	Geometrical Frustration as Paradigm for Low Temperature Physics , Arthur Ramirez
TT 24.1	Di	10:15	(TU H104)	Single-Electron Transport in Nano-Electromechanical Devices , Yaroslav M. Blanter
TT 24.2	Di	10:50	(TU H104)	Nano-Electromechanical Systems with Carbon Nanotubes , Yuval Yaish , Vera Sazonova, Ethan D. Minot, Hande Üstünel, David Roundy, Tomas A. Arias, Paul L. McEuen
TT 28.1	Di	14:00	(TU H104)	Cryogenic Detectors for X-ray Astronomy , Piet de Korte

Fachsitzungen

TT 1	Superconductivity - Fabrication, Technical Optimization and Characterization	Fr 10:15–13:00	TU H104	TT 1.1–1.11
TT 2	Correlated Electrons - Metal Insulator Transition	Fr 10:15–13:00	TU H2053	TT 2.1–2.11
TT 3	Correlated Electrons - Heavy Fermions	Fr 10:15–13:00	TU H3027	TT 3.1–3.11

TT 4	Symposium Superconducting Cuprates	Fr	14:00–17:45	TU H104	TT 4.1–4.10
TT 5	Superconductivity - Mechanisms, Phase Diagram, Competing Order	Fr	18:00–19:00	TU H104	TT 5.1–5.4
TT 6	Correlated Electrons - (General) Theory I	Fr	14:00–16:15	TU H2053	TT 6.1–6.9
TT 7	Correlated Electrons - (General) Theory II	Fr	16:30–18:45	TU H2053	TT 7.1–7.8
TT 8	Posters Transport	Fr	14:00–18:00	Poster TU C	TT 8.1–8.53
TT 9	Solids at Low Temperature - Quantum Liquids, Bose-Einstein Condensates, Ultracold Atoms, ...	Fr	17:00–18:45	TU H3027	TT 9.1–9.6
TT 10	Superconductivity - Tunneling, Josephson Junctions, SQUIDs	Sa	08:30–12:45	TU H104	TT 10.1–10.16
TT 11	Correlated Electrons - Spin Systems and Itinerant Magnets: Theory	Sa	08:45–10:30	TU H2053	TT 11.1–11.7
TT 12	Correlated Electrons - Spin Systems and Itinerant Magnets: Experiment	Sa	10:45–12:45	TU H2053	TT 12.1–12.8
TT 13	Transport - Quantum Coherence and Quantum Information Systems	Sa	08:45–12:45	TU H3027	TT 13.1–13.15
TT 14	Symposium Superconducting Quantum Systems	Sa	13:45–16:45	TU H104	TT 14.1–14.6
TT 15	Superconductivity - Properties, Electronic Structure, Order Parameter I	Sa	14:00–16:45	TU H2053	TT 15.1–15.10
TT 16	Posters Correlated Electrons, Measuring Devices, Cryotechnique	Sa	11:00–16:30	Poster TU C	TT 16.1–16.92
TT 17	Symposium Quantum Magnetism in Molecule-based Materials	Mo	10:15–13:00	TU H104	TT 17.1–17.6
TT 18	Superconductivity - Properties, Electronic Structure, Order Parameter II	Mo	10:00–13:00	TU H2053	TT 18.1–18.10
TT 19	Transport - Nanoelectronics I: Spintronics and Magnetotransport	Mo	10:00–12:15	TU H3027	TT 19.1–19.7
TT 20	Schottky Award Lecture	Mo	12:30–13:15	TU P270	TT 20.1–20.1
TT 21	Symposium Frustrated Systems	Mo	14:00–18:00	TU H104	TT 21.1–21.9
TT 22	Transport - Nanoelectronics II: Quantum Dots and Wires, Point Contacts	Mo	14:00–17:30	TU H2053	TT 22.1–22.13
TT 23	Posters Superconductivity, Solids at Low Temperature	Mo	14:00–18:00	Poster TU D	TT 23.1–23.62
TT 24	Symposium Nanomechanics	Di	10:15–12:50	TU H104	TT 24.1–24.5
TT 25	Correlated Electrons - Low-dimensional Systems: Models	Di	09:45–13:00	TU H2053	TT 25.1–25.13
TT 26	Superconductivity - Heterostructures, Andreev Scattering, Proximity Effect, Coexistence	Di	10:15–11:45	TU H3027	TT 26.1–26.6
TT 27	Solids at Low Temperature - New Materials	Di	12:00–12:30	TU H3027	TT 27.1–27.2
TT 28	Superconductivity - Applications I : Cryodetectors	Di	14:00–16:00	TU H104	TT 28.1–28.7
TT 29	Measuring Devices, Cryotechnique	Di	16:15–16:45	TU H104	TT 29.1–29.2
TT 30	Superconductivity - Applications II : Levitation, SQUID-based Sensors, Devices	Di	16:45–18:15	TU H104	TT 30.1–30.6
TT 31	Correlated Electrons - Low-dimensional Materials I	Di	14:00–16:00	TU H2053	TT 31.1–31.8
TT 32	Correlated Electrons - Low-dimensional Materials II	Di	16:15–18:30	TU H2053	TT 32.1–32.9
TT 33	Transport - Nanoelectronics III: Molecular Electronics	Di	14:00–18:00	TU H3027	TT 33.1–33.15
TT 34	Correlated Electrons - Quantum Impurities, Kondo Physics	Mi	09:45–11:15	TU H104	TT 34.1–34.6
TT 35	Correlated Electrons - Quantum Critical Phenomena	Mi	11:15–13:00	TU H104	TT 35.1–35.7
TT 36	Superconductivity - Vortex Dynamics, Vortex Phases, Pinning	Mi	10:00–13:00	TU H2053	TT 36.1–36.11
TT 37	Transport - Fluctuations and Noise	Mi	10:15–12:15	TU H3027	TT 37.1–37.8

Übersicht über die Sitzungen des Fachverbands Tiefe Temperaturen

Alle angegebenen Veranstaltung finden in Hörsälen der TU Berlin statt.

PV: Plenarvortrag ; ÖAV: Öffentlicher Abendvortrag; HV: Hauptvortrag ; FV: Fachvortrag ; SY:Symposium

SC: Superconductivity ; CE: Correlated Electrons ; TR: Transport ; SLT: Solids at Low Temperature

Freitag, 4.3.05

8:30-9:30 *PV Kouwenhoven*

Vormittag **SYQL** HE101

SY Measurements at the Quantum Limit

10:15-13:00 **TT 1** H104

SC - Fabrication, Technical

Optimization and Characterization

10:15-13:00 **TT 2** H2053

CE - Metal-Insulator Transition

10:15-13:00 **TT 3** H3027

CE - Heavy Fermions

14:00-17:45 **TT 4** H104

SY Superconducting Cuprates

14:00 HV Chesca

14:45 HV Borisenko

15:15 FV Hackl

16:00 FV Uhrig

14:00-16:15 **TT 6** H2053

CE - (General) Theory I

14:00-18:00 **TT 8** TU-C (2.OG)

Posters: Transport

17:00-18:45 **TT 9** H3027

SLT - Quantum Liquids,

BE Condensates,

Ultracold Atoms, ...

17:00 HV Hofstetter

18:00-19:00 **TT 5** H104

SC - Mechanisms, Phase Diagram,

Competing Order

20:00-21:30 *ÖAV Gaub*

Samstag, 5.3.05

Vormittag **SYRS** H3010

SY Renormalization and Scaling

8:30-12:45 **TT 10** H104

SC - Tunneling, Josephson

Junctions, SQUIDs

8:45-10:30 **TT 11** H2053

CE - Spin Systems and

Itinerant Magnets:

Theory

8:45-12:45 **TT 13** H3027

TR - Quantum Coherence and

Quantum Information Systems

10:45-12:45 **TT 12** H2053

CE - Spin Systems and

Itinerant Magnets:

Experiment

13:45-16:45 **TT 14** H104

SY Superconducting

Quantum Systems

13:45 HV Mooij

14:15 HV Martinis

14:45 FV Duty

15:15 FV Wallraff

15:45 FV Fazio

16:15 FV Wilhelm

14:00-16:45 **TT 15** H2053

SC - Properties, Electronic Structure,

Order Parameter I

11:00-16:30 **TT 16** TU-C (2.OG)

Posters: Correlated Electrons,

Measuring Devices, Cryotechnique

17:00-18:00 *PVe Cesarisky & Ekert*

18:15-21:15 Welcome evening for all participants

Montag, 7.3.058:30-9:30 *PVe Norton & Kroemer*10:15-13:00 **TT 17** H104
SY Quantum Magnetism
in Molecule-based Materials10:15 *HV Broholm*10:50 *HV Harrison*11:30 *FV Lang*12:00 *FV Honecker*10:00-13:00 **TT 18** H2053
SC - Properties, Electronic
Structure, Order Parameter II10:00 *HV Dahm*12:00 *HV Goll*10:00-13:00 **TT 19** H3027
TR - Nanoelectronics I:
Spintronics and Magnetotransport11:00 *HV van Wees*11:30 *HV Murakami*12:30-13:15 **TT 20** P270
Schottky Award Lecture by *Belzig*14:00-18:00 **TT 21** H104
SY Frustrated Systems14:00 *FV Brenig*14:25 *HV Lhuillier*14:50 *FV Fulde*15:15 *FV Moessner*15:40 *FV Troyer*16:20 *HV Ramirez*16:45 *FV Hemberger*17:10 *FV Lemmens*17:35 *FV Geck*14:00-17:30 **TT 22** H2053
TR - Nanoelectronics II:
Quantum Dots and Wires,
Point Contacts14:00-18:00 **TT 23** TU-D (3.OG)
Posters: Superconductivity,
Solids at Low Temperature18:00-19:45 **Allgemeine Mitgliederversammlung der DPG**20:00-21:30 *ÖAV Dosch***Dienstag, 8.3.05**8:30-9:30 *PV Braun-Munzinger*10:15-13:00 **TT 24** H104
SY Nanomechanics10:15 *HV Blanter*10:50 *HV Yaish*11:30 *FV Kotthaus*12:00 *FV Shnirman*9:45-13:00 **TT 25** H2053
CE - Low-dimensional
Systems: Models10:15-11:45 **TT 26** H3027
SC - Heterostructures,
Andreev Scattering,
Proximity Effect, Coexistence12:00-12:30 **TT 27** H3027
SLT - New Materials14:00-16:00 **TT 28** H104
SC - Applications I: Cryodetectors14:00 *HV de Korte*14:00-16:00 **TT 31** H2053
CE - Low-dimensional Materials I14:00-18:00 **TT 33** H3027
TR - Nanoelectronics III:
Molecular Electronics16:15-16:45 **TT 29** H104
Measuring Devices, Cryotechnique16:15-18:30 **TT 32** H2053
CE - Low-dimensional Materials II16:45-18:15 **TT 30** H104
SC - Applications II: Levitation,
SQUID-based Sensors, Devices18:30-19:45 **TT-Mitgliederversammlung** H205320:00-21:30 *ÖAV Keller*

Mittwoch, 9.3.058:30-9:30 *PV Sarachik*Ganztägig **SYUA** HU Audimax
SY Mesoscopic Physics of Ultracold Atoms9:45-11:15 **TT 34** H104
CE - Quantum Impurities,
Kondo Physics10:00-13:00 **TT 36** H2053
SC - Vortex Dynamics,
Vortex Phases, Pinning10:15-12:15 **TT 37** H3027
TR - Fluctuations and Noise11:15-13:00 **TT 35** H104
CE - Quantum Critical
Phenomena**Mitgliederversammlung des Fachverbands Tiefe Temperaturen**

Di 18:30–19:45 TU H2053

Tagesordnung

1. Frühjahrstagung 2005, Statistik
2. Themenkreise
3. Frühjahrstagung 2006, Termine, HV, Symposien
4. Neuwahl des Fachverbandsvorsitzenden TT
5. Verschiedenes

Fachsitzungen

– Haupt-, Fach-, Kurzvorträge und Posterbeiträge –

TT 1 Superconductivity - Fabrication, Technical Optimization and Characterization

Zeit: Freitag 10:15–13:00

Raum: TU H104

TT 1.1 Fr 10:15 TU H104

Boron-doped Diamond Films — ●H.C. FREYHARDT¹, K. WINZER², D. BOGDANOV², P.J. WILBRANDT¹, M. MALCHOW¹, L. SCHÄFER³, and J. WURM⁴ — ¹Institut für Materialphysik und — ²1. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — ³Fraunhofer-Institut Schicht u. Oberflächentechnik, Bienroder Weg 54E, 38108 Braunschweig — ⁴METAKEM GmbH, Achtehnmorgenweg 3, 61250 Usingen

After superconductivity was reported in bulk high-pressure synthesized B containing diamond, B-doped diamond films were deposited on polycrystalline W and single-crystalline Si substrates by a hot-filament activated chemical vapour deposition process. The polycrystalline films exhibit lattice constants which are slightly larger than for pure diamond. Whereas films on W are under compressive stresses, films on Si are almost stress-free. The nominal B-concentration varied between 2700 and 5200 ppmB and was checked by SIMS and Raman spectroscopy. Superconductivity was observed in all samples with a transition temperature T_c up to 3.3K for 5200 ppmB. The T_c increases with the B content and the transition width was found to be 0.2K for the best sample. Upper critical fields $B_{C2}(0)$ are scaling with T_c and reach 3.6T. It will be discussed whether superconductivity can be described by a BCS-like behaviour.

TT 1.2 Fr 10:30 TU H104

Superconductivity on boron-doped diamond plates — ●DMITRIJ BOGDANOV¹, KLAUS WINZER¹, and CHRISTOPH WILD² — ¹I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — ²Fraunhofer Institut für Angewandte Festkörperphysik, Tullastr. 72, 79018 Freiburg i. Br.

We study boron-doped diamond plates prepared by the microwave-plasma-CVD technique. In contrast to diamond films on silicon substrates the absence of a substrate allows unequivocal measurements of the electrical resistivity and of the Hall coefficient of the doped diamond. The samples show semiconducting behaviour in the non-superconducting state down to the critical temperatures between $0,4 \text{ K} < T_C < 4 \text{ K}$. The upper critical fields $B_{C2}(0)$ scale with the transition temperatures T_C ; their values are up to 3 tesla. The hole concentrations were determined by the measurements of the Hall coefficient at temperatures near T_C . The correlation of the calculated density of states $N(E_F)$ and T_C will be compared with different theoretical models.

TT 1.3 Fr 10:45 TU H104

Superconductivity in nominally undoped La based T'-structure cuprates — ●YOSHIHARU KROCKENBERGER^{1,2}, AKIO TSUKADA¹, HIDEKI YAMAMOTO¹, DIRK MANSKE², MICHIO NAITO³, and LAMBERT ALFF⁴ — ¹NTT Basic Research Laboratories, 3-1 Morinosato-Wakamiya, Atsugi, Kanagawa 243-0198, Japan — ²Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — ³Department of Applied Physics, Tokyo University of Agriculture and Technology, 2-24-16 Naka-cho, Koganei, Tokyo 184-8588, Japan — ⁴Vienna University of Technology, ISAS, Applied Electronic Materials, Gusshausstr. 27-29/366,A-1040 Vienna, Austria

La_2CuO_4 in the T-structure is classified as the "Mott-insulating" parent compound of the high-temperature superconductors. However, La_2CuO_4 with Nd_2CuO_4 (T') structure has not yet been synthesized and investigated due to the ionic size driven structural instability to the T-phase. We report the synthesis of $\text{La}_{2-x}\text{RE}_x\text{CuO}_4$ with the T' structure by molecular beam epitaxy, using isovalent substituents RE = Sm, Eu, Gd, Tb, Lu, and Y for La stabilizing the T' phase. Surprisingly, all these nominally undoped T'-compounds show metallic behavior and even become superconducting at critical temperatures up to 25K. The observed smooth decrease of the resistivity of samples grown in increasingly reducing atmosphere suggests that for these materials the expected Mott-insulating state is not obtained even close to the undoped compound. The phase

diagram of the electron-doped T'-compounds therefore seems to depend strongly on details of the crystal structure.

TT 1.4 Fr 11:00 TU H104

Preparation and characterization of UPd_2Al_3 thin films in (100) orientation — ●MICHAEL FOERSTER, CHRISTIAN HERBERT, MARTIN JOURDAN, and HERMANN ADRIAN — J.-Gutenberg-Universität Mainz

We prepared for the first time high quality thin films of the Heavy-Fermion superconductor UPd_2Al_3 in a*-axis orientation employing MBE methods. The natural (001) growth direction can be changed to (100) by using YAlO_3 (010) and (112) substrates. The samples were characterized in respect of their crystalline and superconducting properties. Buffer layers of naturally a*-axis oriented UNi_2Al_3 with thickness $\approx 100\text{\AA}$ resulted in clearly improved film quality. These new samples enable tunneling experiments on UPd_2Al_3 in a*-axis direction, which are of high interest to further investigate the symmetry of the unconventional sc-order parameter in this model system for Heavy-Fermion superconductivity.

TT 1.5 Fr 11:15 TU H104

Density of critical current of Nb and NbN thin film bridges — ●KONSTANTIN ILIN¹, MICHAEL SIEGEL¹, ALEXEI SEMENOV², HEINZ-WILHELM HÜBERS², and ANDREAS ENGEL³ — ¹Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe, Karlsruhe, Germany — ²DLR Institut für Planetenforschung, Berlin, Germany — ³Physics-Institute of the University of Zürich, Zürich, Switzerland

We present results of a systematic study of the critical current in superconducting Nb and NbN thin film bridges. The bridges with a width from 50 nm to $10\mu\text{m}$ were patterned from thin superconducting films by means of electron-beam lithography and ion milling. For both materials the nominal critical current density extrapolated to zero temperature varied with the bridge width and thickness. We attribute these variations to a fabrication-enhanced reduction of the effective, superconducting cross-section of the bridges with respect to their geometric cross-section and to an uneven distribution of the super-current over the superconducting core of the bridge. In very thin bridges, i.e. 5 nm and 8 nm for NbN and Nb, respectively, the nominal current density increased drastically when the bridge width became smaller than 500 nm. We associate the enhancement of the critical current in those bridges with the crossover from depinning of magnetic vortices to either their nucleation or breaking of Cooper pairs.

TT 1.6 Fr 11:30 TU H104

Laserablation und Charakterisierung von MgB_2 Filmen — ●CHRISTIAN LEIRER, ANDREAS HEINRICH und BERND STRITZKER — Universität Augsburg, EPIV, 86135 Augsburg

Seit der Entdeckung der Supraleitung in MgB_2 wurden unterschiedliche Verfahren zu dessen Herstellung entwickelt. Bei der Herstellung dünner Filme spielte die Laserablation bisher eine untergeordnete Rolle, da die erhaltenen Schichten deutlich schlechtere supraleitende Eigenschaften gegenüber dem Bulk-Material aufwiesen. Wir wollen hier eine modifizierte Methode der Lasseablation vorstellen, mit der es uns möglich ist, eine Sprungtemperatur von 38,5 K zu erreichen, was nahezu dem Wert des Bulk-Materials entspricht. Dies gelingt mit einem besonderen in-situ Annealingverfahren. Die erzielten Sprungtemperaturen liegen deutlich über den bisher mit PLD erreichten Werten. Zudem gelang es uns durch teilweise Abschattung des Substrates gegenüber dem Plasma, in diesem Bereich ein verbessertes Schichtwachstum zu erhalten. Das in-situ Annealingverfahren wird vorgestellt und die Mechanismen des Abschattungseffektes werden diskutiert. Weiter berichten wir über die Korrelation zwischen Plasmaeigenschaften während der Ablation, strukturellen sowie magnetfeldabhängigen supraleitenden Eigenschaften.

TT 1.7 Fr 11:45 TU H104

Superconductivity in nanocrystalline mechanically alloyed MgB₂ bulk samples and Fe sheathed multifilamentary tapes — ●OLAF PERNER¹, WOLFGANG HÄSSLER¹, CLAUS FISCHER¹, MARKO HERRMANN¹, GÜNTER FUCHS¹, KONSTANTIN NENKOV¹, BERNHARD HOLZAPFEL¹, LUDWIG SCHULTZ¹, and JÜRGEN ECKERT² — ¹Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, PF 270116, D-01171 Dresden — ²TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

The application of the mechanical alloying (MA) technique for MgB₂ powder preparation can be regarded as an optimal tool to obtain a nanocrystalline microstructure due to grain refinement as well as to control the exact stoichiometry of the MgB₂ compound. Subsequently hot pressed bulk samples as well as by the powder-in-tube technique fabricated tapes show enhanced magnetic flux pinning in the superconducting state resulting in high critical current density J_c values.

In order to investigate the role of grain boundaries and impurities on superconductivity in MgB₂ a series of bulk samples with different preparation parameters as well as impurity doping with oxides were characterized by transport and magnetization measurements as well as analytical transmission electron microscopy. The results will be described in detail and compared with the model of vortex dynamics.

The multifilamentary MgB₂ tapes exhibit high values of the critical current density J_c of 35 kA/cm² and 9 kA/cm² in external magnetic fields of 7.5 T and 10 T, respectively, at 4.2 K due to a homogeneous, nanocrystalline microstructure and small sized impurities.

TT 1.8 Fr 12:00 TU H104

In-situ RHEED-Charakterisierung und elektrische Eigenschaften von YBa₂Cu₃O₇-Schichten — ●A. HIRSCH, M. KARGER, F. LUDWIG und M. SCHILLING — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, TU-Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig

Zur Herstellung von Bauelementen aus Hochtemperatursupraleitern wie Josephson-Kontakte und supraleitende Quanteninterferometer (SQUIDS) sind dünne Schichten hoher epitaktischer Qualität erforderlich.

Mit den Methoden der statistischen Versuchsplanung wird das Wachstum von YBa₂Cu₃O₇ auf SrTiO₃-Einkristallsubstraten mittels gepulster Laser-Deposition (PLD) in Hinblick auf die strukturellen und elektrischen Eigenschaften untersucht. Insbesondere wird ein Zusammenhang zwischen den aus in-situ RHEED-Untersuchungen gewonnenen epitaktischen Eigenschaften der Schichten und den elektrischen Eigenschaften Übergangstemperatur T_c , kritische Stromdichte j_c bei 77 K und relativen Widerstandsverhältnis $R(300\text{ K})/R(100\text{ K})$ geprüft. Desweiteren wird der Einfluss von kontinuierlicher bzw. Intervall-Deposition auf die Schichtqualität diskutiert. Ein Überblick über die Ergebnisse wird gegeben.

TT 1.9 Fr 12:15 TU H104

J_c enhancement in YBa₂Cu₃O_{7-x} thin films by metal doping — ●J. HÄNISCH, C. CAI, R. HÜHNE, B. HOLZAPFEL und L. SCHULTZ — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Due to the sharp cube textures in RABiTS (rolling assisted biaxially textured substrates) tapes, grain boundaries are not the only J_c limiting

factor anymore and flux pinning is now again a focus for further improvement of coated conductors in higher magnetic fields.

In this work, we present a comparative study of the influence of different metallic dopants (D: Ir, Ti, Zr and Hf) on $J_c(B)$. Quasi-multilayer films of 40x(6.5 uc YBCO/n uc D) were prepared by pulsed laser deposition with a stoichiometric YBCO target and a metal target for the dopant, n being in the range of 0.04...0.3. In the case of Ir, nano-particles of BaIrO₃ are growing epitaxially inside the YBCO film. Due to their larger lattice parameter of 4.1 Å compared to 3.9 Å (*b*-axis) in YBCO, the YBCO structure is under lateral stress. A certain degree of disorder on the Ba sites is expected because of the non-stoichiometry after precipitation. Both introduce extended and random defects respectively and lead to an enhancement in pinning force density and irreversibility field.

In addition, Zn doping is investigated as a possibility to enhance J_c in thin films. At doping levels of $x < 0.05\%$, an increase in J_c in higher magnetic fields was found.

TT 1.10 Fr 12:30 TU H104

Cube textured Cu-based substrates for HTS coated conductors — ●RAINER NAST, BERNHARD OBST, GUNTER KOTZYBA, and WILFRIED GOLDACKER — Forschungszentrum Karlsruhe, Institut für Technische Physik, Postfach 3640, 76021 Karlsruhe

As alternative substrate tapes for coated conductor, cube textured copper based tapes instead of nickel are possible candidates to achieve high critical current densities in YBCO. The advantages of Cu are the non-ferromagnetism, the larger thermal and electrical conductivity and the lower cost of Cu in comparison to Ni. In this work, we report about the texturing of pure copper and different copper alloys, such as Cu-Sn, Cu-Mn and a dispersion hardened Cu-B4C tape. The annealing temperature have been optimized to get a high volume fraction of the cube texture as sharp as possible. The maximum of the cube texture deviation histograms is at 3.8° for Cu and 4.4° for Cu-B4C. In addition a continuous Ni overlayer was plated on Cu to avoid the diffusion of Cu and to improve the oxidation resistance for the following growth of buffer layers and YBCO.

TT 1.11 Fr 12:45 TU H104

Normal and mixed state Hall effect in (Hg_{0.9}Re_{0.1})Ba₂CaCu₂O_{6+δ} fully textured HTSC thin films — ●ABOUELWAF A SALEM, GERHARD JAKOB, and HERMANN ADRIAN — Institut für Physik, Johannes Gutenberg-Universität, 55099

Temperature and magnetic field dependence of the Hall effect in the normal and mixed state of fully textured (Hg_{0.9}Re_{0.1})Ba₂CaCu₂O_{6+δ} (HgRe-1212) HTSC thin films prepared by laser ablation deposition have been studied. The longitudinal resistivity ρ_{xx} and Hall resistivity ρ_{yx} of HgRe-1212 superconductor thin films were measured for a wide range of magnetic fields up to 12 T with the field perpendicular to the *ab* plane and the current in the *ab* plane. A sign change of the Hall resistivity is observed in fields below 3 T in the region close to the superconducting onset temperature. The temperature dependencies $\rho_{xx} \propto T$ and $\rho_{yx} \propto 1/T$ have been observed for HgRe-1212 thin films. Anderson's formula for the Hall angle θ_H , namely $\cot \theta_H = \alpha T^2 + \beta$, remains valid for temperatures T above T_c . In the mixed state a power-law behavior is observed, where ρ_{yx} scales to a power-law function of ρ_{xx} : $\rho_{yx} = A\rho_{xx}^\beta$, with β increasing from 1.0 to 1.7 as the field increases from 1 to 12 T.

TT 2 Correlated Electrons - Metal Insulator Transition

Zeit: Freitag 10:15–13:00

Raum: TU H2053

TT 2.1 Fr 10:15 TU H2053

The orbital degree of freedom in single- and bilayered manganites — ●M. MERZ¹, P. REUTLER², B. BÜCHNER², A. REVCOLEVSKI³, Y. IDZERDA⁴, S. TOKUMITSU⁵, and S. SCHUPPLER⁵ — ¹Inst. für Kristallographie, RWTH-Aachen — ²IFW Dresden — ³Uni. Paris-Sud — ⁴NRL, Washington — ⁵Forschungszentrum Karlsruhe, IFP

Transition metal oxides like the manganites are fascinating materials since their physical properties are intimately connected with an unusual interrelation between spin, charge, and orbital degrees of freedom. Yet, only little is known about the nature of the experimentally observed ordered phases and the principal factors determining the ordering scheme. To better understand the phenomena of charge/orbital ordering (CO/OO) and to isolate the fundamental properties which serve as a driving force for CO/OO we have investigated layered manganites with

x-ray diffraction and near-edge x-ray absorption spectroscopy. The current data demonstrate that the energy difference between $d_{3z^2-r^2}$, $d_{3y^2-r^2}$, and $d_{3x^2-r^2}$ orbitals is very small for single- and bilayered systems and indicate that the orbital degree of freedom is determined not only by crystal field effects but also by orbital coupling.

TT 2.2 Fr 10:30 TU H2053

Local Green's operator and its applications to manganites — ●HORACIO ALIAGA — Theo. III, Uni-Augsburg, D-86135 Augsburg, Germany

An algorithm is presented to calculate the electronic local Green's operator for manganites-related hamiltonians. This algorithm is proved to scale linearly with the number of states in the Hilbert-space, is able of parallel implementation, and outperforms computationally the Exact Di-

agonalization (ED) method for clusters larger than 400 sites. This method together with the Monte Carlo (MC) technique is used to derive new results for the manganites phase diagram for the spatial dimension $D=3$ and half-filling.

TT 2.3 Fr 10:45 TU H2053

Role of lattice distortion and orbital splitting in Mott-Hubbard transitions — ●K. HELD, A. YAMASAKI, R. ARITA, M. FELDBACHER, and O.K. ANDERSEN — MPI for solid state research, Stuttgart

Lattice distortions lift the degeneracy orbitals have e.g. in a cubic phase. By means of a two band model study, we show that even a small splitting of the orbitals can have a dramatic effect, if a system is close to a Mott-Hubbard transition. Then, electronic correlations grossly enhance the splitting. There can be one or two transition in which the two split bands become insulating. We also report on realistic LDA+DMFT (local density approximation + dynamical mean field theory) calculations for the pressure-induced Mott-Hubbard transition in LaMnO_3 at room temperature. Our conclusion is that the Jahn-Teller and GdFeO_3 distortion and its change are essential for the Mott-Hubbard transition.

TT 2.4 Fr 11:00 TU H2053

Electronic gap closure and structural changes in YTiO_3 and LaTiO_3 at high pressures — ●INGO LOA¹, X. WANG¹, K. SYASSEN¹, M. HANFLAND², T. LORENZ³, H. ROTH³, and Y.-L. MATHIS⁴ — ¹Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart — ²European Synchrotron Radiation Facility, F-38043 Grenoble — ³II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — ⁴Forschungszentrum Karlsruhe, ISS/ANKA, D-76021 Karlsruhe

LaTiO_3 and YTiO_3 are two Mott-Hubbard-type insulators that are characterized by a single $3d$ electron occupying t_{2g} orbitals. Both compounds adopt a distorted perovskite-type structure at ambient pressure. We have investigated the pressure-induced changes in the electronic excitation gaps of LaTiO_3 and YTiO_3 by infrared reflection and absorption spectroscopy. These experiments evidence a pressure-induced insulator-to-metal transition in LaTiO_3 near 11 GPa ($T = 300$ K) while YTiO_3 remains insulating to at least 20 GPa. For YTiO_3 we observe a continuous down-shift of the absorption edge from 0.7 eV at ambient conditions to 0.4 eV at 17 GPa. Like in the case of LaTiO_3 this indicates an evolution towards a metallic state at high pressures. The associated structural changes were determined by synchrotron x-ray powder diffraction. We will present detailed information on the equations of state as well as the variations of bond lengths and bond angles as a function of pressure. For YTiO_3 we observe hardly any variation in bond angles with pressure, which makes it attractive as a model system for theoretical investigations.

TT 2.5 Fr 11:15 TU H2053

Relevance Of Structural Distortions To The Metal Insulator Transition Of Doped LaTiO_3 — ●H. ROTH¹, K. KORDONIS¹, A. KOMAREK¹, M. Cwik¹, N. SCHITTNER¹, J. BAIER¹, M. KRIENER¹, T. LORENZ¹, N. JOHANNSEN¹, T. ZABEL¹, A. EL FILALI¹, G. ANDRÉ², M. BRADEN¹, and A. FREIMUTH¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Labaroatore Léon Brillouin, Saclay

LaTiO_3 is an antiferromagnetic insulator. Hole-doping suppresses T_N and induces a metal-insulator transition (MIT). We present a systematic study of magnetization, specific heat and resistivity of $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ and $\text{LaTiO}_{3+\delta}$. While $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ shows a MIT at a hole concentration $n = x \approx 4\%$, the oxygen-doped $\text{LaTiO}_{3+\delta}$ stays insulating up to a much higher charge-carrier concentration $n = 2\delta \approx 8\%$. Thus, the MIT of doped LaTiO_3 cannot be described by band filling alone. X-ray and neutron diffraction show that the orthorhombic splitting ϵ decreases upon doping, too. Both, the magnetic and the metal insulator transition scale with the size of ϵ , indicating that the orbital splitting is crucial for the magnetic and transport behaviour. Another aspect of the MIT in the studied systems is the coexistence of antiferromagnetic order and metallic behaviour in the intermediate doping range ($x \approx 0.05, 0.04 \leq \delta \leq 0.1$).

Supported by the DFG through SFB 608

TT 2.6 Fr 11:30 TU H2053

Charge order, orbital order, and electron localization in the Magnéli phase Ti_4O_7 — ●V. EYERT, U. SCHWINGENSCHLÖGL, and U. ECKERN — Institut für Physik, Universität Augsburg

The metal-insulator transition of the Magnéli phase Ti_4O_7 is studied by means of augmented spherical wave (ASW) electronic structure calculations as based on density functional theory and the local density ap-

proximation. The results show that the metal-insulator transition arises from a complex interplay of charge order, orbital order, and singlet formation of those Ti $3d$ states which mediate metal-metal bonding inside the four-atom chains characteristic of the material. Ti_4O_7 thus combines important aspects of Fe_3O_4 and VO_2 . While the charge ordering closely resembles that observed at the Verwey transition, the orbital order and singlet formation appear to be identical to the mechanisms driving the metal-insulator transition of vanadium dioxide.

TT 2.7 Fr 11:45 TU H2053

Local Structure of V_2O_3 in the vicinity of the metal-insulator transition — ●P. PFALZER¹, M. KLEMM¹, M. L. DENBOER² und S. HORN¹ — ¹Universität Augsburg, Lehrstuhl für Experimentalphysik II, Universitätsstr. 1, 86135 Augsburg — ²Queens College of CUNY, 65-30 Kissena Blvd., Flushing, New York 11367, USA

We have measured the temperature dependence of the local structure of V_2O_3 close to the metal-insulator transition (MIT). Polarization dependent EXAFS-measurements give evidence that the emergence of the insulating state is directly connected to the trigonal distortion of the O coordination octahedra, which is determined by the distance of the V atoms along the hexagonal c-axis. While this V-V pair-distance shows a sharp jump exactly at the temperature of the MIT, the properties of the Vanadium bonds in the a-b (basal-)plane are smeared out and no abrupt changes are detected at the MIT. Even in the metallic phase the full trigonal symmetry is not recovered, but a local monoclinic distortion — although significantly reduced in size — persists up to room temperature. This suggests that the driving forces for the MIT are due to interactions between V ions in the basal plane, leading to the insulating state e.g. via changes in hybridization.

TT 2.8 Fr 12:00 TU H2053

Thermal Conductivity, Thermopower, and Figure of Merit of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ — ●M. KRIENER, K. BERGGOLD, I. KLASSEN, T. LORENZ, C. ZOBEL, and A. FREIMUTH — II. Physikalisches Institut, Universität zu Köln, 50937 Köln

Cobaltates attract strong interest because Co ions have the possibility to occur in different spin states. Especially, LaCoO_3 shows a temperature-induced spin-state transition whose microscopic origin is still discussed controversially. Recently, the layered cobaltate $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ attracted much interest due to its superconductivity and the water-free compound Na_xCoO_2 due to its possible relevance for thermoelectric cooling. Na_xCoO_2 has a low electrical resistivity ρ , a low thermal conductivity κ , and a large thermopower S , leading to a rather large thermoelectric figure of merit $ZT = S^2T / \kappa\rho$ which should approach unity for an effective thermoelectric cooling. In this talk we present a systematic study of the figure of merit on a series of single crystals of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$. Substituting La^{3+} in LaCoO_3 by Sr^{2+} drives the compound from a nonmagnetic insulator through a spin-glass phase ($x \geq 0.04$) to a ferromagnetic metal for $x \geq 0.18$ [1]. The entire series of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ has rather low κ values, whereas S strongly decreases with increasing x . For intermediate Sr concentrations in the spin-glass region we find notably large values of Z indicating that Co-based materials could be promising candidates for thermoelectric cooling.

[1] M. Kriener *et al.*, Phys. Rev. B **69**, 094417 (2004)

Supported by the DFG through SFB 608.

TT 2.9 Fr 12:15 TU H2053

Modelling the magnetic susceptibility of LaCoO_3 — ●THOMAS MÖLLER^{1,2} and ERWIN MÜLLER-HARTMANN¹ — ¹Institut für Theoretische Physik, — ²II. Physikalisches Institut, Universität zu Köln

LaCoO_3 is a non-magnetic insulator, which develops a Curie susceptibility above ~ 100 K. According to the Hund's rules the 5D -quintet with $S = 2$ (high spin) should form the ground state for the $3d^6$ electron configuration of Co^{3+} . A sufficiently large cubic crystal field breaks Hund's first rule, and the ground state becomes non-magnetic ($S = 0$, low spin). However, this high-spin / low-spin scenario is not in agreement with the experimental results [1]. Radwański and Ropka [2] suggested another model for LaCoO_3 . Here, the ground state is the high spin state, but this multiplet is split by spin orbit coupling and a trigonal Jahn-Teller distortion in such a way that a non-magnetic ground state develops. We calculated the magnetic susceptibility in this model and find a strong anisotropy where the Curie susceptibility disappears in the plane perpendicular to the Jahn-Teller distortion and only a large van-Vleck term remains. For a D_{4h} distortion, this can be explained by pure symmetry. A vanishing Curie susceptibility is found also in case of a D_{3d} distortion,

but here the reason is still unclear. Due to its strong anisotropy the T-dependence of the averaged susceptibility $\bar{\chi} = \frac{1}{3}\chi_{\parallel} + \frac{2}{3}\chi_{\perp}$ differs from that observed in LaCoO₃.

[1] Zobel *et al.*, Phys. Rev. B **66**, 020402(R) (2002)

[2] Radwański and Ropka, Solid State. Comm. **112**, 621 (1999)

TT 2.10 Fr 12:30 TU H2053

Unconventional temperature-dependence of charge order in La_{1.8}Sr_{0.2}NiO₄ — ●J. SCHLAPPA¹, C. SCHÜSSLER-LANGEHEINE¹, C.-F. CHANG¹, Z. HU¹, M. BENOMAR¹, E. SCHIERLE², H. OTT^{1,2}, E. WESCHKE², G. KAINDL², A. TANAKA³, M. BRADEN¹, and L. H. TJENG¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Institut für Experimentalphysik, Freie Universität Berlin — ³ADSM, Hiroshima University, Japan

We report on a detailed study of charge order in Sr-doped La₂NiO₄, using the new technique of resonant soft x-ray diffraction at the Ni L_{2,3} and La M_{4,5} resonances. For La_{2-x}Sr_xNiO₄ we observe a decrease of the coherence length of charge order, as determined from the width of the corresponding superstructure peak, not only when the system is heated up, but also when it is cooled below ≈ 65 K. While the superstructure-peak height decreases towards higher temperatures in a way resembling usual 2nd-order phase transitions, the change in the integrated intensity is much smaller, thus showing a behavior that is significantly different from that of the order parameter of other phase transitions. This means that upon heating the charge order breaks into smaller and smaller domains, while inside these domains the character of the order, as given by its period length and the energy dependence of the superstructure peak across the resonance, is conserved. A similar behavior is found upon cooling. A possible reason for this loss of coherence at low-temperatures is the influence of the disorder potential formed by the dopant atoms; a frustra-

tion caused by a competing magnetic order appears unlikely considering the observed temperature dependence.

TT 2.11 Fr 12:45 TU H2053

Effect of pressure on the electric transport properties of RNiO₃ — ●R. LENGSDORF¹, J.A. ALONSO², D.I. KHOMSKI¹, H. MICKLITZ¹, and M.M. ABD-ELMEGUID¹ — ¹II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln — ²Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain

The temperature-induced metal-insulator (MI) transition in the RNiO₃ series has been ascribed to an opening of a small charge transfer gap at $T < T_{MI}$ which is intimately connected with either a slight but abrupt expansion of the unit cell volume or an orthorhombic (*Pbnm*) to monoclinic (*P2_{1/n}*) structural transition for large (R=Pr,..., Eu) and small (R=Dy,..., Lu) R³⁺ ions, respectively. The monoclinic symmetry in the insulating state implies two independent Ni-sites and the presence of charge ordering. Experimental evidence for such a charge ordered state in larger R³⁺ nickelates has recently been reported (e.g. EuNiO₃ and NdNiO₃ thin films), supporting the importance of charge ordering for the occurrence of the temperature-induced MI transition. For a deeper understanding of the mechanism of the MI transition in the RNiO₃ series, we have studied the effect of pressure on the transport properties of some selected RNiO₃ (R=Sm, Eu, Y and Lu) oxides. While the monoclinic structure of YNiO₃ ($T_{MI}=582$ K and $T_N=138$ K) and LuNiO₃ ($T_{MI}=599$ K and $T_N=125$ K) remains stable up to 14 GPa and 16 GPa, respectively, the pressure-temperature dependence of the electrical resistance clearly indicates a transition to a metallic state already at $p \geq 5$ GPa. Possible mechanisms responsible for the pressure-induced insulator-metal transition in RNiO₃ series will be discussed.

TT 3 Correlated Electrons - Heavy Fermions

Zeit: Freitag 10:15–13:00

Raum: TU H3027

TT 3.1 Fr 10:15 TU H3027

Multiband Superconductivity in the heavy fermion PrOs₄Sb₁₂ — ●GABRIEL SEYFARTH¹, JEAN-PASCAL BRISON¹, MARIE-AUDE MÉASSON², JACQUES FLOUQUET², KOICHI IZAWA³, Y. MATSUDA³, H. SUGAWARA⁴, and H. SATO⁴ — ¹CRTBT-CNRS, 38042 Grenoble, France — ²CEA-Grenoble, 38054 Grenoble, France — ³ISSP, Chiba 277-8581, Japan — ⁴Tokyo Metropolitan University, Tokyo 192-0397, Japan

In our contribution we show that several experimental measurements indicate that the superconducting phase of PrOs₄Sb₁₂ [1] involves quasiparticles of different effective masses and different gap amplitudes, i.e. it has a multiband character, like it is observed in the archetype of this class of superconductors, MgB₂ [3]. These evidences come a) from He₂(T) calculations (published in [5]) that reproduce the small positive curvature at low fields, assuming the existence of two different electronic bands, b) from Andreev-reflection measurements in Au-PrOs₄Sb₁₂ junctions and c) from the low field dependence of thermal transport measurements in the superconducting phase at very low temperatures (50mK). They are supported by dHvA measurements [6], which reveal a large spread of effective masses on the different sheets of the Fermi surface of this strongly correlated system. The discussion will include other experimental results which were interpreted in terms of unconventional superconductivity [2],[4].

References :

[1] E. D. Bauer (2002) Phys. Rev. B 65 100506 [2] E. Chia (2003) PRL 91 247003 [3] F. Giubileo (2001) PRL 87 177008 [4] K. Izawa (2003) PRL 90 117001 [5] M.-A. Measson (2004) Phys. Rev. B 70 064516 [6] H. Sugawara (2003) Acta Physica Polonica B 34 1125

TT 3.2 Fr 10:30 TU H3027

Competition between antiferromagnetism and superconductivity in CeCu₂Si₂ — ●O. STOCKERT¹, E. FAULHABER², N. STÜSSER³, K. PROKES³, W. SCHMIDT⁴, G. ZWICKNAGL⁵, H.S. JEEVAN¹, M. DEPPE¹, M. LOEWENHAUPT², C. GEIBEL¹, and F. STEGLICH¹ — ¹Max-Planck-Institut für Chem. Physik fester Stoffe, D-01187 Dresden, Germany — ²Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — ³Hahn-Meitner-Institut, D-14109 Berlin, Germany — ⁴Institut Laue-Langevin, F-38042 Grenoble, France — ⁵Institut für Math. Physik, TU Braunschweig, D-38106 Braunschweig, Germany

We report on neutron scattering experiments on magnetically ordered

CeCu₂Si₂ single crystals exhibiting A- and A/S-phase anomalies. Below $T_N \approx 0.8$ K antiferromagnetic order has been detected with a propagation vector $\tau \approx (0.215 \ 0.215 \ 0.53)$ at $T = 50$ mK. The magnetic order is due to nesting of the Fermi surface as indicated by renormalized band-structure calculations. The observation of incommensurate antiferromagnetic order as the nature of the A-phase in CeCu₂Si₂ suggests that a spin-density-wave instability is the origin of the quantum critical point in CeCu₂Si₂. Elastic high-resolution neutron scattering on both, A- and A/S-type crystals, reveal the long-range nature of the antiferromagnetic order in the A/S-crystal, but yield a considerable line broadening for the A-type crystal pointing to a finite domain size or correlation length. However, in energy scans no increased width of the magnetic peaks has also been detected. Extensive measurements, performed on the A/S-crystal also in magnetic fields, show that in this crystal antiferromagnetism and superconductivity seem to exclude each other on a microscopic scale.

TT 3.3 Fr 10:45 TU H3027

Tunneling spectroscopy on epitaxial superconducting UNi₂Al₃ thin films — ●ANDREY ZAKHAROV, MARTIN JOURDAN, and HERMANN ADRIAN — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55128 Mainz, Germany

Tunneling spectroscopy experiments on thin film planar junctions of the heavy-fermion superconductor UNi₂Al₃ were performed. Employing an in vacuo process it was possible to prepare cross-junctions with a*-axis oriented epitaxial thin films of UNi₂Al₃ as a base electrode, artificial insulating layer of AlO_x as a barrier and a well-known superconducting metal (Pb or In) as a counter electrode. The typical tunneling densities of states of the superconducting counter electrodes including strong coupling features were observed, proving the contacts to be in the tunneling regime with an essentially pin-hole free barrier. In the normal magnetically ordered state of the heavy-fermion compound a pseudogap was observed. First result of direct probing the superconducting density of states of UNi₂Al₃ are presented.

TT 3.4 Fr 11:00 TU H3027

Drude Response of Heavy Fermions in UNi₂Al₃ — ●MARC SCHEFFLER¹, MARTIN DRESSEL¹, MARTIN JOURDAN², and HERMANN ADRIAN² — ¹II. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart — ²Institut für Physik, Universität Mainz, 55099 Mainz

The defining mass enhancement of the charge carriers in heavy-fermion compounds goes hand in hand with an equivalent decrease of the charge carrier relaxation rate. This relaxation rate can be identified from characteristics in the frequency-dependent conductivity: a roll-off in the real part $\sigma_1(\omega)$ and a maximum in the imaginary part $\sigma_2(\omega)$, two core predictions of the Drude model of metallic conduction.

Recently we succeeded with the first direct measurements of a Drude response in heavy-fermion UPd₂Al₃, revealing an extremely low relaxation rate in the GHz range. Now we present results on the related compound UNi₂Al₃ in the same frequency (45 MHz to 20 GHz) and temperature (1.65 K to 300 K) ranges. Again, at low temperatures we find a Drude behavior at GHz frequencies. Thus we can directly observe the relaxation rate as a function of temperature and use this to discuss the charge carrier density.

TT 3.5 Fr 11:15 TU H3027

Kondo-ion electron spin resonance of isotope clean ¹⁷⁴YbRh₂Si₂ — ●J. WYKHOFF¹, J. SICHELSCHEIDT¹, G. KNEBEL², G. LAPERTOT², J. FLOUQUET², J. FERSTL¹, H.-A. KRUG VON NIDDA³, C. GEIBEL¹, and F. STEGLICH¹ — ¹Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — ²Département de Recherche Fondamentale sur la Matière Condensée, SPSMS, CEA Grenoble, 38054 Grenoble, France — ³Experimentalphysik V, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The heavy-fermion compound YbRh₂Si₂ is located very close to a magnetic field induced quantum critical point. The unexpected observation of electron spin resonance (ESR) of the Kondo-ion Yb³⁺ below the Kondo temperature ($T_K \simeq 25$ K) might be a direct verification of the localized moment scenario of quantum criticality. We present the ESR of isotope clean ¹⁷⁴YbRh₂Si₂ which was prepared at the CEA Grenoble. Its T behavior is very similar compared to that of YbRh₂Si₂. Especially, for the ESR linewidth an exponential behavior above $T \simeq 12$ K and a progressive reduction by decreasing T down to the lowest accessible $T = 1.7$ K could be confirmed in ¹⁷⁴YbRh₂Si₂. However, ¹⁷⁴YbRh₂Si₂ shows a smaller residual linewidth and a strongly reduced thermal line broadening in the whole T region. Assuming a smaller disorder in ¹⁷⁴YbRh₂Si₂ these observations further support our previous finding that introducing disorder in YbRh₂Si₂ by La- or Ge-doping causes a more effective Yb³⁺ ESR relaxation. The question arises whether an ESR bottleneck effect could be responsible for the extremely narrow linewidth.

TT 3.6 Fr 11:30 TU H3027

Magnetic structure vs. crystallographic disorder in single crystalline UPt₂Si₂ — ●S. SÜLLOW¹, A. OTO¹, A. LOOSE², J. KLENKE², R. FEYERHERM², R.W.A. HENDRIKX³, and J.A. MYDOSH^{3,4} — ¹IFP, TU Braunschweig, Braunschweig, Germany — ²BENSC, HMI, Berlin, Germany — ³Leiden University, Leiden, The Netherlands — ⁴MPI-CPS, Dresden, Germany

We present a detailed investigation of the crystallographic structure, lattice disorder and magnetic order of a single-crystal of the moderately mass-enhanced U intermetallic UPt₂Si₂. Utilizing the bright contrast between U, Pt and Si in neutron scattering, we establish the lattice symmetry to be $P4/nmm$ (CaBe₂Ge₂-lattice). Moreover, the observation of an anomalously large thermal displacement factor U_{11}/U_{22} for the Pt(2) and Si(2) sites at low temperatures indicates frozen-in disorder on these sites. The material undergoes an antiferromagnetic transition below $T_N = 32.1$ K, with ferromagnetically coupled a - b -planes and an antiferromagnetic stacking along the c axis. In addition, as result of the crystallographic disorder we observe magnetic clusters up to $T_{irr} = 34$ K. The existence of the clusters explains the previously observed anomalous antiferromagnetic domain pinning in the compound [1]. Moreover, the disorder bears relevance to the electronic transport properties of the compound, which are commonly metallic along the a axis, but disorder dominated in c direction.

[1] A. Otop *et al.*, J. Appl. Phys. 95 (2004) 6702

TT 3.7 Fr 11:45 TU H3027

Magnetic field-induced non-Fermi-liquid resistivity in YbAgGe single crystals — ●PHILIPP G. NIKLOWITZ¹, GEORG KNEBEL¹, SERGEY L. BUDKO², PAUL C. CANFIELD², and JACQUES FLOUQUET¹ — ¹SPSMS/CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble cedex 9, France — ²Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

Hexagonal YbAgGe has recently been recognised as a new heavy-

fermion (HF) system with $T_K = 24$ K, γ of a few hundred mJ/molK² and planar magnetic anisotropy $\chi_{ab}/\chi_c \approx 3$ at low temperatures. Two magnetic transitions below 1 K can be fully suppressed with fields $H < 10$ T. In going from low to higher H and T , the $H - T$ phase diagram down to 0.4 K shows a first-order transition from an antiferromagnetically ordered phase to a second magnetically ordered phase and then a second-order phase transition to a paramagnetic (field-polarised) phase. We have investigated YbAgGe for the first time down to 50 mK by measuring the resistivity ρ of single crystals in fields up to 14 T. Our results extend the $H - T$ phase diagram to the lowest temperatures for $H \perp c$ and $H \parallel c$. Whereas at low H , $\rho(T)$ reveals a temperature exponent $n \geq 2$, close to and beyond the critical field of the second-order phase transition we find $1 < n < 1.5$ and strong enhancement of the temperature dependence of $\rho(T)$, before Fermi-liquid behaviour is recovered above 10 T. Particularities in the appearance of the unconventional form of $\rho(T)$ will be discussed considering the HF nature and structural aspects of YbAgGe. YbAgGe appears to be one of few Yb-based stoichiometric systems, where quantum-critical behaviour may be induced by a magnetic field.

TT 3.8 Fr 12:00 TU H3027

Optical spectroscopy of the mixed valence semiconductor TmSe — ●MICHAEL DUMM¹, BORIS GORSHUNOV¹, DANIEL FALTERMEIER¹, PHILIPP HAAS¹, MARTIN DRESSEL¹, and TAKESHI MATSUMURA² — ¹Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart — ²Physics Department, Tohoku University, Sendai 980-77, Japan

Among mixed-valence compounds TmSe has attracted particular interest because of its unusual physical properties. For instance, beyond unique magnetic properties this semiconductor shows no signs of activated behavior in the temperature dependence of the dc conductivity. We investigated the dynamical conductivity of TmSe at $5 \text{ K} \leq T \leq 300 \text{ K}$ by employing infrared and quasi-optical Terahertz techniques in a broad frequency range $10 \text{ cm}^{-1} \leq \nu \leq 10000 \text{ cm}^{-1}$ covering all relevant energy scales. At high temperatures, the optical spectra reveal signatures of a two-component free-carrier response originating on the one hand from light d -electrons and on the other hand from heavy f -electronic states hybridized with the charge carriers in the conduction band. Going towards lower temperatures, the heavy carrier response starts diminishing and a gap-like feature builds up below 100 cm^{-1} . On the basis of a detailed analysis of our optical and dc data, we will discuss the origin of the gap. Furthermore, we will compare the results obtained on TmSe to those measured on other Kondo insulators like YbB₁₂ and SmB₆.

TT 3.9 Fr 12:15 TU H3027

Geometrical Frustration in Rare-Earth Face-Centered Cubic Crystals — ●VERONIKA FRITSCH, JOE D. THOMPSON, and JOHN L. SARRAO — Los Alamos National Laboratory, Los Alamos, New Mexico 87544, USA

In a 3-dimensional solid the simplest form of magnetic frustration is spins on a tetrahedron with antiferromagnetic coupling. A face-centered cubic (fcc) lattice is a simple example of a network of edge-sharing tetrahedra; however, most fcc compounds exhibit well-defined magnetic order, dominated by next-neighbor (nn) and next-nearest-neighbor (nnn) interactions. To minimize the effects of nnn interactions and maximize frustration, the network of edge-sharing tetrahedra has to be divided into sub-networks of corner-sharing tetrahedra, as is realized in pyrochlore and spinel structures. A further example of a fcc -lattice split in two sub-networks of corner-sharing tetrahedra are the intermetallic ternaries $REInCu_4$ ($RE = \text{heavy rare-earth}$). Here the rare-earth ions occupy a fcc -lattice, where half of the tetrahedra are filled with an In-ions and the other half with a Cu-tetrahedron. The extent of frustration in these systems is determined by the magnetic moment of the rare-earth ion and second by their separation distance, which can be tuned with chemical substitution, e.g. Ni for Cu. We present measurements of electrical resistivity, magnetic susceptibility and specific heat on single crystals of the title compounds with the trivalent rare-earth ions Gd, Dy, Ho and Er, demonstrating geometrical frustration of their spin and orbital angular momentum.

TT 3.10 Fr 12:30 TU H3027

Kondo-lattice type models at finite temperatures with exact diagonalization — ●IVICA ZEREC, BURKHARD SCHMIDT, and PETER THALMEIER — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden

The competition between the RKKY interaction and the Kondo screening in heavy fermion compounds is considered to be the origin of quantum

critical phase transitions. They are generically described by the Doniach phase diagram, which was originally obtained from a simplified version of the Kondo lattice model in one dimension - the Kondo necklace model. We consider a similar model for the 2D systems, derived from the Kondo lattice model neglecting charge degrees of freedom. We use the finite temperature Lanczos method to numerically diagonalize the Hamiltonian matrix for finite clusters and calculate thermodynamic and correlation functions for various values of the coupling constants and the external magnetic field. The results are used to construct the phase diagrams for the finite clusters. These may provide some insight into the physics in the neighborhood of a quantum critical point.

TT 3.11 Fr 12:45 TU H3027

Fluctuation conductivity of thin films and nanowires near a parallel-field-tuned superconducting quantum phase transition

— •NAYANA SHAH¹, ANDREI LOPATIN², and VALERII VINOKUR² —
¹Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — ²Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

TT 4 Symposium Superconducting Cuprates

Zeit: Freitag 14:00–17:45

Raum: TU H104

Hauptvortrag

TT 4.1 Fr 14:00 TU H104

Phase Sensitive Tests with Cuprate Superconductors Based on the Josephson Effect and Andreev bound states — •BORIS CHESCA¹, DIETMAR DÖNITZ¹, DIETER KÖLLE¹, REINHOLD KLEINER¹, A. TSUKADA², MICHIO NAITO², ARIANDO³, and HANS HILGENKAMP³ —
¹Physikalisches Institut-Experimentalphysik II, Universität Tübingen, Germany — ²NTT Basic Research Lab., Japan — ³Faculty of Science and Technology and MESA+ Research Inst., University of Twente, The Netherlands

Junctions formed between two superconductors provide the unique opportunity to obtain information on the symmetry of the superconducting order parameter simultaneously from tunneling of Cooper pairs and of quasiparticles. Indeed, on one hand the d-wave symmetry leads to striking anomalies in the Cooper pair Josephson tunneling in both hole- and electron-doped cuprate junctions: spontaneous appearance of half flux quanta [1] or GHz circulating currents [2], or field enhanced Josephson currents [2-4]. On the other hand, Andreev bound states induced zero-bias conductance peak (ZBCP) in the tunneling spectra of quasiparticles is also a clear signature of d-wave symmetry. We discuss the controversy of ZBCP physics in electron-doped cuprate junctions [5] as well as the importance of the complementary character of these two different phase sensitive tests. We consider two cases: junctions formed between cuprates or between cuprate and conventional superconductors.

[1] C.C. Tsuei and J.R. Kirtley, *Rev. Mod. Phys.* **72**, 969 (2001); [2] B. Chesca et al., *Phys. Rev. Lett.* **88**, 177003 (2002); [3] B. Chesca et al., *Phys. Rev. Lett.* **90**, 057004 (2003); [4] R. R. Schulz, et al., *Appl. Phys. Lett.* **76**, 912 (2000); [5] B. Chesca et al., *Condmat-0402131* (2003).

TT 4.2 Fr 14:30 TU H104

Pseudogap, superconductivity and conservation of states in electron doped HTS: results from tunneling spectroscopy

— •BETTINA WELTER¹, ANDREAS WINKLER¹, LAMBERT ALFF¹, YOSHIO HARU KROCKENBERGER¹, MICHIO NAITO², and RUDOLF GROSS¹ —
¹Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — ²NTT Basic Research Laboratories, Atsugi, Japan

Exploring the doping dependent properties of the electron doped cuprates and comparing them to the hole doped systems will help to understand the origin of superconductivity in these materials. Here, we report on tunneling spectroscopy measurements on grain boundary junctions of electron doped high-temperature superconductors $\text{La}_{2-x}\text{Ce}_x\text{CuO}_4$, $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4$ and $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ with different Ce concentrations around optimal doping. We focus on the pronounced depletion in the density of states near E_F observed in the normal state above B_{c2} and its evolution with temperature, magnetic field and doping [1]. Considerations concerning the conservation of states rule indicate a coexistence of this pseudogap regime and the superconducting state.[2]. As in this context the method of normalization is crucial, we show a detailed comparison of different methods and discuss their justification. [1] L. Alff, Y. Krockenberger, B. Welter, M. Schonecke, R. Gross, D.

We calculate the fluctuation correction to the normal state conductivity in the vicinity of a quantum phase transition from a superconducting to normal state, induced by applying a magnetic field parallel to a dirty thin film or a nanowire with thickness smaller than the superconducting coherence length. We find that at zero temperature, where the correction comes purely from quantum fluctuations, the positive Aslamazov-Larkin contribution, the negative density of states contribution, and the Maki-Thompson interference contribution, are all of the same order and the total correction is negative. Further we show that based on how the quantum critical point is approached, there are three regimes that show different temperature and field dependencies which should be experimentally accessible.

Manske and M. Naito, *Nature* **422**, 698 (2003)

[2] B. Welter, Y. Krockenberger, M. Naito, L. Alff and R. Gross, *Physica C* **388**, 299 (2003)

This work is supported by the DFG through Forschergruppe 538.

Hauptvortrag

TT 4.3 Fr 14:45 TU H104

Angle-Resolved Photoemission Spectroscopy of High- T_c Superconductors: Identifying the Pairing Boson — •SERGEY BORISENKO — Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, Helmholtzstrasse 20, D-01069, Dresden

The search for the pairing mechanism in High-Temperature Superconducting cuprates has converged to the choice between the electron-phonon and electron-electron interactions. This dilemma remains one of the main problems of the modern condensed matter physics. We study HTSC using the Angle-Resolved Photoemission Spectroscopy. Due to the recent improvement of the resolution, this method allows to detect the "fingerprints" of the coupling between the electrons and bosonic excitations conceivably responsible for the pairing. Analysing the momentum, doping and temperature dependences of the electron-boson coupling effects in Bi-based cuprates we make an attempt to identify the pairing boson in high- T_c superconductors.

Fachvortrag

TT 4.4 Fr 15:15 TU H104

Ordering Phenomena in Cuprates — •RUDI HACKL¹, LEONARDO TASSINI¹, FRANCESCA VENTURINI², ANDREAS ERB¹, NAOKI KIKUGAWA³, and TOSHITSU FUJITA³ — ¹Walther-Meissner-Institut, D-85748 Garching — ²Bruker BioSpin AG, CH-8117 Faellanden — ³ADSM, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan

We present results of Raman scattering experiments on hole doped cuprates with $0 \leq p \leq 0.26$. Spectra were measured for temperatures between 4.2 and 330 K as a function of polarization. In all compounds a strong anisotropy of the transport properties develops for doping levels below approximately 0.21. In agreement with recent photoemission experiments electrons with momenta along the diagonal of the copper-oxygen plane always exhibit metallic dynamics except for $p \equiv 0$. In contrast, for electrons moving along the principal axes a metal-insulator transition is found at $x \simeq 0.21$. In addition to this quite general phenomenon, a new type of low-temperature response is found at material-dependent doping levels in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{Y}_{0.97}\text{Ca}_{0.03}\text{Ba}_2\text{Cu}_3\text{O}_{6+x}$. Both the spectral shape and the selection rules provide strong evidence that the new low-energy response originates from the formation of fluctuating one-dimensional charge order. In $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ the lattice apparently helps to stabilize stripes making them visible in a Raman experiment at doping levels up to at least 0.10.

Pause

Fachvortrag

TT 4.5 Fr 16:00 TU H104

Magnetic Excitations in High-Temperature Superconductors — ●GÖTZ S. UHRIG¹, KAI P. SCHMIDT¹, and MARKUS GRÜNINGER² — ¹Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — ²II. Physikalisches Institut, Universität zu Köln, 50937 Köln

Recently, more and more evidence is emerging that the magnetic excitations in high temperature superconductors have a universal character. The resonance mode at \mathbf{Q}_{AF} and the incommensurate satellites need no longer be regarded as mutually exclusive phenomena pertaining to different families of cuprates. This observation revives the interest in the quantitative theoretical description of the magnetic excitations. One route in the quest for such a theory is to consider charge modulated phases like stripes or tiling patterns which are suggested experimentally by scanning tunnel microscopy and theoretically by phenomenological quantum dimer models.

We present a quantitative description of the universal magnetic excitations which is based on charge stripes where the collective magnetic excitations result from dispersing triplon modes. The anisotropy of the dispersion implies the observed two different energy scales. Very good agreement is obtained for realistic coupling parameters which include a sizable cyclic exchange.

Evidence and counter-evidence for the validity of the model proposed and for possible alternatives is discussed.

TT 4.6 Fr 16:30 TU H104

Testing stripe theories: Geometry of spin excitations in the superconducting and normal state of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ — ●VLADIMIR HINKOV¹, BERNHARD KEIMER¹, PHILIPPE BOURGES², STEPHANE PAILHES², YVAN SIDIS², ALEXANDRE IVANOV³, ANDREY KULAKOV¹, CHENGTIAN LIN¹, DAPENG CHEN¹, and CHRISTIAN BERNHARD¹ — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²Laboratoire Leon Brillouin, Saclay, France — ³Institut Laue Langevin, Grenoble, France

The physics of high-temperature cuprate superconductors exhibits a two-dimensional (2D) character due to the layered structure. An influential theory predicts a further reduction of dimensionality: In the CuO_2 -layers charge and spin are supposed to separate spontaneously forming one-dimensional (1D) stripes of antiferromagnetically ordered spins separated by charge rivers. Such stripe arrangements should become visible by virtue of their quasi-1D spin excitations. We use inelastic neutron scattering (V. Hinkov et al., Nature 430, 650) to investigate the in-plane geometry of spin excitations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ with T_c of 90K, 61K and 35K, respectively. We use fully untwinned samples, as the signal from twinned crystals contains contributions from both perpendicular twin domains. We demonstrate, that the spin excitations are 2D and form a ring in reciprocal space, thus excluding simple, 1D arrangements of stripes. However, amplitude and width are modulated along the ring. Therefore, configurations of stripes are possible with strong orientational fluctuations, which can be quantified by our data. Further, we show that a great deal of the observed modulation originates from the normal state.

TT 4.7 Fr 16:45 TU H104

Novel neutron resonance mode in $d_{x^2-y^2}$ superconductors — ●ILYA EREMIN¹, DIRK K. MORR², ANDREY V. CHUBUKOV³, KARL BENNEMANN¹, and MICHAEL R. NORMAN⁴ — ¹Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany — ²Department of Physics, University of Illinois at Chicago, Chicago, IL 60607 — ³Department of Physics, University of Wisconsin, Madison, WI 53706 — ⁴Materials Science Division, Argonne National Laboratory, Argonne, IL 60439

We show that a new resonant magnetic excitation at incommensurate

momenta, observed recently by inelastic neutron scattering experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$, is a *spin exciton*. Its location in the magnetic Brillouin zone and its frequency are determined by the momentum dependence of the particle-hole continuum. We identify several features that distinguish this novel mode from the previous resonance mode observed near $\mathbf{Q} = (\pi, \pi)$, such as its intensity maximum which occurs in a different part of the magnetic Brillouin zone.

TT 4.8 Fr 17:00 TU H104

Investigation of HTSC with ARPES using the circularly polarized light. — ●VOLODYMYR ZABOLOTNYI, SERGEY BORISENKO, ALEXANDER KORDYUK, JOCHEN GECK, JÖRG FINK, MARTIN KNUPFER, and BERND BÜCHNER — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

There exist certain theoretical suggestions that in copper-oxide based high-temperature superconducting materials, the so-called time-reversal and rotational symmetry-breaking phase should be observed. To reveal this effect a set of experiments with circularly polarized light has been done. Anticipated effect has not been observed and therefore the answer whether this phase exists still remains unclear. Instead a new effect was discovered. We observe the dichroism of different signs on the bonding and antibonding components of the CuO -band in lead doped BISCO samples. Here we present the detailed behaviour of the dichroic signal in the 1st and partly 2nd Brillouin zones, as well as the temperature dependence for the optimally- and over-doped samples. Some plausible explanations of the effect are given.

TT 4.9 Fr 17:15 TU H104

Lattice dynamics and electron-phonon coupling in $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ — ●K.-P. BOHNEN¹, V. PANKOKE² und R. HEID¹ — ¹Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Wissenschaftliches Rechnen, P.O.B. 3640, D-76021 Karlsruhe

Recently the lattice dynamics of $\text{YBa}_2\text{Cu}_3\text{O}_7$ has been calculated successfully with modern ab-initio density functional methods [1]. However, the superconducting properties depend sensitively on the oxygen content thus it is of great interest to study the lattice dynamics and the electron-phonon coupling as function of doping. Here we present results for the Ortho-II phase of $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ which has been possible to treat in detail with density-functional perturbation approach. The structure, lattice dynamics and electron-phonon coupling has been determined and will be compared with available experimental data as well as with results for $\text{YBa}_2\text{Cu}_3\text{O}_7$. The calculations indicate that the oxygen-apex modes are most strongly affected by doping.

[1] K.-P. Bohnen, R. Heid, M. Krauss, Europhys. Lett. **64**, 104 (2003)

TT 4.10 Fr 17:30 TU H104

Fermi-liquid based theory for the in-plane magnetic anisotropy in untwinned cuprates — ●DIRK MANSKE¹ and ILYA EREMIN² — ¹Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — ²Freie Universität Berlin, Institut für Theoretische Physik, 14195 Berlin

Using a generalized RPA-type theory we calculate the in-plane anisotropy of the magnetic excitations in hole-doped high- T_c superconductors. Extending our earlier Fermi-liquid based studies on the resonance peak by inclusion of orthorhombicity, we still find two-dimensional spin excitations, however, being strongly anisotropic. This reflects the underlying anisotropy of the hopping matrix elements and of the superconducting gap function. We compare our calculations with experimental data on fully untwinned YBCO (V. Hinkov et al., Nature 2004) and find good agreement. Our results are in contrast to earlier interpretations on the in-plane anisotropy in terms of stripes (H. Mook et al., Nature 2000).

TT 5 Superconductivity - Mechanisms, Phase Diagram, Competing Order

Zeit: Freitag 18:00–19:00

Raum: TU H104

TT 5.1 Fr 18:00 TU H104

Interplay between competing and coexisting ground states in electron doped cuprates — ●YOSHIHARU KROCKENBERGER^{1,2}, ANDREAS WINKLER³, BETTINA WELTER³, DIRK MANSKE², MICHIO NAITO⁴, and LAMBERT ALFF⁵ — ¹NTT Basic Research Laboratories, NTT Corporation, 3-1 Wakamiya, Morinosato, Atsugi-shi, Kanagawa 243-0198, Japan — ²Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — ³Walther-Meißner-Institute, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — ⁴Department of Applied Physics, Tokyo University of Agriculture and Technology (TUAT), 2-24-16 Naka-cho, Koganei, Tokyo 184-8588, Japan — ⁵Vienna University of Technology, ISAS, Applied Electronic Materials, Gusshausstr. 27-29/366, A-1040 Wien, Austria

The ground state of superconductors is characterized by the long-range order of condensed Cooper pairs: this is the only order present in conventional superconductors. The high- T_c superconductors, in contrast, exhibit more complex phase behaviour, which might indicate the presence of other competing ground states. Here we report the existence of a second order parameter hidden within the superconducting phase of the underdoped (electron-doped) high- T_c superconductor $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_{4+y}$. The existence of a pseudogap when superconductivity is suppressed excludes precursor superconductivity as its origin. This supports the picture that the physics of high- T_c is determined by the interplay between competing and coexisting ground states.

TT 5.2 Fr 18:15 TU H104

Inhomogeneous charge and spin order in electron-doped high- T_c cuprate superconductors — ●H.-H. KLAUSS¹, D. BAABE¹, H. LUETKENS², D. MIENERT¹, P. ADELMANN³, Y. KROCKENBERGER⁴, L. ALFF⁴, M. NAITO⁵, and F.J. LITTERST¹ — ¹IMNF, TU Braunschweig, Germany — ²PSI, Villigen, Schweiz — ³IFP, FZ Karlsruhe, Germany — ⁴WMI, TU München, Germany — ⁵NTT, Atsugi, Japan

We investigated the relevance of inhomogeneous charge and spin order in the electron-doped high- T_c superconductors $(\text{Nd,Pr})_{2-y}\text{Ce}_y\text{CuO}_4$ with $0.05 \leq y \leq 0.125$ by means of muon spin relaxation ($\mu^+\text{SR}$). In this doping range the samples show long-range antiferromagnetic order below $T \approx 100$ K. In all samples we found inhomogeneous local field distributions, which are consistent with an electronic phase separation on a nanometer length scale. This suggests, in addition to similar results in hole-doped cuprates, that this phenomenon is of general relevance for the physics of cuprate superconductors. We also studied the magnetic and superconducting properties of a 20 nm $\text{Ag}/300$ nm $\text{La}_{1.9}\text{Ce}_{0.1}\text{CuO}_4$ (LCCO) heterostructure by means of low-energy $\mu^+\text{SR}$. For temperatures below $T = 90$ K, the stoichiometrically homogeneous LCCO film exhibits a magnetic layer at the interface to the Ag capping. Energy-dependent low-energy $\mu^+\text{SR}$ reveals that the thickness of this magnetic layer continuously increases from 0 nm to 50 nm with decreasing temperature and that it persists below the superconducting transition at $T_c = 28$ K. In

an applied magnetic field, the LCCO film shows Meissner screening with a magnetic penetration depth of the order of 350 nm proving the coexistence of bulk superconductivity and magnetism in the same sample.

TT 5.3 Fr 18:30 TU H104

Excitation spectrum of d -wave Fermi surface deformation — ●HIROYUKI YAMASE — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569, Stuttgart, Germany

The d -wave Fermi surface deformation ($d\text{FSD}$) is one of possible orders competing with the d -wave singlet pairing, and is generated by forward scattering processes of electrons. We report dynamical properties of the $d\text{FSD}$ and calculate its correlation functions within the random phase approximation. In the normal state, the excitation spectrum shows a low energy peak, which smoothly connects to critical fluctuations of the $d\text{FSD}$ at lower temperature. The competition with the d -wave pairing, however, blocks the critical fluctuations. The whole spectral weight is transferred to high energy where a pronounced peak appears in the d -wave pairing state. This peak is an overdamped collective mode of the $d\text{FSD}$ and can grow to become a resonance mode at moderate finite wavevectors.

TT 5.4 Fr 18:45 TU H104

Photobleaching in $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$ in a simultaneous Raman and transport experiment — ●S. BAHR¹, A. R. GOÑI², J. GUIMPEL³, B. MAIOROV⁴, A. FAINSTEIN³, G. NIEVA³, and C. THOMSEN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — ²ICREA Research Professor, Institut de Ciència de Materials de Barcelona, Campus de la UAB, 08193 Bellaterra, Spain — ³Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, 8400 San Carlos de Bariloche, Río Negro, Argentina — ⁴Superconductivity Technology Center, MS K763, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Persistent photoinduced change of physical properties in the $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$ high temperature superconductor family has for some time been investigated with various, complementary experimental methods. Illumination induced effects are observed in electrical transport as well as in Raman spectra, and more recently, in reflectance anisotropy spectroscopy. While a connection to oxygen deficiencies in the chain plane of the material is obvious in all experiments, the precise mechanism of photobleaching is still uncertain, nor it is clear if all methods probe aspects of the same physical property of the material.

In this study we focus on the explicit connection between electrical transport and optical phenomena by performing a simultaneous experiment. Both the change of resistivity and Raman features in thin films of $\text{GdBa}_2\text{Cu}_3\text{O}_{7-\delta}$ under illumination have been recorded. We present a comparison of the time dependencies and discuss the results in the framework of the oxygen-vacancy picture of photobleaching.

TT 6 Correlated Electrons - (General) Theory I

Zeit: Freitag 14:00–16:15

Raum: TU H2053

TT 6.1 Fr 14:00 TU H2053

Theory of optical spectral weights in Mott insulators with orbital degeneracy — ●PETER HORSCH¹, GINIYAT KHALIULLIN¹, and ANDRZEJ M. OLEŚ^{1,2} — ¹Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — ²Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Krakau, Poland

Introducing partial sum rules for the optical multiplet transitions, we outline a unified approach to magnetic and optical properties of strongly correlated transition metal oxides. On the examples of LaVO_3 and LaMnO_4 we demonstrate how the temperature and polarization dependences of different components of the optical multiplet are determined by the underlying spin and orbital correlations dictated by the low-energy superexchange Hamiltonian.

G. Khaliullin, P. Horsch, and A.M. Oleś, Phys. Rev. B 70, 195103 (2004).

TT 6.2 Fr 14:15 TU H2053

Spectral functions of some frustrated lattice structures with charge degrees of freedom — ●FRANK POLLMANN¹, PETER FULDE¹, and ERICH RUNGE² — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — ²Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, 98684 Ilmenau, Germany

Geometrical frustration of lattices leads to many interesting physical effects. While the magnetic properties of frustrated lattices have already received wide interest, one recently began to explore the charge degrees of freedom. In particular it has been proposed that excitations carrying charge $e/2$ should exist. However, it is not clear whether these excitations can separate from each other or are confined. For a deeper understanding of the dynamics of these charge degrees of freedom we calculated numerically the spectral functions of spinless fermions on finite checkerboard- and kagomé lattices. In both cases the spectral functions indicate a strong non-Fermi liquid behaviour. Furthermore we compare our results with

analogous bosonic systems.

TT 6.3 Fr 14:30 TU H2053

Phase diagram of the half-filled two-dimensional SU(N) Hubbard-Heisenberg model. — ●FAKHER ASSAAD — Universität Würzburg

We investigate the phase diagram of the half-filled SU(N) Hubbard-Heisenberg model with hopping t , exchange J and Hubbard U , on a two-dimensional square lattice. In the large- N limit, and as a function of decreasing values of t/J , the model shows a transition from a d -density wave state to a spin dimerized insulator. A similar behavior is observed at $N=6$ whereas at $N=2$ a spin density wave insulating ground state is stabilized. The $N=4$ model, has a d -density wave ground state at large values of t/J which as a function of decreasing values of t/J becomes unstable to an insulating state with no apparent lattice and spin broken symmetries. In this state, the staggered spin-spin correlations decay as a power-law, resulting in gapless spin excitations at $\vec{q} = (\pi, \pi)$. Furthermore, low lying spin modes with small spectral weight are apparent around the wave vectors $\vec{q} = (0, \pi)$ and $\vec{q} = (\pi, 0)$. This gapless spin liquid state is equally found in the SU(4) Heisenberg ($U/t \rightarrow \infty$) model in the self-adjoint antisymmetric representation. An interpretation of this state in terms of a π -flux phase is offered. Our results stem from projective ($T = 0$) quantum Monte-Carlo simulations on lattice sizes ranging up to 24×24 .

TT 6.4 Fr 14:45 TU H2053

Electron-phonon interaction in strongly correlated materials — ●OLIVER RÖSCH and OLLE GUNNARSSON — Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, 70569 Stuttgart

We study the interplay of electron-phonon and electron-electron interactions for a t - J model with electron-phonon coupling. Using exact sum rules, we find that the effect of the electron-phonon interaction on the phonon self-energy is strongly suppressed at low doping, while there is no corresponding suppression for the electron self-energy or the phonon-induced electron-electron interaction.¹

Photoemission experiments suggest polaronic behavior in undoped cuprates due to coupling to bosons. Calculating the electron-phonon interaction in a shell model, we find sufficiently strong coupling to give polaronic behavior. Using an adiabatic approximation we explain why the broad peak from phonon sidebands shows a dispersion consistent with that of a quasi-particle in a purely electronic model without electron-phonon interaction.²

[1] O. Rösch and O. Gunnarsson, cond-mat/0407064, Phys. Rev. Lett. in press.

[2] O. Rösch and O. Gunnarsson, cond-mat/0410247.

TT 6.5 Fr 15:00 TU H2053

Kombination von Vielteilchen- und Ab-Initio-Methoden zur Berechnung der elektronischen Struktur von Metallen — ●OLAF PESCHEL¹, GERD CZYCHOLL¹ und ILAN SCHNELL² — ¹Universität Bremen, Institut für Theoretische Physik — ²Los Alamos National Laboratory, Theoretical Division

Wir gehen von den Bloch-Wellenfunktionen einer DFT-Hartree-Rechnung (ohne Austausch-Korrelationspotential) aus, mit denen wir die statische Suszeptibilität und dielektrische Funktion in Random Phase Approximation (RPA) berechnen. Die Bloch-Wellenfunktionen transformieren wir zu maximal lokalisierten Wannier-Funktionen, und berechnen bezüglich dieser Basis alle relevanten Hopping- und statisch abgeschirmten Coulomb-Matrixelemente. Wir haben damit den Hamilton-Operator in Zweiter Quantisierung unter Berücksichtigung statischer Abschirmung, mit ab-initio berechneten Parametern. Dies ermöglicht die Anwendung von Verfahren der Vielteilchentheorie.

Konkrete Rechnungen wurden für Li als denkbar einfachstes Metall durchgeführt. Es zeigt sich, daß nur on-site-Beiträge bei den abgeschirmten Coulomb-Matrixelemente relevant sind, so daß wir ein verallgemeinertes Vierband-Hubbard-Modell erhalten. Da die Größe der abgeschirmten Coulomb-Wechselwirkung deutlich geringer als die Bandbreite ist, kann die Selbstenergie in zweiter Ordnung Störungsrechnung (SOPT) berechnet werden. Dadurch wird dynamische Abschirmung mitberücksichtigt. Wir vergleichen die Ergebnisse der SOPT mit denen einer statisch abgeschirmten Hartree-Fock-Rechnung.

TT 6.6 Fr 15:15 TU H2053

Transportgrößen von Systemen schwerer Fermionen in DMFT/NRG — ●CLAAS GRENZEBACH, FRITHJOF ANDERS und GERD CZYCHOLL — Institut für Theoretische Physik, Universität Bremen

Systeme schwerer Fermionen werden durch das periodische Andersonmodell (PAM) beschrieben, welches mittels der dynamischen Molekularfeldtheorie (DMFT) auf ein effektives Einzelstellenproblem (SIAM) abgebildet wird. Dieses behandeln wir mit numerischer Renormierungsgruppentheorie (NRG), einem nicht-störungstheoretischen Verfahren, das sich für Rechnungen mit kleinen, mittleren und großen Wechselwirkungen U eignet und die Kondoskala korrekt wiedergibt.

Damit werden in Abhängigkeit von der Temperatur statische und dynamische Leitfähigkeiten und die Thermokraft berechnet.

TT 6.7 Fr 15:30 TU H2053

Influence of Electron Correlations on Electron Transfer — ●SABINE TORNOW, NING-HUA TONG, and RALF BULLA — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Electron transfer is a basic chemical process and is found, e.g. in corrosion of metals, enzymatic activities, cell metabolism or photosynthesis. The donor and acceptor sites may be transition metal ions (e.g., in some basic biological processes) and are strongly coupled to environmental modes (bath). To include electron correlations and multi electron transfer we propose a new model which extends the spin-boson model. We calculate static and dynamic properties using Wilsons Numerical Renormalization Group method. We discuss the thermal transition rate and discuss polaron, bipolaron and exciton formation.

TT 6.8 Fr 15:45 TU H2053

Arbitrary-range hopping on the Bethe lattice: Exact results for densities of states and dynamical mean-field theory — ●MARCUS KOLLAR¹, MARTIN ECKSTEIN¹, KRZYSZTOF BYCZUK², and DIETER VOLLHARDT¹ — ¹Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg — ²Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 Warszawa, Poland

We develop a new method which relates an arbitrary hopping Hamiltonian on the Bethe lattice to the Hamiltonian with nearest-neighbor hopping [1]. This provides an exact expression for the density of states for any hopping. We present analytic results for the DOS corresponding to hopping between nearest and next-nearest neighbors, and also for exponentially decreasing hopping amplitudes. Conversely it is possible to construct a hopping Hamiltonian on the Bethe lattice for any given DOS. We also derive the exact self-consistency equations arising in the context of dynamical mean-field theory, which lead to a new starting point for studies of the Hubbard-type models with frustration.

[1] M. Eckstein *et al.*, cond-mat/0409730.

TT 6.9 Fr 16:00 TU H2053

A Quantum Central Limit Theorem for Interacting Many Particle Systems and its Applications — ●MICHAEL HARTMANN^{1,2}, GÜNTER MAHLER², and ORTWIN HESS³ — ¹DLR Stuttgart, Pfaffenwaldring 38-40, 70569 Stuttgart — ²Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — ³Advanced Technology Institute, University of Surrey, Guildford GU2 7XH, UK

We present a central limit theorem for the distribution of the total energy in a product state of a quantum many body system with nearest neighbor or next nearest neighbor interactions [1]. Using this result, one can draw estimates on quantities which are functions of the total energy without diagonalizing the Hamiltonian. Interesting examples are the density of states and the partition function [2]. On the other hand, information about the local (subsystem-) states can be obtained, too [3]. An advantage of our approach is its applicability to strongly interacting and frustrated systems.

[1] Hartmann, Mahler and Hess: Lett. Math. Phys. 68 (2004) 103

[2] Hartmann, Mahler and Hess: cond-mat/0406100

[3] Hartmann, Mahler and Hess: Phys. Rev. Lett. 93 (2004) 080402

TT 7 Correlated Electrons - (General) Theory II

Zeit: Freitag 16:30–18:45

Raum: TU H2053

Hauptvortrag

TT 7.1 Fr 16:30 TU H2053

Self-Energy Functionals: A New Approach to Strongly Correlated Electron Systems — ●MICHAEL POTTHOFF — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

Since the seminal work by Luttinger, Ward, Baym and Kadanoff in the sixties, we know about a fundamental variational principle of the form $\delta\Omega[\Sigma] = 0$. This is interesting as it promises an access to the grand potential Ω and the self-energy Σ for a system of interacting fermions and, thereby, to the equilibrium thermodynamics as well as to (one-particle) excitations. While truncations of the functional form were frequently used in the past to construct weak-coupling (“conserving”) approximations, it is surprising that there has not been a single *direct* application of the variational principle until recently. This stands in marked contrast to the widespread Ritz principle $\delta E[\Psi] = 0$ which, however, does not give information on excitation properties.

This talk shows how to make use of the Luttinger-Ward variational principle in various physical situations. In the high- T_c problem, for example, systematic and non-perturbative approaches are needed which accurately treat short-range correlations while directly working in the thermodynamic limit. This can be achieved with a novel variational cluster-perturbation theory. Contacts can be made to the cluster generalizations of the DMFT. For various transition metals and oxides, on the other hand, a local (mean-field) approximation is sufficient. Here the self-energy-functional approach shows up an efficient way to account for the temporal degrees of freedom. Extensions of the method to include phonons, non-local interactions and to disordered systems are discussed.

TT 7.2 Fr 17:00 TU H2053

Collective fields in the functional renormalization group for fermions, Ward identities, and the exact solution of the Tomonaga-Luttinger model — ●FLORIAN SCHÜTZ¹, LORENZ BARTOSCH^{1,2}, and PETER KOPIETZ¹ — ¹Institut für Theoretische Physik, Universität Frankfurt, Robert Mayer-Strasse 8, 60054 Frankfurt — ²Department of Physics, Yale University, P. O. Box 208120 New Haven, CT 06520-8120, USA

We have developed ¹ a new formulation of the functional renormalization group (RG) for interacting fermions. We decouple the interaction by means of a Hubbard-Stratonovich transformation and derive an exact hierarchy of RG flow equations for the irreducible vertices of the resulting coupled field theory involving both fermionic and bosonic fields. The freedom of choosing a momentum transfer cutoff for the bosonic soft modes in addition to the usual band cutoff for the fermions opens the possibility of new RG schemes. In particular, we show how the exact solution of the Tomonaga-Luttinger model emerges from the functional RG if one works with a momentum transfer cutoff. Then the Ward identities associated with the local particle conservation at each Fermi point are valid at every stage of the RG flow and provide a solution of an infinite hierarchy of flow equations for the irreducible vertices. The RG flow equation for the irreducible single-particle self-energy can then be closed and can be reduced to a linear integro-differential equation, the solution of which yields the result familiar from bosonization.

[1] Florian Schütz, Lorenz Bartosch and Peter Kopietz, cond-mat/0409404.

TT 7.3 Fr 17:15 TU H2053

Fermionic renormalization group flow into phases with broken symmetry — ●CARSTEN HONERKAMP¹, MANFRED SALMHOFER², WALTER METZNER¹, and OLIVER LAUSCHER² — ¹MPI Festkörperforschung, Stuttgart — ²Theoretische Physik, Universität Leipzig

We present an extension of the fermionic functional RG which allows us to continue the RG flow into long-range ordered phases. For the example of Cooper pairing we discuss how the divergence of the RG flow without selfenergy corrections is cured and how BCS and Eliashberg gap equations are obtained from the RG. We describe how vertex corrections beyond the mean-field approach and the Kohn-Luttinger mechanism are included in this formalism.

TT 7.4 Fr 17:30 TU H2053

Contractor Renormalization Group Approach to the Strongly-Correlated Hubbard Model — ●SASCHA BREHM¹, ENRICO ARRIGONI^{2,1}, and WERNER HANKE¹ — ¹Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — ²Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria

In a first step, we apply the Contractor Renormalization Technique (CORE) to the 2-D Hubbard Model including bosonic plus fermionic excitations. The resulting Plaquette Boson-Fermion Model (PBFM) displays even qualitative changes (screening, etc.) compared to the so far exclusively considered purely bosonic Plaquette Model (E. Altman and A. Auerbach, Phys.Rev.B 65, 104508 (2002)). This is also shown in the case of the inter-layer Cooper-pair tunnelling theory. The phase diagram for the competing phases is then calculated within the slave-boson technique.

TT 7.5 Fr 17:45 TU H2053

Non-Equilibrium Scaling Analysis of the Kondo Model with Voltage Bias — ●STEFAN KEHREIN — Theoretische Physik III - Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg

We study the scaling equations for the Kondo model with voltage bias. We discuss how their structure changes from the well-known equilibrium form to the non-equilibrium situation for nonzero voltage bias. Our analysis is done using the flow equation method (infinitesimal unitary transformation method) that makes the many-body Hamiltonian increasingly more energy-diagonal (cond-mat/0410341). In particular, it becomes apparent that the conventional expansion of the scaling equations in powers of the running coupling constant needs to be reconsidered carefully in non-equilibrium. Our observations should be of general importance for deriving the scaling flow of similar non-equilibrium quantum many-body problems.

TT 7.6 Fr 18:00 TU H2053

Violation of the Fluctuation-Dissipation Theorem in the Kondo Model with a Non-Equilibrium Initial State — ●DMITRY LOBASKIN and STEFAN KEHREIN — Theoretische Physik III - Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg

The fluctuation-dissipation theorem (FDT) plays a fundamental role in understanding equilibrium quantum many-body problems. However, the FDT does in general not hold in non-equilibrium situations. In this talk we present exact results for the violation of the FDT in the Kondo model where the impurity spin is frozen for all negative times, and set free to relax towards its equilibrium value at positive times. Exact results at the Toulouse point of this model (cond-mat/0405193) make it possible to investigate the FDT violation on all time scales: for times much later than the initial non-equilibrium preparation, for times immediately after the relaxation starts, and for the crossover between these two regimes. General aspects of the FDT and the reason for its violation in non-equilibrium are discussed as well.

TT 7.7 Fr 18:15 TU H2053

Selbstenergie-Funktional-Theorie für wechselwirkende Elektronensysteme mit Unordnung — ●MATTHIAS BALZER und MICHAEL POTTHOFF — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland D-97074 Würzburg

Die Selbstenergie-Funktional-Theorie¹ bietet einen nicht-perturbativen Zugang zur Berechnung wechselwirkender Elektronensysteme. Approximative Lösungen können variationell unter Verwendung eines Referenzsystems bestimmt werden. Wir stellen hier die Verallgemeinerung der Theorie auf ungeordnete Systeme vor. Dazu wird ein erweitertes Funktional von Unordnungs- und Wechselwirkungs-Selbstenergie betrachtet, ein entsprechendes Variationsprinzip aufgestellt und gezeigt, wie dieses durch Bezugnahme auf ein Referenzsystem zur Konstruktion von Approximationen angewendet werden kann. Die Wahl des Referenzsystems bestimmt den Charakter der Approximation. Z.B. ergibt sich als optimale lokale Näherung die DMFT-CPA. Darüberhinaus sind aber auch einfachere und dennoch konsistente Näherungen konstruierbar. Um die Anwendbarkeit der Theorie zu demonstrieren, diskutieren wir eine Zwei-Platz-

(Mean-Field-)Näherung zur Bestimmung des $T=0$ -Phasendiagramms des Anderson-Hubbard-Modells mit binärer Legierungsunordnung.

¹ M. Potthoff, Eur. Phys. J. B 32, 429 (2003)

TT 7.8 Fr 18:30 TU H2053

Localization of non-interacting electrons in thin layered disordered systems — ●V. Z. CEROVSKI, R. K. BROJEN SINGH, and M. SCHREIBER — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

Localization of electronic states in disordered thin layered systems

with b layers is studied using the transfer-matrix method and finite-size scaling of the inverse smallest Lyapunov exponent. The results support the one-parameter scaling theory of localization for disorder strengths W studied and $b = 1, \dots, 6$. The obtained results for the localization length are in good agreement with both the analytical results of the self-consistent theory of localization and the numerical scaling studies of the two-dimensional Anderson model. The localization length near the band center grows exponentially with b for a fixed W but no localization-delocalization transition takes place.

TT 8 Posters Transport

Zeit: Freitag 14:00–18:00

Raum: Poster TU C

TT 8.1 Fr 14:00 Poster TU C

Spin transport in disordered single-wall carbon nanotubes — ●NITESH RANJAN, N. NEMEC, and G. CUNIBERTI — Molecular Computing Group, Universität Regensburg, D-93040 Regensburg, Germany

The effects of vibrations on the linear conductance of single-wall carbon nanotubes can be described by the Anderson model of disorder [1]. Indeed, there are also indications that multi-wall carbon nanotubes effectively behave as a disordered single-wall system as far as transport properties are concerned [2]. With this motivation, we investigate spin transport in ferromagnetically contacted disordered single-wall carbon nanotubes (within the tight binding model) in the coherent regime. Different models for the ferromagnetic leads are employed ranging from wide-band leads to fcc(111) surfaces (as in the case of cobalt). Results as a function of disorder strength and Fermi energy in the leads are given for realistic tube lengths of several hundred nanometers.

[1] M. Gheorghe *et al.*, *cond-mat/0411192*, (2004).

[2] R. Egger and A. O. Gogolin, *Phys. Rev. Lett.* **87**, 066401 (2001).

TT 8.2 Fr 14:00 Poster TU C

Vibrational effects on the linear conductance of carbon nanotubes — ●RAFAEL GUTIERREZ¹, MARIETA GHEORGHE¹, ALESSANDRO PECCHIA², ALDO DI CARLO², and GIANAURELIO CUNIBERTI¹ — ¹Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg — ²INFM and Dept. of Electrical Engineering, University of Rome “Tor Vergata”, I-00133 Rome

Carbon nanotubes (CNTs) has become a paradigm for studying electronic transport on low dimensions. They have a high potential for applications in the emerging field of molecular electronics. The main body of research on electronic transport in CNTs in the last decade has mainly focused on elastic transport. The influence of vibrational excitations on charge propagation in CNTs has not been however addressed in detail. We present a density-functional-based study on the influence of structural lattice fluctuations on the *elastic* electronic transport in carbon nanotubes in the linear response regime. Structural distortions are considered as a random field; the linear conductances can be calculated after appropriate averaging over this field. Results obtained from a frozen-phonon-like approximation are compared with classical molecular dynamics simulations. We demonstrate that the average effect of structural fluctuations can be captured by the Anderson model of disorder. Further, the influence of single vibrational modes on the electronic transport can be extracted with our approach as well as the role of zero-point quantum fluctuations.

TT 8.3 Fr 14:00 Poster TU C

DMRG calculations of non-equilibrium transport in one dimensional strongly correlated lattice models — ●GÜNTER SCHNEIDER and PETER SCHMITTECKERT — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe

We study non equilibrium transport in one dimensional strongly correlated lattice models using real time dynamics within Density Matrix Renormalization Group (DMRG). In particular we calculate the finite bias conductance beyond Landauer-Büttiker theory for various model nano structures.

TT 8.4 Fr 14:00 Poster TU C

Percolative Transport in $\text{Ag}_{2+\delta}\text{Se}$ with High Silver Excess — ●M. VON KREUTZBRÜCK¹, K. ALLWEINS¹, B. MÖGWITZ², C. KORTE², J. JANEK², and L. KIENLE³ — ¹Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen — ²Physikalisch-Chemisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 58, D-35392 Giessen — ³Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart

Since the appearance of an unusual linear and large magnetoresistance (MR) effect in the narrow gap silver chalcogenides $\text{Ag}_{2+\delta}\text{Se}$ and $\text{Ag}_{2+\delta}\text{Te}$ shown by Xu et al. in 1997 research has drawn much attention to establish new routes for the design of magnetoresistive sensors. We investigated the galvanomagnetic transport properties of polycrystalline Ag_xSe thin films with silver excess in the range from $x = 1.5$ to 18. The results prove that the silver excess controls the transition from linear magnetoresistance (MR) behaviour to the quadratic ordinary MR and the temperature for the metal-semiconductor transition. We observe for $2 < x < 2.3$ a steep rise of the conductivity and interpret this result as a consequence of the percolation of nanoscale silver networks within the semiconducting matrix. To verify our model we performed an estimation on the basis of a FEM-model of both cubic silver selenide grains with nanoscopic silver films in the grain boundary and silver precipitates within the narrow-band matrix. The simulation proves the presence of the coexistence of silver paths on the nanoscale and single silver precipitates, which is also indicated by first TEM investigations.

TT 8.5 Fr 14:00 Poster TU C

Spin relaxation in Quantum Dots induced by Nyquist Noise — ●FLORIAN MARQUARDT¹ and VENIAMIN A. ABALMASSOV² — ¹Department of Physics, Yale University, New Haven 06520, USA — ²Institute of Semiconductor Physics SB RAS and Novosibirsk State University, 630090 Novosibirsk, Russia

We analyze the spin relaxation rate T_1^{-1} for an electron inside a quantum dot that is subject to the Nyquist voltage fluctuations of the confining metallic gates. In combination with spin-orbit coupling, this leads to a relaxation rate that depends on the direction of the magnetic field and the impedance matrix of the gate circuit, providing possibilities for distinguishing this mechanism from other sources of relaxation.

[1] F. Marquardt and V. A. Abalmassov, *cond-mat/0404749* (2004)

TT 8.6 Fr 14:00 Poster TU C

Periodic Field Emission from an Isolated Nano-Scale Electron Island — ●D.V. SCHEIBLE¹, C. WEISS², J.P. KOTTHAUS¹, and R.H. BLICK³ — ¹Center for NanoScience and Fakultät für Physik der Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — ²Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — ³Department of Electrical & Computer Engineering, University of Wisconsin-Madison, 1415 Engineering Drive, Madison, Wisconsin 53706

We observe field emission from an isolated nano-machined gold island. The island is able to mechanically oscillate between two facing electrodes, which provide recharging and detection of the emission current. We are able to trace and reproduce the transition from current flow through a rectangular tunneling barrier to the regime of field emission. A theoretical model via a master-equation reproduces the experimental data and shows deviation from the Fowler-Nordheim description due to the island's electric isolation.

[1] D. V. Scheible et al., *Phys. Rev. Lett.* **93**, 186801 (2004).

TT 8.7 Fr 14:00 Poster TU C

Zero-Bias Anomaly in Disordered Multiwall Carbon Nanotubes — •N. KANG, L. LU, Z. W. PAN, and S. S. XIE — Institute of Physics, Chinese Academy of Science, Beijing, People's Republic of China

Multiwall carbon nanotubes (MWNTs) provide a unique system for studying electron-electron (e-e) interaction effects in disordered wires. We have studied tunneling of electrons into MWNTs as a function of voltage and temperature. The conductance of MWNTs exhibits a strong suppression at low energies, showing a sign of strong e-e correlation. At high energy, the differential conductance obeys a power law behavior, which is predicted by the environmental quantum fluctuation theories. At lower energy, we observed a crossover to an exponential dependence, in accordance with recent theoretical calculation. For an analytic description of our data at low temperatures, it would require a nonperturbative theory for the e-e interaction, being consistent with our previous transport measurements on the same batch of MWNTs [1,2].

[1] N. Kang, et al., Phys. Rev. B 66, 241403 (2002). [2] N. Kang, et al., Phys. Rev. B 67, 33404 (2003).

TT 8.8 Fr 14:00 Poster TU C

Nonequilibrium transport in nanostructured palladium-nickel alloy films — •JAKOB BRAUER¹, HEIKO B. WEBER¹, and HILBERT V. LÖHNEYSEN^{2,3} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik — ³Physikalisches Institut, Universität Karlsruhe

We investigated electronic transport properties of short nanostructured metallic bridges. Our samples consisted of short palladium-nickel alloy films contacted by thick gold electrodes acting as reservoirs, thereby establishing a nonequilibrium electronic distribution under applied bias[1]. The nickel concentration of the alloy was chosen near the onset of ferromagnetic ordering. The motivation for this was to study the interplay between electronic nonequilibrium distribution and exchange splitting. We measured the dependency of the resistance on magnetic field, bias and temperature. Our data show a zero-bias anomaly, which depends on the magnetic field in a nontrivial fashion.

[1] H.B. Weber *et al.*, PRB 63 (2001) 165426

TT 8.9 Fr 14:00 Poster TU C

Theoretical analysis of the conductance histograms of Au atomic contacts — •MARKUS DREHER¹, JAN HEURICH², CARLOS CUEVAS², ELKE SCHEER¹, and PETER NIELABA¹ — ¹Physics Department, University of Konstanz, 78457 Konstanz, Germany — ²Institut für Theoretische Festkörperphysik, University of Karlsruhe, 76128 Karlsruhe, Germany

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 8.10 Fr 14:00 Poster TU C

Electron transport in metallic multi-island geometries: Coulomb blockade and quantum fluctuations — •BJÖRN KUBALA¹, GÖRAN JOHANSSON², and JÜRGEN KÖNIG¹ — ¹Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²MC2, Chalmers University of Technology, S-412 96 Göteborg, Sweden

Experiments on coupled single-electron transistors investigate, how charging effects on one island are modified by capacitive and tunnel coupling to other islands [1]. We developed a method to study electron transport through such systems, driven by finite thermal or voltage bias. Based on real-time transport theory [2], all diagrams up to second order in tunneling coupling are automatically generated and evaluated. This computational approach captures all different sequential and cotunnel-

ing processes.

In particular, we find a class of cotunneling processes involving correlated tunneling onto two different islands. These can be linked to tunneling rates for an SET in a noisy environment -constituted by another SET- as calculated within a $P(E)$ theory. We will discuss applications to different setups and strength and limitations of our method.

[1] R. Schäfer et al., cond-mat/0205223; Physica E 18, 87, (2003); K. W. Lehnert et al., Phys. Rev. Lett. 91, 106801 (2003).

[2] H. Schoeller and G. Schön, Phys. Rev. B 50, 18 436 (1994); J. König, H. Schoeller, and G. Schön, Phys. Rev. Lett. 78, 4482 (1997).

TT 8.11 Fr 14:00 Poster TU C

Competition of Coherence and Decoherence: the Phase Diagram of the Non-Equilibrium Kondo Model — •STEFAN KEHREIN — Theoretische Physik III - Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg

We study the Kondo effect in quantum dots in a non-equilibrium state due to an applied dc-voltage bias. Using the method of infinitesimal unitary transformations (flow equations), we develop a perturbative scaling picture that naturally contains both equilibrium coherent and non-equilibrium decoherence effects (cond-mat/0410341). The competition of these effects determines the phase diagram of the non-equilibrium Kondo model, and e.g. establishes a large single-channel Kondo physics dominated regime for asymmetrically coupled quantum dots. We present results for the conductance, the local density of states and the spin-spin correlation function at various points in this phase diagram.

TT 8.12 Fr 14:00 Poster TU C

Density of states of interacting electrons in quasi one-dimensional metallic wires — •WOLFGANG KÖRNER¹, PETER SCHWAB², and HERMANN GRABERT¹ — ¹Albert-Ludwigs-Universität Freiburg — ²Universität Augsburg

Based on the quasiclassical Green's function approach [1] we determine the tunneling density of states $\rho(\varepsilon)$ of a diffusive metallic nanowire in presence of electron-electron interactions. The perturbative result by Altshuler and Aronov, $\rho(\varepsilon) \propto \varepsilon^{-1/2}$, is extended to the nonperturbative regime near the Fermi edge where $\rho(\varepsilon) \propto \sqrt{\varepsilon} \exp(-\varepsilon_0/\varepsilon)$, in accordance with calculations based on the nonlinear σ -model [2]. Further extensions, including contributions from the spin triplet channel, will also be discussed.

[1] P. Schwab and R. Raimondi, Ann. Phys. (Leipzig) 12, 471-516 (2003)

[2] J. Rollbühler and H. Grabert, Phys. Rev. Lett. 87, 126804 (2001)

TT 8.13 Fr 14:00 Poster TU C

A Gate-Controlled Atomic Quantum Switch — •FANGQING XIE¹, LAURENT NITTLER¹, STEFAN BRENDENBERGER¹, CHRISTIAN OBERMAIR¹, and THOMAS SCHIMMEL^{1,2} — ¹Institute for Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe Germany

An atomic-scale quantum conductance switch is demonstrated which allows to open and close an electrical circuit by the controlled and reproducible reconfiguration of silver atoms within an atomic-scale junction [1]. The only movable parts of the switch are the contacting atoms. The switch is entirely controlled by an external electrochemical voltage applied to an independent third gate electrode. Controlled switching was performed between a quantized, electrically conducting "on-state" exhibiting a conductance of $G_0 = 2e^2/h$ ($\approx 1/12.9k\Omega$) or preselectable multiples of this value and an insulating "off-state" [2].

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

[2] F.-Q. Xie, Ch. Obermair and Th. Schimmel, Solid State Communications 132, 437-442 (2004).

TT 8.14 Fr 14:00 Poster TU C

Supersymmetry for disordered systems with interaction — •GEORG SCHWIETE¹ and KONSTANTIN B. EFETOV^{1,2} — ¹Institut für Theoretische Physik III, Ruhr-Universität Bochum — ²L. D. Landau Institute for Theoretical Physics, Moscow

Considering disordered electron systems we suggest a scheme that allows to include an electron-electron interaction into a supermatrix sigma-model [1]. The method is based on replacing the initial model of interacting electrons by a fully supersymmetric model. Although this replacement is not exact, it is a good approximation for a weak short range interac-

tion and arbitrary disorder. The replacement makes the averaging over disorder and further manipulations straightforward and we come to a supermatrix sigma-model containing an interaction term. The structure of the model is rather similar to the replica one, although the interaction term has a different form. We study the model by perturbation theory and renormalization group calculations. We check the renormalizability of the model in the first loop approximation and in the first order in the interaction. In this limit we reproduce the renormalization group equations known from earlier works. We hope that the new supermatrix sigma-model may become a new tool for non-perturbative calculations for disordered systems with interaction.

[1] G. Schwiete, K. Efetov, cond-mat/0409546

TT 8.15 Fr 14:00 Poster TU C

Cotunneling and coherent tunneling through quantum dots — ●BERNHARD WUNSCH, MICHAEL TEWS, and DANIELA PFANNKUCHE — 1. Institut für Theoretische Physik, Universität Hamburg

We study transport through a quantum dot coupled to two electronic reservoirs. Including all transport processes up to fourth order in tunneling [1] we go systematically beyond a master equation approach with transition rates obtained from Fermi's Golden rule. Thus we are able to describe transport structures within the coulomb blockade regime due to cotunneling which allow to measure the excitation spectrum of the dot. In particular we identify peaks in the differential conductance inside the coulomb blockade which are due to a sequential tunneling process out of an excited state allowed by a previous inelastic cotunneling event [1]. Furthermore we investigate the effect of coherent tunneling, where different transport channels may interfere with each other and the quantum dot may be in a superposition of eigenstates [3].

[1] J. König, J. Schmid, H. Schoeller, and G. Schön, Phys. Rev. B **54** 16820 (1996)

[2] M. Tews, Annalen der Physik **13** 249-304 (2004)

[3] D. Boese, W. Hofstetter, and H. Schoeller, Phys. Rev. B **66** 125315 (2002)

TT 8.16 Fr 14:00 Poster TU C

Switching an Electrical Current with Atoms: the Reproducible Operation of a Multi-Atom Relay — ●FANGQING XIE¹, CHRISTIAN OBERMAIR¹, and THOMAS SCHIMMEL^{1,2} — ¹Institute for Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

The demonstration of a multi-atom quantum point contact relay is reported, which can be reversibly switched between a quantized conducting "on-state" and an insulating "off-state" by applying an electrochemical control potential to a separate, third electrode, the control or gate electrode [1,2]. The transition occurs directly from the conducting "on-state" at $5G_0$ ($G_0 = 2e^2/h$ being the conductance quantum) to the insulating "off-state". No stable intermediate levels are observed during the switching process, indicating a reproducible bistable reconfiguration of one single multi-atom contact rather than a deposition and dissolution of different parallel contacts. The results demonstrate the feasibility and reproducible operation of a configurable electronic device based on a multi-atom contact, which exhibits the functionality of an atomic relay or a transistor, opening intriguing perspectives for electronics and logics on the atomic scale.

[1] F.-Q. Xie, Ch. Obermair and Th. Schimmel, Solid State Communications **132**, 437-442 (2004).

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

TT 8.17 Fr 14:00 Poster TU C

Aharonov-Bohm Interferometry with Quantum Dots — ●STEFAN LEGEL¹, JÜRGEN KÖNIG², JAN MARTINEK³, and GERD SCHÖN¹ — ¹Universität Karlsruhe — ²Ruhr-Universität Bochum — ³Institute of Molecular Physics, PAS, Poznan, Poland

The manifestations of quantum coherence are in the foundations of the physics of mesoscopic systems. The presence of quantum coherence is detectable through interference experiments.

We study electron transport through a closed Aharonov-Bohm interferometer containing two single-level quantum dots. We address the question how electron-electron 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 8.18 Fr 14:00 Poster TU C

Adiabatic Pumping through interacting Quantum Dots — ●JANINE SPLETTSTOESSER^{1,2}, MICHELE GOVERNALE¹, ROSARIO FAZIO¹, and JÜRGEN KÖNIG² — ¹Scuola Normale Superiore, Pisa — ²Ruhr-Universität Bochum

There has been much recent experimental and theoretical interest in adiabatic quantum pumping through mesoscopic electronic devices such as quantum dots. A systematic framework exists to analyze such a system in the non-interacting limit starting from the so-called Brouwer's formula. In interacting systems a general formalism to describe adiabatic pumping is not available until now. Using the nonequilibrium-Green-function approach for transport through interacting systems (by Jauho, Wingreen and Meir), we write a formula to calculate adiabatic pumping through an interacting quantum dot.

TT 8.19 Fr 14:00 Poster TU C

Conductance Measurements on Ferromagnetic Breakjunctions — ●CÉCILE BACCA, MAGDALENA HÜFNER, H.-F. PERNAU, and ELKE SCHEER — Fachbereich Physik, Universität Konstanz

We investigate lithographically fabricated breakjunctions of ferromagnetic metals. With the help of a three-point bending mechanism, the bridges can be opened to a single-atom contact, broken to a vacuum-tunnel contact and closed again repeatedly at low temperatures ($T \leq 4.2\text{K}$). 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. However, the details of the magnetoconductance curves are not yet fully understood. In order to separate the contributions of the different possible effects (magnetostriction, TMR, BMR, AMR,...) we analyse the magnetoconductance as a function of the symmetry of the contact, of the free-standing bridge length, and for different materials (Co, Ni). In parallel we calculate [2] the magnetization state as a function of the geometry of the contact, the film thickness and its magnetic history. [1] J.M. Krasns 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 8.20 Fr 14:00 Poster TU C

Exactly solvable model of three interacting particles in an external magnetic field — E. P. NAKHMEDOV^{1,2}, ●K. MORAWETZ^{1,2}, M. AMEDURI³, A. YURTSEVER⁴, and C. RADEHAUS¹ — ¹Chemnitz University of Technology, 09107 Chemnitz, Germany — ²Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — ³Weill Cornell Medical College in Qatar, Qatar Foundation, Doha, Qatar — ⁴Azerbaijan Academy of Sciences, Institute of Physics, H. Cavid 33, 370143 Baku, Azerbaijan

The quantum mechanical problem of three identical particles, moving in a plane and interacting pairwise via a spring potential, is solved exactly in the presence of a magnetic field. Calculations of the pair-correlation function, mean distance and the cluster area show a quantization of these parameters. Especially the pair-correlation function exhibits a certain number of maxima given by a quantum number. We obtain Jastrow prefactors which lead to an exchange correlation hole of liquid type, even in the presence of the attractive interaction between the identical electrons. [1] E. P. Nakhmedov, K. Morawetz, M. Ameduri, A. Yurtsever, C. Radehaus, Phys. Rev. B **67** (2003) 205106

TT 8.21 Fr 14:00 Poster TU C

Spin-dependent transport through quantum dots with three ferromagnetic leads — ●DANIEL URBAN, MATTHIAS BRAUN, and JÜRGEN KÖNIG — Institut für Theoretische Physik III, Ruhr-Universität Bochum

We examine a single-level quantum dot weakly tunnel-coupled to three ferromagnetic leads. A current between two leads gives rise to spin accumulation and spin blockade. Two effects allow to modify the spin on the dot by changing the magnetization direction of the floating third lead.

The first of these effects is anisotropic spin damping. Spin components in the direction of the third lead have an increased lifetime. The second is

an exchange field arising in the presence of ferromagnetism and Coulomb interaction [1]. It causes precession of the accumulated spin [2].

Transport through the system depends on the spin on the dot and can thus be controlled by the third lead in a transistor-like manner.

[1] J. König and J. Martinek, Phys. Rev. Lett. **90**, 16 (2002).

[2] M. Braun and J. König and J. Martinek, to appear in Phys. Rev. B, (2004), cond-mat/0404455.

TT 8.22 Fr 14:00 Poster TU C

Transport properties of ferromagnetically filled multiwall carbon nanotubes — ●H. VINZELBERG, M. MILNERA, I. MÖNCH, D. ELEFANT, A. LEONHARDT, J. SCHUMANN, and B. BÜCHNER — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstr. 20, D 01069 Dresden, Germany

In conventional semiconductor electronics the spin of the electrons is an unused quantity. However, spin dependent devices have a significant potential for data storage technology and future electronics. Due to their large spin-flip scattering length carbon nanotubes (CNTs) represent a promising candidate for spin dependent electronic devices. High magnetoresistance effects were recently discovered on ferromagnetically contacted CNTs. Ferromagnetically filled multiwall CNTs (MWCNTs) exhibit interesting magnetic properties. However, transport measurement results exist only on as grown two dimensional arrays of aligned Fe-filled MWCNTs. Here we investigate single ferromagnetically filled MWCNT devices produced by using an AC-electrophoresis deposition on predefined Au- or Ti- microfinger structures. The measured magnetotransport data show a broad spectrum of behaviour: positive and negative magnetoresistance, oscillations and shoulders.

TT 8.23 Fr 14:00 Poster TU C

Absence of fractional conductance quantization in ferromagnetic atomic contacts — ●MICHAEL HÄFNER¹, DIEGO FRUSTAGLIA², and JUAN-CARLOS CUEVAS^{1,3} — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Quantum Transport and Information, Scuola Normale Superiore, 56126 Pisa, Italy — ³Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, 28049 Madrid, Spain

In this work we present a theoretical analysis of the current through atomic contacts of magnetic 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 8.24 Fr 14:00 Poster TU C

Thermopower of single-molecule devices — ●JENS KOCH¹, FELIX VON OPPEN¹, YUVAL OREG², and ERAN SELA² — ¹Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — ²Department of Condensed Matter Physics, Weizmann Institute for Science, Rehovot 76100, Israel

We investigate the thermopower of single molecules weakly coupled to metallic leads. We model the molecule in terms of the relevant electronic orbitals and phonons corresponding to either internal vibrations or to oscillations of the molecule as a whole. The thermopower is computed by means of rate equations including both sequential-tunneling and cotunneling processes.

The sign of the thermopower reveals whether electronic transport through the molecule occurs via the LUMO or the HOMO. It is found that the thermopower is sensitive to higher-order processes such as cotunneling. Under certain conditions, it allows one to access the electronic and phononic excitation spectrum of the molecule in a linear-response measurement. In particular, we find that phonon features are more pronounced for weak lead-molecule coupling.

TT 8.25 Fr 14:00 Poster TU C

Theory for transport through a single magnetic molecule: endohedral N@C₆₀ — ●FLORIAN ELSTE and CARSTEN TIMM — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

We present a theory for transport through a single magnetic N@C₆₀ molecule in a break junction, weakly coupled to the metallic leads. Since transport through a single C₆₀ molecule has been demonstrated and the synthesis of endohedral fullerenes is also feasible, such an experiment is possible with present-day technology. Employing a density-matrix formalism we derive rate equations for the occupation probabilities of the many-particle states of the molecule. We calculate the current-voltage characteristics and predict novel interesting structures in the differential conductance dI/dV , which are very different from what is seen for electrons coupled to molecular vibrations. Our results reveal Coulomb-blockade behavior as well as a fine structure of the Coulomb-blockade peaks in dI/dV due to the exchange coupling of the C₆₀ spin to the spin of the encapsulated nitrogen atom.

TT 8.26 Fr 14:00 Poster TU C

Electronic Transport Measurements on Mass-Selected Silicon Clusters — ●JOCHEN GREBING, FELIX VON GYNZ-REKOWSKI, BERND BRIECHLE, GERD GANTEFÖR, and ELKE SCHEER — University of Konstanz, 78467 Konstanz, Germany

We present a setup to study electronic transport properties of single or a few clusters.

Using a magnetron sputter source, clusters can be produced and then be soft-landed on opened adjustable metallic electrodes fabricated with a MCB technique [1]. By closing the junction a single or a few clusters shall be contacted and their electronic transport properties, i.e. current-voltage curves, shall be examined *in situ*. According to theoretical calculations a nonlinear behavior is expected for a bias > 0.5 V for Si₄ clusters contacted with Al leads [2]. A systematic investigation of this system shall provide information to verify these calculations. As a further project these Si₄ clusters shall be gated using a sandwich MCB technique which is currently being developed.

[1] MCB: Mechanically Controllable Breakjunction

[2] C. Roland et al., Phys. Rev. B **66**, 035332 (2002)

TT 8.27 Fr 14:00 Poster TU C

Electronic Transport through C₆₀ — ●TOBIAS BÖHLER, JOCHEN GREBING, and ELKE SCHEER — FB Physik - Universität Konstanz

The electronic transport through a single or a few C₆₀ 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 temperature the experiment shows evidence that the conductance of a single C₆₀ molecule between gold contacts is in the order of a tenth of G_0 . This can be seen in opening and closing curves and also in time-dependent fluctuations of the conductance. However, the thermal fluctuations of the electrodes hamper the acquisition of meaningful current-voltage characteristics. Therefore we present an improved setup to measure the differential conductance at low temperatures.

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

TT 8.28 Fr 14:00 Poster TU C

Influence of laser irradiation on the transport in molecular wires — ●S. WELACK, U. KLEINEKATHÖFER, and M. SCHREIBER — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

New features of molecular wires can be observed when they are irradiated by laser fields. This can be done by periodically oscillating light fields but also by short laser pulses. Here we restrict ourselves to periodic laser fields though the current propagation method is well suited for short laser pulses as well. The theoretical foundation used for these investigations is the density matrix formalism based on a splitting of the full system into a relevant part and a thermal bath. Recently we have developed a formalism which is based on a time-convolutionless projection-operator approach which includes the interaction with time-dependent laser fields non-perturbatively and is valid at low temperatures [1]. This theory including further extensions is used in the current project for the determination of electron transport through molecular wires. Similar to studies of other groups [2] the coupling between the leads and the wire shall be treated perturbatively. From the population dynamics the current through the molecular wire is determined.

- [1] U. Kleinekathöfer, J. Chem. Phys. **121**, 2505 (2004).
 [2] J. Lehmann, S. Kohler, V. May and P. Hänggi, J. Chem. Phys. **121**, 2278 (2004).

TT 8.29 Fr 14:00 Poster TU C

Electronic and Optoelectronic Properties of Single-Molecule Junctions — •JOACHIM REICHERT¹, CAO QI¹, HARALD FUCHS¹, IVAN STICH², and DOMINIK MARX³ — ¹Physikalisches Institut, Westfälische Wilhelms-Universität Münster, D - 48149 Münster — ²Center for Computational Material Science, Slovak University of Technology, Ilkovicova 3, 812 19 Bratislava — ³Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D - 44780 Bochum

Recent developments and advances in atomic-scale imaging and manipulation techniques enables access to a new field of single molecule experiments. Electronic transport measurements through single organic molecules which are immobilized by self assembling techniques between two metallic electrodes (e.g. mechanically controlled breakjunction [1]) as well as tunnelling experiments through molecular films with STM have proven the ability of organic molecules to act as functional parts in nanoscale-devices. Especially scanning near-field optical microscopy (SNOM) with its ability to apply an optical field to a molecular system in a controlled manner enlarges the range of experimental available properties in metal-anchored molecular junctions. With a combination of these techniques we want to study the electronic/optoelectronic properties of single molecules covalently linked between a metallic substrate and a SNOM-tip to improve the understanding of electronic transport through single molecules.

[1] J. Reichert, R. Ochs, D. Beckmann, H.B. Weber, M. Mayor, H. v. Löhneysen, Phys.Rev.Lett. **88**, 176804 (2002). [2] H.-U. Danzebrink, U. C. Fischer, NATO ASI Series 242, 255, 303 (1993).

TT 8.30 Fr 14:00 Poster TU C

Discrete low-bias conductance fluctuations in molecular break-junctions — •JAN U. WÜRFEL, MARK ELBING, MARCEL MAYOR, and HEIKO B. WEBER — Institut für Nanotechnologie, FZ Karlsruhe

We investigate the electronic transport properties of gold-molecule-gold junctions using the mechanically-controllable break-junction (MCBJ) technique. We have shown in former studies that under certain conditions single-molecule contacts could be achieved [1]. Here, we study the longterm stability (up to days) of stable and reproducible contacts, which show discrete transitions in the conductance at low bias (~ 10 mV). Some of the conductance values could be identified as integer multiples of a fixed value. This may suggest an integer number of molecules contributing. The findings are discussed.

[1] Phys. Rev. Lett., **88**, 176804 (2002)

TT 8.31 Fr 14:00 Poster TU C

A perturbative expansion of shot noise in quantum dots and molecules — •MATTHIAS HETTLER¹, JASMIN AGHASSI^{1,2}, AXEL THIELMANN¹, JÜRGEN KÖNIG³, and GERD SCHÖN^{1,2} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — ²Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ³Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We study current and shot noise in perturbation theory in the coupling of a mesoscopic object (e.g. quantum dot or molecule) to metallic electrodes. We explicitly account for the electronic interactions and the resulting many-body states of the molecule/quantum dots, and allow for relaxation of the excited states. We present in some detail the diagrammatic technique that allows for the computation of the noise to second order in the molecule-electrode coupling. In particular, we discuss the influence of co-tunneling processes as well as the effect of intermolecular (interdot) couplings and relaxation on the shot noise. Furthermore, we find the Fano factor to be very sensitive to the tunnel-coupling strength, which may serve as a spectroscopic tool for the various coupling strengths.

TT 8.32 Fr 14:00 Poster TU C

Nanoscale electrodes on cleaved edge semiconductor surfaces for molecular electronics applications — •SEBASTIAN STROBEL¹, SEBASTIAN LUBER¹, DIETER SCHUH¹, WERNER WEGSCHEIDER², and MARC TORNOW¹ — ¹Walter Schottky Institut, TU München, 85748 Garching, Germany — ²Institut für Angewandte und Experimentelle Physik, U Regensburg, 93040 Regensburg, Germany

Current efforts in molecular electronics target at novel concepts for future nano-electronics thereby aiming at a fundamental understanding of charge transfer mechanism in (bio-) molecular "wires" such as DNA. Starting point is the preparation of suitable nanogap - electrodes that serve as electrical contacts to the molecules.

We present a novel strategy based on a semiconductor heterostructure grown by molecular beam epitaxy that consists of a AlGaAs layer into which a thin layer of GaAs (5 - 20 nm) is embedded. After cleaving the structure an atomically flat plane is obtained. Subsequent selective etching of the GaAs layer perpendicular to that plane and evaporation of a few nanometer thick metal film yields the nano-gap electrodes.

We successfully bridged nano-gap electrodes with single, 30 nm diameter colloidal Au nano-particles by AC electric trapping. The resulting drop in resistance of up to seven orders of magnitude verified the electrical functionality of our devices. First measurements on electrodes functionalized with organic self-assembled monolayers will be presented.

TT 8.33 Fr 14:00 Poster TU C

Multiphoton photofieldemission in electromigrated nanogaps — •S. DANTSCHER¹, D. WOLPERT¹, W. PFEIFFER¹, J. U. WÜRFEL², and H. B. WEBER² — ¹Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg — ²FZ Karlsruhe, Institut für Nanotechnologie, PO-Box 3640, 76021 Karlsruhe

The combination of nanocontacts and laser excitation offers the possibility of studying photoinduced nonequilibrium transport phenomena and therefore also electron dynamics on the nanometer scale. Using the method of electromigration, contacts with electrode distances in the range of several nanometers can be produced. For relatively large gaps no tunnel current is detectable, i.e. with a moderate applied DC bias, that avoids field emission, these junctions carry no significant current.

We have investigated photocurrents in such contacts under illumination with ultrashort femtosecond laserpulses. The use of a microscope objective as focusing element provides focal radii down to $2\mu\text{m}$ resulting in maximum intensities during the pulses of $10^{10}\text{W}/\text{cm}^2$. Under these conditions and with bias voltages in the range of $\pm 5\text{V}$ photo induced currents are detected. The intensity dependences exhibit power laws with exponents up to 3, indicating that multiphoton excitation is responsible for the detected current. Moreover the multiphoton order depends on the actual junction parameters, such as the applied bias. This suggests that the photocurrent flows in the nanogap. The observed bias dependence is attributed to photofieldemission, i.e. the multiphoton photocurrent is influenced by the static field distribution in the gap. In addition, also dynamic field effects might affect the signals.

TT 8.34 Fr 14:00 Poster TU C

Molecular conductance at finite voltage: bias driven evolution of Kohn-Sham-orbitals — •MAX KOENTOPP, FERDINAND EVERS, FLORIAN WEIGEND, MARK ELBING, ROLF OCHS, MARCEL MAYOR, and HEIKO WEBER — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Ground state density functional theory calculations yield the exact electron density if the exact exchange-correlation functional is employed.

The evolution of the equilibrium density with parametric changes in the Hamiltonian, e.g. realized by a change in the electrostatic potential, can provide crucial information about transport properties, like the Coulomb blockade.

To test our ideas, we perform model calculations using TURBOMOLE for a diode molecule, which exhibits a structure of a double quantum dot and has been investigated experimentally [1]. In particular, we investigate the origin of the characteristic peak structure in the differential conductance. Our results are consistent with the interpretation that the stepwise increase of the conductance occurs when the number of occupied levels of one of the dots, that have an energy above the lowest unoccupied level of the other dot, increases by one.

[1] M. Elbing, R. Ochs, M. Mayor, H. Weber, M. Koentopp, F. Evers, F. Weigend, Proc. Nat. Acad. Sci. USA, submitted.

TT 8.35 Fr 14:00 Poster TU C

Manipulating a molecule's conformation with gates: a molecular switch — •ANDREAS ARNOLD, MAX KOENTOPP, FERDINAND EVERS, and OLIVER RUBNER — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Molecules can undergo a conformational change when being charged. For molecules connected to external leads their excess charge becomes a parameter that can be tuned by means of a gate. Therefore, the mole-

cular conformation can be controlled at will, which may prove useful for potential applications, e. g. a molecular switch. We present a calculation based on density functional theory using TURBOMOLE for the model system bipyridine. Our calculation shows, that the equilibrium angle between the two benzene rings can indeed be controlled by the gate voltage. In particular, adding an excess charge of 2 electrons to the molecule takes the system from a strongly tilted, low conductance state over into an almost planar, high conductance configuration.

TT 8.36 Fr 14:00 Poster TU C

Perfekte Quanteninformationsbertragung in Spinketten — ●PETER KARBACH und JOACHIM STOLZE — Institut für Physik, Universität Dortmund, 44221 Dortmund

Gekoppelte Spins $1/2$ werden in der Quanteninformationsverarbeitung viel diskutiert, in letzter Zeit zunehmend auch als Mittel zum *Transport* von Quanteninformation. Hierbei spielen eindimensionale Systeme (Spinketten) naturgemäß eine besonders wichtige Rolle. Die kürzlich gefundene *perfekte* Abbildung eines Zustands zwischen dem ersten und letzten Spin einer speziellen inhomogenen XX-Kette (Christandl et al., PRL **92**, 187902 (2004)) kann verallgemeinert werden auf die „Spiegelung“ eines Zustands zwischen den beiden Hälften der Kette (Albanese et al. quant-ph/0405029). Wir zeigen, wie die beiden einzigen bisher bekannten Ketten mit perfekter Spiegelung eines Zustands nahezu beliebig verallgemeinert werden können. Hierzu muss nur das Einteilchen-Energiespektrum der Spinkette in der Darstellung wechselwirkungsfreier spinloser Fermionen gewisse Eigenschaften besitzen. Wir diskutieren Beispiele perfekt spiegelnder Spinketten und demonstrieren deren Eigenschaften; z.B. sind alle Autokorrelationen dieser Systeme für beliebige Temperaturen strikt periodisch.

TT 8.37 Fr 14:00 Poster TU C

Long Josephson junctions as vortex qubits — ●A. KEMP, A. N. PRICE und A. V. USTINOV — Physikalisches Institut III, Universität Erlangen-Nürnberg, Erwin-Rommel-Str 1., 91058 Erlangen, Germany

We have investigated the properties of Josephson vortices in annular Josephson junctions of circumference comparable to the Josephson penetration depth, at millikelvin temperatures. The fluctuation-induced activation of these vortices exhibits a systematic magnetic field and temperature dependence. We evaluate the height of the potential barrier between two spatially separated vortex states in long heart-shaped junctions. Reproducibility of the initial vortex state is guaranteed through the use of current injectors. Such injected fluxons are manipulated by means of homogeneous magnetic fields produced by microstrips carrying rectangular pulses. Low temperature microwave transmission characteristics show that such microstrips offer the possibility to control the barrier height of a vortex qubit on sub-nanosecond timescales.

TT 8.38 Fr 14:00 Poster TU C

Driven two-level system in a photonic crystal — ●GEESCHE BOEDECKER und CARSTEN HENKEL — Institut für Physik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam

We discuss a specific system-reservoir model with strong coupling and long-range temporal memory in the bath. The model can be physically realized with a coherently driven two-level system embedded in a photonic crystal. The problem differs from the usual spin-boson setting in several respects: the bath is essentially at zero temperature, its spectral density is zero in some finite frequency interval (photonic bandgap), and the two-level system is only coupled to near-resonant bath modes (rotating wave approximation). Its emission spectrum has been characterized only in the weak coupling limit in the quantum optics literature. We discuss here numerically exact simulation schemes for this non-Markovian problem and compare them to approximations based on the path integral formulation.

TT 8.39 Fr 14:00 Poster TU C

Bi- and tripartite entanglement in a flux-qubit triangle — ●JOHANNES FERBER und FRANK WILHELM — LMU München, Department für Physik, and CeNS

We are investigating a system of three superconducting flux qubits, inductively coupled by a surrounding loop or via shared lines.

We derive the possible coupling strength between the qubits and determine the energy level structure. We show, that for a proper and physical choice of parameters, the system shows strong three-qubit entanglement, quantified by the 3-tangle of the system [1].

Systems consisting of three qubits provide the possibility of examining

quantum nonlocality using GHZ-states in a potentially more convenient way than the two-qubit Bell inequality. Based on our results, we discuss the feasibility of such a GHZ-experiment using flux qubits. Moreover, we outline applications of three-bit interactions to the acceleration of quantum algorithms.

[1] V. Coffmann, J. Kundu, and W. K. Wothers, Phys. Rev. A **61**, 052306 (2000).

TT 8.40 Fr 14:00 Poster TU C

Continuous measurement of two spin qubits in quantum dots — ●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 investigate counting statistics of the currents with respect to signatures of entanglement of the spins.

TT 8.41 Fr 14:00 Poster TU C

Fabrication of superconducting qubit structures — ●GEORG WILD, TOBIAS HEIMBECK, HERIBERT KNOGLINGER, KARL MADEK, MATTEO MARIANTONI, CHRISTIAN PROBST, ACHIM MARX, and RUDOLF GROSS — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Solid state based quantum bits (qubits) promise to be producible using present day micro- and nanofabrication technologies thus allowing scalability up to systems comprising a large number of qubits. Superconducting qubits are advantageous because of the superconducting energy gap. Superconducting qubits based on Josephson junctions where the Josephson coupling energy is larger than the charging energy are usually called flux qubits. We are fabricating flux qubits with different designs based on Al/Al₂O₃ tunnel junctions. Measurements on various test structures (Josephson junctions, SQUIDs, qubits) help to analyze and further optimize the system parameters and to compare the different qubit variants. Flux qubits require an external magnetic field bias generating half a flux quantum in the ring defining the qubit to reach the degeneracy point. To shift this degeneracy point to zero field a π -shift element has to be inserted into the ring. We have started to develop a process to fabricate π -shifters based on superconductor/ferromagnet/superconductor Josephson junctions where a thin ferromagnetic NiPd layer is embedded between two Nb layers. This work was supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft.

TT 8.42 Fr 14:00 Poster TU C

Low temperature setup for characterization of superconducting qubits — ●KARL MADEK, TOBIAS HEIMBECK, HERIBERT KNOGLINGER, MATTEO MARIANTONI, CHRISTIAN PROBST, GEORG WILD, ACHIM MARX, and RUDOLF GROSS — Walther-Meissner-Institut, 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 quantum bits suggesting sufficiently large decoherence times. In order to experimentally investigate superconducting qubits well shielded low temperature measurement setups are required. We have established a dilution unit with several layers of mumetal and cryoperm shields and several stages of low pass filters at different temperatures in the biasing lines. A semirigid coaxial cable with thermally anchored attenuators is used for microwave spectroscopy on superconducting devices. Furthermore, the whole setup is placed in a shielded room. Measurements of the escape rate of Josephson junctions out of the zero voltage state using a current ramping technique serve to evaluate the quality of the shielding. The observation of a crossover from the quantum tunneling regime to the thermal regime shows the negligibility of noise. This work was supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft.

TT 8.43 Fr 14:00 Poster TU C

Quantum state transfer in arrays of flux qubits — ●ANDRIY LYAKHOV and CHRISTOPH BRUDER — Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, CH-4056, Basel, Switzerland

In this work, we describe a possible experimental realisation of Bose's idea to use spin chains for short distance quantum communication [1]. Josephson arrays have been proposed and analyzed as transmission channels for systems of superconducting charge qubits [2]. Here, we consider a chain of persistent current qubits [3], that is appropriate for state transfer with high fidelity in systems containing flux qubits. We calculate the fidelity of state transfer for this system. In general, the Hamiltonian of this system is not of XY-type, and we analyze the magnitude and the effect of the terms that break XY-symmetry.

[1] S. Bose, Phys. Rev. Lett. **91**, 207901 (2003).

[2] A. Romito, R. Fazio, and C. Bruder, quant-ph/0408057.

[3] L.S. Levitov *et al.*, cond-mat/0108266.

TT 8.44 Fr 14:00 Poster TU C

Probing superconducting phase qubits — ●JÜRGEN A. LISENFELD, CHRISTIAN COQUI, ALEXANDER LUKASHENKO, ALEXANDER KEMP, ABDUFARRUKH A. ABDUMALIKOV, and ALEXEY V. USTINOV — Physikalisches Institut III, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Solid-state quantum bits based on current-biased Josephson junctions have recently been shown as very promising. They require appropriate galvanic isolation of the junctions 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 tunnelling to the other well changes the magnetic flux in the qubit, which is measured by a dc-SQUID. In current experiments, we investigate the operation of such qubits. Another crucial point is the coupling of qubits, which we study in a system of two capacitively coupled current-biased junctions. One effect which appears here is phase-locking, resulting in the formation of voltage steps in the current-voltage characteristics. Another feature of the coupled system is the appearance of entangled macroscopic quantum states, which we try to observe by using microwave spectroscopy.

TT 8.45 Fr 14:00 Poster TU C

Decoherence during Two-Qubit Gates — ●MARKUS J. STORCZ, FRANK HELLMANN, CALIN HRELESCU, and FRANK K. WILHELM — Physics Department and CeNS, Ludwig-Maximilians-Universität München, Theresienstr. 37, D-80333 München

Superconducting solid-state quantum bits (qubits) are promising candidates for the realization of a *scalable* quantum computer. However, they are limited by decoherence due to the many extra degrees of freedom of a solid-state system.

We investigate a system of two qubits in a setup that is typical for *pseudospin* solid-state qubits such as charge or flux systems. We evaluate the decoherence properties and gate quality factors (GQF) in the presence of a common and two uncorrelated baths coupling to an arbitrary mixture of σ_z and σ_x and evaluate the decoherence rates and GQF for non-ideal, i.e. non identical qubits, realized in experimental setups. We emphasize the importance of symmetries to minimize decoherence during a quantum gate operation and explore memory effects of the environment between gate pulses.

Moreover, we investigate a setup of a chain of superconducting qubits with capacitive (flux qubits) or inductive (charge qubits) nearest neighbor coupling. Errors due to $1/f$ noise, which is picked up by the coupling elements, are anticipated to be the dominating source of errors in this setup. We propose to encode the qubits into a Decoherence Free Subspace (DFS) that provides full protection against coupling errors.

TT 8.46 Fr 14:00 Poster TU C

Quantum phase transitions in a 2-qubit system — ●HENRYK GUTMANN¹, FRANK WILHELM¹, and GERGELY ZARÁND² — ¹Department für Physik and CeNS, LMU, 80333 München — ²Department of Theoretical Physics, Budapest University of Technology and Economics, H-1521 Budapest, Hungary

For describing local as well as common decoherence effects we investigate a setup of two coupled spins influenced by two local bosonic baths as well as a common one. Here we are interested to go beyond the usual weak coupling regime, as we want to focus on the transition from quantum mechanical behaviour to classical localization of the

spins, as well as the emergence and disappearance of entanglement. We start with a quite generic two-spin generalization of the spin-boson model, *i.e.* where the environmental influences, the spin interactions and the spin Hamiltonian do not commute with each other. In order to eliminate the environmental Hamiltonian terms we unitarily transfer the spin-boson Hamiltonian onto the anisotropic Kondo model, using a technique given in Ref.[1]. Therefrom we derive scaling equations in first order perturbation theory. Considering the corresponding fixed point Hamiltonian we receive first qualitative insights in the different dissipative phase regimes. To get more reliable results we present higher order scaling equations by applying *operator product expansions* on the generated products of the renormalized spin couplings.

[1]: T.A. Costi and G. Zaránd, Phys. Rev. B **59**, 12398 (1999).

TT 8.47 Fr 14:00 Poster TU C

Electromagnetic Full-Wave Simulation of a Superconducting Microstrip Resonator — ●M. MARIANTONI¹, M.J. STORCZ², W.D. OLIVER³, F.K. WILHELM², A. MARX¹, and R. GROSS¹ — ¹Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, D-85748 Garching, Germany — ²Physics Department and CeNS, LMU München, D-80333 München, Germany — ³MIT Lincoln Laboratory, Lexington, MA 02420, USA

A fundamental phenomenon in nature is the interaction between light and matter. This process can be observed letting interact a single photon with a single atom. In the last decade several experiments with quantum optical systems have been realized giving rise to a broad research activity in the field called cavity-Quantum-ElectroDynamics (cQED). We propose an experimental realization making use of solid state devices, the role of atom being played by a superconducting flux qubit. The flux qubit interacts with a microwave-photons field inside a cavity. The cavity is fabricated on-chip using a superconducting microstrip resonator. The properties of the microstrip resonator have been simulated making use of a microwave software based on the transmission-line-matrix method. The software has been adapted for simulating correctly superconducting films in the microwave regime. Particular attention has been paid to the internal quality factor of the resonator taking into account residual surface resistances as well as dielectric and radiation losses. Our simulations show that an internal quality factor of about 10^6 should be achievable. This work is supported by the DFG through SFB 631.

TT 8.48 Fr 14:00 Poster TU C

Noise in a non-adiabatic electron pump — ●MICHAEL STRASS, SIGMUND KOHLER, and PETER HÄNGGI — Institut für Physik, Universität Augsburg

We investigate the electron transport in a two-terminal device consisting of two sites driven by an external AC field. The current and the associated noise are computed numerically within a Floquet approach which is also valid for non-adiabatic driving [1]. As a result, we find maxima of the pump current at the multi-photon resonances even if no voltage is applied. The transport in this setup can be optimized tuning the ratio of the intrasite coupling and the coupling of the sites to the leads. As a measure of the relative noise strength and therefore the transport properties, we study the Fano factor as a function of driving frequency and amplitude. At the multi-photon resonances, the Fano factor shows distinct minima.

The numerically exact solution is in addition compared to analytical results obtained within a high-frequency approximation [2]. This also provides a physical understanding of the current and noise suppressions observed for specific driving parameters. Possible experimental realizations of the system at hand are molecular wires in laser fields, quantum double-wells in heterostructures driven by electrical fields, and coupled quantum dots exposed to microwave radiation.

[1] S. Camalet, S. Kohler, and P. Hänggi, Phys. Rev. B **70**, 155326 (2004)

[2] S. Kohler, S. Camalet, M. Strass, J. Lehmann, G.-L. Ingold, and P. Hänggi, Chem. Phys. **296**, 243 (2004).

TT 8.49 Fr 14:00 Poster TU C

Fluctuations in meander-like superconducting nanostructures — •ANDREAS ENGEL¹, ANDREAS SCHILLING¹, ALEXEI SEMENOV², HEINZ-WILHELM HÜBERS², KONSTANTIN IL'IN³, and MICHAEL SIEGEL³ — ¹Physik Institut der Universität Zürich, Winterthurerstr. 190, 8057 Zürich, Schweiz — ²Deutsches Zentrum für Luft- und Raumfahrt, Rutherfordstr. 2, 12489 Berlin — ³Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe, Hertzstrasse 16, 76187 Karlsruhe

In superconducting films or wires thermal and quantum fluctuations play an increasingly important role, once one or more dimensions become of the order of the superconducting coherence length or less. Examples are thermal and quantum phase-slips in one-dimensional superconducting wires [1]. We experimentally studied fluctuations in NbN superconducting meanders 5 nm thick and 84 nm wide, biased with transport currents very close to the critical current $I_c(T)$. In this operating regime such structures have been shown to be very fast and sensitive optical and near-infrared single-photon detectors [2]. The sensitivity is however limited by dark count events caused by superconducting fluctuations. We will discuss various fluctuation models and compare the temperature and current dependence with experimental results.

[1] C.N. Lau et al., Phys. Rev. Lett., **87**, 217003 (2001), and refs. therein.

[2] A. Semenov et al., Eur. Phys. J. AP, **21**, 171 (2003).

TT 8.50 Fr 14:00 Poster TU C

Full Counting Statistics in a Mach-Zehnder Interferometer — •HEIDI FÖRSTER¹, SEBASTIAN PILGRAM², and MARKUS BÜTTIKER¹ — ¹Département de Physique Théorique, Université de Genève — ²Institute of Theoretical Physics, ETH Zürich

We investigate theoretically an electronic Mach-Zehnder interferometer under the influence of dephasing by coupling the interferometer arms to a fluctuating potential [1]. Here we deal with a one-channel quantum coherent transport problem, whereas counting statistics in many channel conductors is to leading order in the channel number independent of dephasing. Using the scattering matrix approach we write down a generating function, that is statistically averaged over the fluctuating potential. We discuss the effect of dephasing on the first three cumulants, and compare with the limiting cases of a fast and a slowly fluctuating potential. In the latter case we show the complete generating function under influence of dephasing.

[1] H. Förster, S. Pilgram, and M. Büttiker (in preparation)

TT 8.51 Fr 14:00 Poster TU C

Noise-assisted tunneling in a quantum dot: high-frequency shot noise measurement of a quantum point contact — FRANCK BALESTRO¹, EUGEN ONAC¹, LAURENS W. VAN BEVEREN¹, RONALD HANSON¹, •UDO HARTMANN², YULI V. NAZAROV¹, and LEO P. KOUWENHOVEN¹ — ¹Kavli Institute of Nanoscience Delft and ERATO Mesoscopic Correlation Project, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands — ²Physics Department and CeNS, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany

TT 9 Solids at Low Temperature - Quantum Liquids, Bose-Einstein Condensates, Ultracold Atoms, ...

Zeit: Freitag 17:00–18:45

Raum: TU H3027

Hauptvortrag

TT 9.1 Fr 17:00 TU H3027

Ultracold Atoms in Optical Lattices: Tunable Quantum Many-Body Systems — •WALTER HOPSTETTER — Theoretische Physik A, RWTH Aachen, Templergraben 55, 52056 Aachen

Cold atoms in optical lattices offer an exciting new laboratory where quantum many-body phenomena can be realized which are out of reach in solids. They can even serve as quantum simulators for notoriously difficult problems like high-temperature superconductivity. In this talk I will focus on recent developments and new results in multi-component systems: Fermionic atoms with SU(N) symmetry have exotic superfluid and flavor-ordered ground states. I will discuss symmetry breaking, collective modes and detection issues, e.g. in Bragg scattering. On the other hand, bosonic multi-flavor ensembles allow for engineering of quantum spin hamiltonians which are interesting from a quantum computation

We measured tunneling through a quantum dot (QD) induced by shot noise of a quantum point contact (QPC). The influence of the bias voltage through the QPC and the transmission of it have been explored.

We provide a theoretical model based on the description of photon-assisted tunneling (PAT). In contrast to PAT, we do not describe the environment of the QD as a continuous wave source (e.g. a microwave) of irradiation. Instead, we apply a temperature-dependent P(E) theory to calculate tunneling rates through the QD.

TT 8.52 Fr 14:00 Poster TU C

Phase relaxation by a fluctuating gauge field — •THOMAS LUDWIG¹ and ALEXANDER D. MIRLIN^{1,2} — ¹Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — ²Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

We investigate the effect of transverse gauge field fluctuations on the transport properties of a disordered electron system. In particular, we show that very slow fluctuations with frequencies smaller than the inverse dephasing time play an important role in suppressing the amplitude of mesoscopic conductance fluctuations. This is due to ensemble averaging by the measurement if the duration of the measurement is the longest time scale of the system. We also highlight the close connection between mesoscopic conductance fluctuations and weak localization.

TT 8.53 Fr 14:00 Poster TU C

Linear response approach to conductance of strongly correlated 1D systems: A DMRG study — •DAN BOHR^{1,2} and PETER SCHMITTECKERT² — ¹Department of Micro and Nanotechnology, Technical University of Denmark, DK-2800 Kgs. Lyngby — ²Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe

The calculation of transport properties has received much attention over the years. Recently improved experimental techniques has renewed the interest for studying transport properties of strongly correlated 1D quantum systems. We study the conductance through 1D interacting lattice systems using the Kubo formalism for conductance. In this work we calculate the conductance for the well-known non-interacting system, coupled to leads, as well as fully interacting systems coupled to leads. The first serves as a benchmark for the performance of DMRG (density matrix renormalization group) in this context as well as clarifying the finite size scaling needed to extract meaningful results. We show that indeed DMRG can be used successfully in such calculations, and consider the accuracy of this approach.

point of view. I will also discuss effects of reduced dimensionality, in particular polaronic Luttinger liquids in 1d Fermi-Bose systems.

TT 9.2 Fr 17:30 TU H3027

1/N-Expansion for Interacting Bose Gas — •FLAVIO NOGUEIRA¹ and AXEL PELSTER² — ¹Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany — ²Fachbereich Physik, Universität Duisburg-Essen, Essen, Germany

We study the interacting Bose gas by treating a field-theoretic model with N complex fields via a $1/N$ expansion. The resulting excitation spectrum follows from solving a self-consistent equation which contains a temperature-dependent effective interaction. Thermal fluctuations generate an anomalous scaling behavior in the excitation spectrum which leads to a second-order phase transition. Finally, we determine within our $1/N$ approach the temperature dependence of both the condensate

density and the superfluid density.

TT 9.3 Fr 17:45 TU H3027

Quantum Monte Carlo simulations of fermions with attractive interactions confined on optical lattices — ●F. KARIM POUR¹, F. DE LEÓN¹, M. RIGOL^{1,2}, and A. MURAMATSU¹ — ¹Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany — ²Physics Department, University of California, Davis, CA 95616, USA

We present numerical simulations for the negative U Hubbard model for fermions confined on one- (1D) and two-dimensional (2D) lattices. In the 1D case we calculate the exponents related to diagonal and off-diagonal quasi-long range order for different trapping potentials and compare them with the corresponding ones in periodic system. In 2D we characterize the crossover region between the BCS and BEC regimes. Finally, we discuss the possibility of coexistence of diagonal and off-diagonal long range order in the presence of a trapping potential.

TT 9.4 Fr 18:00 TU H3027

Non-equilibrium dynamics of hard-core bosons on 1D lattices: short vs large time results. — ●M. RIGOL^{1,2} and A. MURAMATSU² — ¹Physics Department, University of California, Davis, CA 95616, USA — ²Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany

Based on an exact treatment we study the non-equilibrium dynamics of hard-core bosons on one-dimensional lattices. Starting from a pure Fock state we find that quasi-long range correlations develop very fast in the system, and they lead to the emergence of quasi-condensates at finite momentum [1]. The exponent observed in the power-law decay of the one-particle density matrix, which develops dynamically, is the same that has been proven to be universal in the equilibrium case [2]. We also study the time evolution of clouds of hard-core bosons when they are released from a harmonic trap. In this case we show that the momentum distribution of the free expanding hard-core bosons approaches to the one of noninteracting fermions, in contrast to the known behavior in equilibrium systems [3].

[1] M. Rigol and A. Muramatsu, cond-mat/0403387, to appear in Phys. Rev. Lett. (2004)

[2] M. Rigol and A. Muramatsu, Phys. Rev. A **70**, 031603(R) (2004); ibid. cond-mat/0409132.

[3] M. Rigol and A. Muramatsu, cond-mat/0410683

TT 9.5 Fr 18:15 TU H3027

New superfluidity theory: a weakly interacting but non-dilute Bose gas — ●JEAN-BERNARD BRU¹ and STEFAN ADAMS² — ¹FB Mathematik und Informatik, Johannes Gutenberg-Universität, D-55099 Mainz — ²Max-Planck-Institut für Mathematik in den Naturwissenschaften Inselstraße 22, D-04103 Leipzig

The first microscopic theory of superfluidity was originally found in 1947 by Bogoliubov in three revolutionary papers on the theory of interacting Bose gas. His Weakly Imperfect Bose Gas (WIBG) coming from the truncation of a full interacting Bose gas was a starting point for this theory. However, only very few rigorous results concerning his WIBG and ansatz were previously done until 1998-2000 where a first rigorous analysis of this Bogoliubov model (WIBG) was found at all temperatures and densities. The aim of this talk is to do a more deep analysis of the Bogoliubov theory, including all recent studies (2001) and some new criticizes (2002-2004). Actually, this more detailed analysis gives rise to a new microscopic theory of superfluidity at all temperatures (2004) then introduced at the end of this talk.

In particular, the talk should be concluded by the corresponding phase diagram of this new theory: it exhibits the "Landau-type" excitation spectrum in the presence of a depleted Bose condensation for small temperatures with the formation of "Cooper-type pairs", even at zero-temperature (experimentally, an estimate of the fraction of condensate in liquid ⁴He at T=0 K is 9 %).

TT 9.6 Fr 18:30 TU H3027

Magnetoelastic Coupling in the Spin Dimer System TiCuCl₃ — ●N. JOHANNSEN¹, T. LORENZ¹, A. VASILEV², A. OOSAWA³, and H. TANAKA⁴ — ¹II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln — ²Department of Low-Temperature Physics, Moscow State University, Moscow 119899, Russia — ³Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan — ⁴Department of Physics Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan

We present high-resolution measurements of the thermal expansion and the magnetostriction on a single crystal of TiCuCl₃ which shows a field-induced magnetic order. In this material Cu²⁺ ions form S=1/2 spin dimers with an antiferromagnetic coupling. The spin gap between the singlet ground state and the first excited triplet state amounts only to about 0.65 meV. Therefore, a moderate magnetic field $H > 6$ T induces antiferromagnetic order with a staggered magnetization perpendicular to the applied field. The phase transition causes pronounced anomalies of opposite signs in the field and temperature dependencies of different lattice directions signaling a large magnetoelastic coupling. These anomalies allow for a precise determination of the phase boundaries, which turns out to be extremely sensitive to pressure, e.g. the transition field may change up to $\pm 200\%/GPa$ depending on the direction of uniaxial pressure. This drastic effect can be unambiguously traced back to changes of the intradimer coupling under pressure, whereas the interdimer couplings remain essentially unchanged. On the other hand, a replacement of the Ti by smaller K ions causes a strong change in the interdimer couplings.

TT 10 Superconductivity - Tunneling, Josephson Junctions, SQUIDS

Zeit: Samstag 08:30–12:45

Raum: TU H104

TT 10.1 Sa 08:30 TU H104

High- T_c SQUIDS With an Unusual Current-Phase Relation — ●CHRISTOF SCHNEIDER¹, GERMAN HAMMERL², GENNADIJ LOGVENOV¹, THILO KOPP¹, JOHN KIRTLEY³, PETER HIRSCHFELD⁴, HELENE RAFFY⁵ und JOCHEN MANNHART¹ — ¹Lehrstuhl für Experimentalphysik VI, Institut für Physik, Universität Augsburg, D-86135 Augsburg — ²IBM Zurich Research Laboratory, CH 8803 Rueschlikon, Switzerland — ³IBM Thomas J. Watson Research Center, P.O.Box 218, Yorktown Heights, New York 10598, USA — ⁴Department of Physics, University of Florida, Gainesville, Florida 32611, USA — ⁵Laboratoire de Physique des Solides, Université de Paris-Sud, 91405 Orsay, France

Current-voltage characteristics of SQUIDS show as a function of the applied magnetic field a periodic variation of the critical current. Usually, the periodicity corresponds to one flux quantum $\Phi_0 = h/2e$. In this contribution we present measurements of high- T_c SQUIDS showing a characteristic periodicity of the critical current of $1/2 \times \Phi_0$ in small magnetic fields. The interpretation of the phase-sensitive experiments is consistent with higher harmonics of the current-phase relation for the Josephson current. They are also consistent with a finite interaction between Cooper pairs, leading to a quartet formation of electrons as a possible admixture to the superconducting condensate.

TT 10.2 Sa 08:45 TU H104

Experimental observation of moving 4π -kinks in Josephson-junction arrays — ●JUDITH PFEIFFER, MARCUS SCHUSTER, ABDUFARRUKH A. ABDUMALIKOV, and ALEXEY V. USTINOV — Physikalisches Institut III, Universität Erlangen-Nürnberg, 91058 Erlangen

We experimentally study the dynamics of kinks (magnetic vortices) in annular parallel arrays of underdamped Josephson junctions with different discreteness. Parallel arrays of Josephson junctions are described by the discrete sine-Gordon-model. For small discreteness parameters, we measured very precise phase locking resonances. For systems with higher discreteness, we observe bunched states of two moving kinks, which form either a 4π -kink or various bound states of two phase locked 2π -kinks with finite distance between them. To our knowledge, this is the first experimental observation of dynamically stable 4π -kinks, which have been predicted for discrete sine-Gordon systems by Peyrard and Kruskal [1]. Our numerical results agree quantitatively with the experimental data.

[1] M. Peyrard, M. D. Kruskal *Phys. Ref. D* **14** (1984), 88

TT 10.3 Sa 09:00 TU H104

Thermally induced injection of vortices in narrow long Josephson junctions — ●ABDUFARRUKH A. ABDUMALIKOV¹, MIKHAIL V. FISTUL², and ALEXEY. V. USTINOV¹ — ¹Physikalisches Institut III, Universität Erlangen-Nürnberg, D-91058 Erlangen — ²Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum

We report an experimental and theoretical study of a novel resistive state in ultra-narrow long Josephson junctions induced by thermal fluctuations. In the presence of an externally applied magnetic field, the hysteretic current-voltage characteristics show a low-voltage branch emerging directly from the superconducting state. We explain this feature by random injection of vortices into the junction in the presence of a large high-frequency damping. We obtain the current-voltage characteristics by calculating the dc bias dependent activation rate of the vortex injection. This activation rate is determined by a surface barrier that is controlled by an external magnetic field. Our theoretical analysis, taking into account thermally induced injection of vortices, quantitatively agrees with experimental results.

TT 10.4 Sa 09:15 TU H104

Arbitrary fractional Josephson vortices — ●EDWARD GOLDOBIN, DIETER KOELLE und REINHOLD KLEINER — Physikalisches Institut – Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen

Recently we have suggested and demonstrated experimentally that one can create an arbitrary κ -discontinuity in a long Josephson junction (LJJ) made of conventional superconductors, such as Nb, using a pair of tiny current injectors[1]. In this way one can create and study arbitrary fractional vortices which carry the flux $0 \dots \Phi_0$ proportional to κ or to $2\pi - \kappa$. While for semifluxons ($\kappa = \pi$) a vortex and an antivortex are mirror symmetric, for arbitrary κ -vortices the symmetry is broken. We study several

simplest ground states and investigate the boundaries of their stability.

Since κ -vortices are pinned (for $\kappa \neq 2\pi n$) they cannot be moved by a Lorentz force which is induced by an applied bias current — the bias current only changes the shape of κ -vortex. If the bias current is removed, the vortex returns to its original shape performing decaying oscillations around its equilibrium shape. The frequency of these oscillations can be calculated and depends on κ . Using several coupled κ -vortices at some distance from each other one can design artificial “molecules” and 1D “crystals” with programmable eigen-frequencies (energy-bands) with typical frequencies somewhat below the Josephson plasma frequency.

[1] E. Goldobin et al., *Phys. Rev. Lett.* **92** 057005 (2004).

TT 10.5 Sa 09:30 TU H104

Discrete Breathers in Josephson Ladders — ●MARCUS SCHUSTER and ALEXEY V. USTINOV — Physikalisches Institut III, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen

We present an extensive study of intrinsic localized modes in ladder arrays of small underdamped Josephson junctions. These modes are time periodic localized dynamic states (named discrete breathers) which have recently been found in a large class of nonlinear lattices (see Ref. [1] for a review).

In experiments and numerical simulations, we investigate the spontaneous formation of intrinsic localized modes and their resonant interaction with linear oscillatory waves of the arrays. We furthermore study the propagation of the extended linear waves (Josephson plasmons) through the localized modes. Numerical simulations indicate the occurrence of a Fano resonance which arises from the time periodic scattering potential formed by the discrete breather. As a consequence, the resonant reflection of linear waves from the intrinsic localized mode is found.

[1] D. Campbell, S. Flach, and Y. S. Kivshar, *Physics Today*, January (2004), 43.

TT 10.6 Sa 09:45 TU H104

SIFS junctions for Semifluxon Qubits — ●M. WEIDES¹, H. KOHLSTEDT¹, R. WASER¹, E. GOLDOBIN², D. KOELLE², R. KLEINER², and V. RYAZANOV³ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich — ²Physikalisches Institut – Experimentalphysik II, Universität Tübingen — ³Institute for Solid State Physics, Chernogolovka, Russia

There are several approaches to realize qubits using π or $0-\pi$ Josephson junctions (JJs). Such JJs can be fabricated using a ferromagnetic barrier of thickness d_F between two superconductors, i.e. SFS or SIFS structures. Due to damped spatial oscillations of the order parameter in the F-layer, d_F determines the phase coupling (0 or π) and the critical current density j_c of such JJs. We fabricated SIFS multilayers Nb/Al₂O₃/Cu₄₀Ni₆₀/Nb by magnetron sputtering. Similar JJs without an F-layer (SIS JJs) show $j_c \sim 2.5$ kA/cm², low sub gap current and a large superconducting gap. In SIFS JJs the first side maximum of $j_c(d_F)$ corresponds to the π ground state and is clearly seen in our samples. For applications such as digital logic and qubits, a figure of merit is $V_c = I_c R_n$ in the π state, which for our SIFSs is about $10 \mu V$ — the highest value obtained so far for SIFS JJs. The appearance of a degenerated semifluxon state at the boundary between $0-\pi$ parts¹ is interesting both for fundamental studies and applications. In the quantum limit, semifluxons could be used as quiet qubits or as a playground for testing quantum mechanics. We propose a way of designing $0-\pi$ SIFS junctions for the investigation of semifluxons.

¹ E. Goldobin et al., *Phys. Rev. B* **66**, 100508 (2002).

TT 10.7 Sa 10:00 TU H104

Josephson junctions with nonlinear damping for qubit-RSFQ circuit applications — ●A. B. ZORIN, M. I. KHABIPOV, D. V. BALASHOV, R. DOLATA, F.-I. BUCHHOLZ, and J. NIEMEYER — Physikalisches-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The overdamped Josephson tunnel junctions with resistive shunts are the key elements of the Rapid Single-Flux-Quantum (RSFQ) circuits enabling processing of information presented in quantized leaps of the Josephson phase. The normal metal shunts generate significant current noise even in the quiescent (zero-voltage) state of the Josephson junctions, so an application of such circuits for readout of a Josephson qubit is

problematic because of dramatic dephasing. We demonstrate that shunting of tunnel junctions by Superconductor-Insulator-Normal metal (S-I-N) structures having pronounced nonlinear I - V characteristics can ensure both sufficient damping for proper functioning of the circuit and negligibly small noise in the quiescent state. Superconducting Nb/AlO_x/Nb junctions shunted by Nb/AlO_x/AuPd junctions of S-I-N type were fabricated and, in agreement with our model, exhibited non-hysteretic I - V characteristics at temperatures down to at least 1.4 K.

TT 10.8 Sa 10:15 TU H104

Epitaxial growth of Al/AlO_x/Al trilayers for Josephson junction fabrication — ●J. EROMS, A.H. VERBRUGGEN, C.J.P.M. HARMANS, A.V.D. ENDEN, P.F.A. ALKEMADE, A.R.H.F. ETTEMA, H.W. ZANDBERGEN, and J.E. MOOIJ — Kavli Institute of Nanoscience Delft, Delft University of Technology, Delft, The Netherlands

Superconducting qubit circuits are mainly built from aluminum based Josephson junctions fabricated by shadow evaporation or in a trilayer process. The aluminum films are polycrystalline in both cases. Charge noise and critical current fluctuations limit the performance of present qubits made from those devices. To achieve a defect free barrier, we explore epitaxial aluminum films as a base material for Josephson junctions. We grow Al/AlO_x/Al trilayers on Si (111) wafers in a molecular beam epitaxy system. The films are characterized *in situ* with RHEED and after growth with high-resolution TEM, Kikuchi backscattering and X-ray reflectivity measurements. The bottom Al layer grows epitaxially on the Si substrate, the oxide barrier appears amorphous, but very smooth, and the top Al layer is polycrystalline, but with Al (111) planes still parallel to the Si (111) planes.

TT 10.9 Sa 10:30 TU H104

1/f noise measurements on sub-micron Josephson junctions — ●J. EROMS, J.H. PLANTENBERG, R.N. SCHOUTEN, A.H. VERBRUGGEN, C.J.P.M. HARMANS, and J.E. MOOIJ — Kavli Institute of Nanoscience Delft, Delft University of Technology, Delft, The Netherlands

Superconducting qubits belong to the most promising systems in solid state quantum information processing. They are explored by a number of groups in different configurations, and control of single and two-qubit systems is progressing rapidly. However, decoherence is still a serious issue. Low-frequency fluctuations in the critical current are believed to be an important source of decoherence, as was pointed out e.g. in Ref. 1. This article also gives a universal noise figure based on noise measurements published over the last two decades. To characterize and improve our junction fabrication we have therefore measured 1/f noise in the tunnel resistance of sub-micron Josephson junctions at temperatures down to 300 mK. We used a bridge configuration of two identical junctions and measured the voltage noise with a cross-correlation technique. The noise in our devices was significantly lower than the value expected from the data in Ref. 1.

[1] D.J. Van Harlingen *et al.*, Phys. Rev. **B 70**, 064517 (2004).

TT 10.10 Sa 10:45 TU H104

Experiments with Josephson vortex ratchets — ●EDWARD GOLDOBIN¹, MARKUS BECK¹, DIETER KOELLE¹, REINHOLD KLEINER¹ und MICHAEL SIEGEL² — ¹Physikalisches Institut – Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen — ²Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe, Hertzstr. 16, 76187 Karlsruhe

We investigate experimentally a Josephson vortex ratchet — a fluxon in an asymmetric periodic potential driven by a force with zero time average. The highly asymmetric periodic potential is created in underdamped annular long Josephson junction by means of a current injector[1]. Experimental characterization shows good asymmetry of the constructed potential. We have measured the ratchet effect for driving forces with different spectral content. At low frequencies (~ 100 Hz) we obtained smooth rectification curves $V_{dc}(I_{ac})$ for different amplitudes of the potential and driving shapes. For monochromatic high frequency drive the rectified voltage becomes quantized. At very high frequencies we also observe half-period dynamics, current reversal and chaotic behavior. Such effects can be reproduced in simulation and associated with the inertial mass of a fluxon.

[1] E. Goldobin *et al.*, Phys. Rev. E **63**, 031111 (2001).

TT 10.11 Sa 11:15 TU H104

Elektrische Untersuchung serieller intrinsischer Josephsonkontaktarrays an dünnen $Tl_2Ba_2CaCu_2O_{8+x}$ Schichten auf r-cut Saphir und 20° vicinalem $LaAlO_3$ — ●MICHAEL MANS¹, ALEXANDER GRIB², MATTHIAS BÜENFELD¹, RALF BECHSTEIN¹, FRANK SCHMIDL¹, HENRIK SCHNEIDEWIND³ und PAUL SEIDEL¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743-Jena, Deutschland — ²Physics Department, Kharkov National University, 61077 Kharkov, Ukraine — ³IPHT Jena, Albert - Einstein - Str. 9, 07745-Jena, Deutschland

Zur Messung intrinsischer Josephson-Effekte wurden TBCCO Schichten zum einen auf Saphir hergestellt und zu Mesas strukturiert, zum anderen auf 20° vicinalem $LaAlO_3$ hergestellt und zu brückenartigen Strukturen strukturiert. Für eine Anwendung dieser Kontaktarrays ist es wichtig eine Synchronisation der Kontakte zu erreichen. Aus diesem Grund haben wir die Arrays in Resonatoren platziert. Die Mesas zeigen sehr große Widerstände an der TBCCO-Gold Grenzflächen der Topelektrode, die jedoch durch Anlegen einer geeigneten Spannung gezielt verändert werden können. So sind die zuvor nicht messbaren Äste der U-I-Kennlinie sichtbar zu machen. Für die brückenartigen Kontaktarrays wird gezeigt, wie sich ein zusätzlicher normalleitender Shunt auf die Möglichkeit der Synchronisation auswirkt. Sie wurden hierzu mit Goldschichten versehen und in einem Resonator platziert. Numerische Simulationen an einem geschunteten Array aus 5 Kontakten zeigen deren erfolgreiche Synchronisation. Diese Arbeit wurde gefördert durch die DFG (Nr. Se 664/10-3)

TT 10.12 Sa 11:30 TU H104

Novel Josephson Effect in Triplet Superconductor - Ferromagnet - Triplet Superconductor Junctions — ●BORIS KASTENING¹, DIRK K. MORR^{1,2}, DIRK MANSKE³, and KARL BENNEMANN¹ — ¹Institut fuer Theoretische Physik, Freie Universitaet Berlin, 14195 Berlin, Germany — ²Department of Physics, University of Illinois at Chicago, Chicago, IL, U.S.A. — ³Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

We predict a new type of Josephson effect to occur in Triplet Superconductor - Ferromagnet - Triplet Superconductor Josephson junctions. In addition to the dependence of I_J on the phase difference between the superconductors, we show that a novel dependence on the relative orientation between the ferromagnetic moment and the \mathbf{d} -vectors describing the superconducting pairing symmetry exists. This dependence can be used to build Josephson switches, in which the Josephson current can either be turned on or off or can be made to exhibit a square-wave oscillation.

TT 10.13 Sa 11:45 TU H104

Intrinsic tunneling in perovskite derivatives: From superconductivity to ferroelectricity — ●Y. KOVAL¹, F. CHOWDHURY¹, P. MÜLLER¹, F. LICHTENBERG², and J. MANHART² — ¹Physikalisches Institut III der Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany — ²Experimentalphysik VI der Universität Augsburg, D-86135 Augsburg, Germany

There is a variety of extensions of the basic perovskite crystalline structure. Intercalating the perovskite octahedra with additional layers can result in superconductivity in the high- T_c materials, or in ferromagnetism in some Ruddlesden-Popper phases. In many cases the crystalline sheets of the layered structure alternate between conducting and insulating regions. As a consequence, electrical transport perpendicular to the layers is provided by tunneling. This can range from intrinsic Josephson effects in the high- T_c superconductors to interesting permanent memory effects in titanate based layered perovskites. We present a summary of our recent results.

TT 10.14 Sa 12:00 TU H104

Magneto-resistance of a mesoscopic DC SQUID — ●PAUL GOLDBART, DAVID PEKKER, DAVID HOPKINS, and ALEXEY BEZRADIN — Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, U.S.A.

We analyze an all-superconducting mesoscopic DC SQUID, comprising a pair of thin-film strips connected by a pair of parallel ultra-narrow wires. We focus on the magneto-resistance of the device in the size range in which the strips are narrower than the penetration depth (i.e. the mesoscopic regime), and especially on the low-magnetic-field regime, in which no vortices are present in the strips. The resistance originates in dissipative order-parameter fluctuations in the wires, and its magnetic-

field dependence comes from the phase-gradient of the order parameter in the strips, associated with screening currents. We present a theory of the magnetoresistance of this mesoscopic DC SQUID, based on the Langer-Ambegaokar-McCumber-Halperin theory of intrinsic resistance. We compare this theory with recent experimental data, and discuss why the device can be regarded as a superconducting phase gradiometer.

TT 10.15 Sa 12:15 TU H104

Supraleitende dünne Scheiben und SQUIDs mit und ohne Vortizes. — •ERNST HELMUT BRANDT — Max-Planck-Institut für Metallforschung, Stuttgart

Für supraleitende dünne Filme in Form runder oder rechteckiger Scheiben mit und ohne zentralem Loch und radialem Schlitz wird die Verteilung von Supraström und lokalem Magnetfeld berechnet aus der Maxwell-London-Theorie mit beliebiger magnetischer Eindringtiefe $\Lambda = \lambda^2/d$. Die Ströme können hervorgerufen werden a) durch ein senkrecht angelegtes Magnetfeld, b) durch im Loch eingefangenen Magnetfluss, c) durch Vortizes. Die Anwendung auf SQUIDs (Superconducting Quantum Interference Devices) wird diskutiert. Außerdem wird eine sehr effektive numerische Methode vorgestellt zur Berechnung des idealen periodischen Vortextgitters in Filmen beliebiger Dicke aus der Ginzburg-Landau-Theorie.

TT 10.16 Sa 12:30 TU H104

Sheet current density distribution in a SQUID washer probed by vortices — •DIETMAR DOENITZ¹, MATTHIAS RUOFF¹, RAINER STRAUB¹, ERNST HELMUT BRANDT², JOHN R. CLEM³, REINHOLD KLEINER¹ und DIETER KOELLE¹ — ¹Universität Tübingen, Physikalisches Institut - Experimentalphysik II, Auf der Morgenstelle 14, D-72076 Tübingen — ²Max-Planck-Institut für Metallforschung, D-70506 Stuttgart — ³Ames Laboratory - DOE and Department of Physics and Astronomy, Iowa State University, Ames Iowa 50011, USA

We use Low Temperature Scanning Electron Microscopy (LTSEM) to image vortices in YBCO washer SQUIDs. The imaging is based on the electron-beam-induced local displacement of vortices, which is detected as a flux change $\Delta\Phi$ in the SQUID. The function $\Phi(\vec{r})$ describing the amount of flux a single vortex couples into the SQUID hole is directly measured by the SQUID. The scalar stream function $G(\vec{r}) = \frac{1}{\Phi_0} \cdot \Phi(\vec{r})$ determines contrast C ($\propto |\vec{\nabla}G|$) and direction \hat{d} ($\parallel \vec{\nabla}G$) of the vortex signals. When there is a ring current I flowing around the SQUID loop, the vortex-free sheet current density distribution is $\vec{J} = I \cdot (\hat{z} \times \vec{\nabla}G)$, leading to $|\vec{J}(\vec{r})| \propto C$ and $\vec{J} \perp \hat{d}$. This allows to extract full information on the sheet current density distribution at every position a vortex has been imaged, thus using the vortices as local detectors for \vec{J} . Our experimental results from vortex imaging are in very good agreement with numerical calculations of $\vec{J}(\vec{r})$.

TT 11 Correlated Electrons - Spin Systems and Itinerant Magnets: Theory

Zeit: Samstag 08:45–10:30

Raum: TU H2053

TT 11.1 Sa 08:45 TU H2053

Derivation of the quantum-nonlinear- σ -model for antiferromagnets in a uniform magnetic field — •NILS HASSELMANN and PETER KOPIETZ — Institut für Theoretische Physik, Universität Frankfurt, Robert-Mayer-Strasse 8, 60054 Frankfurt/Main

We reconsider the derivation of the quantum-nonlinear- σ -model for antiferromagnets in a magnetic field. The standard assumption is that the term $(\partial_\tau \mathbf{n})^2$ in the action is replaced in presence of a magnetic field \mathbf{H} by $(\partial_\tau \mathbf{n} - i\mathbf{H} \times \mathbf{n})^2$. Here, \mathbf{n} (with $\mathbf{n}^2 = 1$) represents the staggered moments while τ is the imaginary time. We show that this result is incorrect in that it does not take account of the fact that a uniform magnetic field generates a finite uniform magnetization. We present the correct form of the non-linear- σ -model describing the gapless spin excitations near the antiferromagnetic ordering wavevector.

TT 11.2 Sa 09:00 TU H2053

String Picture of a Frustrated Quantum Magnet and Dimer Model — •YING JIANG and THORSTEN EMIG — Institut für Theoretische Physik, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln

We study the effect of quantum dynamics on geometrically frustrated magnets for a transverse field Ising model at finite temperatures. We develop a microscopic derivation of the Landau-Ginzburg-Wilson (LGW) action for this model and show that it can be interpreted as the free energy of a 3D elastic lattice of non-crossing strings. As a first application, we quantitatively predict the phase diagram and correlations, confirming excellently a key prediction of recent simulations about the existence of unusual phase transitions and an ordered phase. We discuss implications of our string picture for the understanding of the effect of quenched disorder in such quantum frustrated systems.

TT 11.3 Sa 09:15 TU H2053

Renormalization of spin-wave velocity and frustration in Heisenberg Quantum antiferromagnets — •FRANK KRÜGER and STEFAN SCHEIDL — Institut für Theoretische Physik, Uni Köln

Frustrated quantum antiferromagnets exhibit nontrivial quantum phase transitions which are the subject of extensive current research. We characterize the Néel phase for a two-dimensional Heisenberg model as a

function of spin S and the frustration between nearest and next-nearest exchange couplings on a square lattice. We extend the renormalization group approach by Chakravarty, Halperin and Nelson [Phys. Rev. B **39**, 2344 (1989)] to account for the discrete lattice structure. As a consequence, we obtain a renormalization of the spin-wave velocity and the frustration strength, which become significant well before the Néel order becomes instable.

TT 11.4 Sa 09:30 TU H2053

Quantum Fluctuations and Excitations in Magnetic Quasicrystals — •STEFAN WESSEL¹ and IGOR MILAT² — ¹Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart — ²Institut für Theoretische Physik, ETH Zürich, 8093 Zürich, Schweiz

We study the effects of quantum fluctuations and the excitation spectrum for the antiferromagnetic Heisenberg model on the octagonal tiling, a two-dimensional quasicrystal structure. Using a combination of quantum Monte Carlo and numerically solved spin-wave theory, a non-trivial inhomogeneous magnetic ground state is found. A hierarchical structure in the values of the staggered moments is observed which arises from the self-similarity of the quasiperiodic lattice. The magnetic excitation spectrum consists of magnon-like low-energy modes, as well as dispersionless high-energy states of multifractal nature. The dynamical spin structure factor exhibits linear-soft modes at low energies, self-similar structures with bifurcations emerging at intermediate energies, and flat bands in high-energy regions. This generic model is a first step towards understanding magnetic quasicrystals such as the recently discovered Zn-Mg-Ho icosahedral structure.

TT 11.5 Sa 09:45 TU H2053

Kollektive Spinanregungen in der Gutzwillernäherung des Hubbardmodells — •FALK GÜNTHER und GÖTZ SEIBOLD — BTU Cottbus

Auf der Grundlage der spinrotationsinvarianten Slave-Boson-Formulierung des Hubbardmodells untersuchten wir die kollektiven Anregungen eines itineranten Ferromagneten. Die Entwicklung des Ennegefunktionalen um den Sattelpunkt bis zur 2. Ordnung erlaubt die Berechnung dynamischer Korrelationsfunktionen in einer RPA-ähnlichen Näherung. Das ferromagnetische Anregungsspektrum wurde untersucht

und die Dispersionsrelation der Spindichtewellen ermittelt. Im Vergleich zur HF-Theorie stellen wir stark eingeschränkte Phasenbereiche für das Auftreten von Ferromagnetismus fest.

TT 11.6 Sa 10:00 TU H2053

Tunneling Transport Through Single Molecular Magnets — ●CHRISTIAN ROMEIKE, MAARTEN R. WEGEWIJS, and HERBERT SCHOELLER — Institut für Theoretische Physik A, RWTH Aachen

We investigate tunneling transport through a single molecular magnet Mn_{12} . It is known that the low temperature properties ($T \approx 1K$) can be described by a spin Hamiltonian incorporating an easy axis anisotropy and the effect of quantum tunneling of magnetization (QTM). We study using master equations how the high spin ($S = 10$) and the QTM influence the electron transport. We find negative differential conductance effects and complete current suppression for finite bias voltage in many possible situations. Our results apply to molecular magnets that are described by the same type of Hamiltonian.

TT 11.7 Sa 10:15 TU H2053

Control of Local Relaxation Behavior in Closed Bipartite Quantum Systems — ●HARRY SCHMIDT and GÜNTER MAHLER — Institut für Theoretische Physik 1, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart

TT 12 Correlated Electrons - Spin Systems and Itinerant Magnets: Experiment

Zeit: Samstag 10:45–12:45

Raum: TU H2053

TT 12.1 Sa 10:45 TU H2053

Small Angle Neutron Scattering Study of the Magnetic Phase Diagram of MnSi at High Pressure — ●C. PFLEIDERER^{1,2}, D. REZNIK^{2,3}, L. PINTSCHOVUS², and H. v. LÖHNESEN^{1,2} — ¹Physikalisches Institut, Wolfgang-Gaede Str. 1, D-76128 Karlsruhe, Germany — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — ³Laboratoire Leon Brillouin, CEA Saclay, F-91191 Gif-sur-Yvette Cedex, France

The electrical resistivity of the itinerant-electron magnet MnSi suggests as function of pressure an abrupt change from a Fermi liquid to an extended non-Fermi liquid phase above $p_c = 14.6$ kbar. Recently we reported the existence of partial magnetic order in a small pocket of the regime of the non-Fermi liquid phase, where the partial order is characterised by scattering intensity everywhere on the surface of a small sphere in reciprocal space. Here we report a small angle neutron scattering study of the magnetic state of MnSi at pressures up to 22 kbar and magnetic field up to 1 T. Above the critical pressure long-range helical order may be stabilised in magnetic field, where the pressure dependence of the pinning potential of the helical order and key features of hysteresis loops provide microscopic hints consistent with the formation of a stable new phase.

TT 12.2 Sa 11:00 TU H2053

Observation of a Griffiths phase in paramagnetic $La_{1-x}Sr_xMnO_3$ — ●JOACHIM DEISENHOFER¹, D. BRAAK², H.A. KRUG VON NIDDA¹, J. HEMBERGER¹, R.M. EREMINA³, V.A. IVANSHIN⁴, A.M. BALBASHOV⁵, A. LOIDL¹, T. KIMURA⁶, and Y. TOKURA⁶ — ¹EP V, Center for Electronic Correlation and Magnetism, University of Augsburg, 86135 Augsburg, Germany — ²TP II, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — ³E.K. Zavoisky Physical-Technical Institute, 420029 Kazan, Russia — ⁴Kazan State University, 420008 Kazan, Russia — ⁵Moscow Power Engineering Institute, 105835 Moscow, Russia — ⁶Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

We report on the discovery of a new phase boundary above magnetic ordering in low doped $La_{1-x}Sr_xMnO_3$ by means of ESR and susceptibility measurements. The observed triangular phase regime in the paramagnetic state is identified as a realization of a Griffiths phase, where disorder in the ferromagnetic bonds leads to the existence of a temperature scale above T_C . The influence of quenched disorder to allow for the occurrence of a Griffiths phase becomes evident by its appearance within the Jahn-Teller distorted orthorhombic structure.

We investigate the decoherence of a spin 1/2 weakly coupled to an environment of many spins 1/2 with and without coupling. The total system is closed, its state is pure and evolves under Schrödinger dynamics. Nevertheless, the considered spin reaches a quasi-stationary equilibrium state.

We find that this state depends strongly on the coupling to the environment on the one hand and on the coupling within the environmental spins on the other. In particular we focus on spin star geometries with interaction $\hat{H}^{int} = \sum_{i,j} \sum_{\nu} \gamma_{ij}^{(\nu)} \hat{\sigma}_i \otimes \hat{\sigma}_j^{(\nu)}$ with random γ_{ij} to investigate the effect of intra-environmental coupling on the central spin. By changing the dynamics of the environment its effect as a bath on the central spin is changed and may even be adjustable to some degree. The relaxation behavior is related to the distribution of the energy eigenvectors of the total system.

TT 12.3 Sa 11:15 TU H2053

Magnetic Excitations in Layered Manganites — ●D. SENFF¹, M. BENOMAR¹, F. KRÜGER², S. SCHEIDL², Y. SIDIS³, P. REUTLER^{4,5}, A. REVCOLEVSKI⁵ und M. BRADEN¹ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Institut für Theoretische Physik, Universität zu Köln, Germany — ³Laboratoire Léon Brillouin, France — ⁴IfW Dresden, Germany — ⁵Laboratoire de Physico-Chimie de l'Etat Solide, Université

The most prominent member of the series $La_{1-x}Sr_{1+x}MnO_4$ is the half-doped compound with $x=0.5$. This system exhibits a very stable charge/orbital ordering, which at lower temperatures is accompanied by an antiferromagnetic ordering of ferromagnetic zig-zag chains, usually called CE-type order. We present the results of our experimental and theoretical work on the spin-wave spectrum in this phase.

Using inelastic neutron scattering we mapped out a large part of the magnetic excitation spectrum, which consists of one acoustic and two optic bands. All parts of the observed spectrum can be well described within linear spin-wave, taking account only two nearest-neighbor exchange constants, one ferromagnetic coupling J_{\parallel} and an antiferromagnetic interaction J_{\perp} . Our experimental data proof, that the intrachain coupling J_{\parallel} is the dominant magnetic interaction in this system and we thus conclude that the CE-type ordering is driven by the underlying orbital ordering.

In addition, we want to discuss the spin-wave spectrum of the parent system $LaSrMnO_4$ ($x=0$), which exhibits conventional G-type AFM-ordering, and compare the different coupling constants in these two compounds.

TT 12.4 Sa 11:30 TU H2053

Weak Itinerant Ferromagnetism and Half-Metallic State among Filled Skutterudites: MFe_4Sb_{12} ($M = Na, K, Ca, Ba$) — ●A. LEITHE-JASPER, W. SCHNELLE, H. ROSNER, M. BAENITZ, A. RABIS, A.A. GIPPIUS, E.N. MOROZOVA, J.A. MYDOSH, and Y. GRIN — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The chemical, structural and magnetic properties of alkali and alkaline-earth metal compounds with filled-skutterudite structure, MFe_4Sb_{12} ($M = Na, K, Ca, Ba$), are described [1,2]. X-ray and neutron diffraction and elemental analysis established the crystal structure without defects and disorder on the cation site. The electronic structure is calculated by LMTO and FPLO methods. Quantum chemical calculations (electron localization function, ELF) reveal the covalent character of both Fe-Sb and Sb-Sb interactions. Electronic structure calculations within the LDA exhibit a band ferromagnetic ground state and predict a half-metallic behaviour for $M = Na, K$. In contrast to Ca/Ba Fe_4Sb_{12} , the alkali-metal skutterudites are itinerant electron ferromagnets with small magnetic moments ($\approx 0.25 \mu_B/Fe$ atom) and $T_C \approx 85$ K. Yet, the paramagnetic moments of all four compounds are between 1.5 and 1.7 μ_B per

Fe atom, indicating similar Stoner-factors.

- [1] A. Leithe-Jasper et al. Phys. Rev. Lett. 91, 037208 (2003).
 [2] A. Leithe-Jasper et al. Phys. Rev. B, in print (1 Dec 2004).

TT 12.5 Sa 11:45 TU H2053

Specific Heat, Electronic State and Einstein Phonon Modes of Filled Iron Antimony Skutterudites: $M\text{Fe}_4\text{Sb}_{12}$ ($M = \text{Na, K, Ca, Ba, La, Yb}$) — •W. SCHNELLE, H. ROSNER, A. LEITHE-JASPER, M. BAENITZ, J.A. MYDOSHI, and Y. GRIN — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Filled skutterudites adopt crystal structures with weakly bonded fillers M which can move in an oversized cavity. While the compounds $\text{NaFe}_4\text{Sb}_{12}$ and $\text{KFe}_4\text{Sb}_{12}$ are weak itinerant electron ferromagnets below $\approx 80\text{K}$ [1,2], the isostructural alkaline-earth and the La and Yb-filled compounds are paramagnets down to 2K. Specific heat measurements at low temperatures reveal electronic terms γ ranging from 100 to 200 mJ/molK², irrespective of the ground state. A field dependence of γ is only found for $\text{LaFe}_4\text{Sb}_{12}$. In addition, an Einstein term to $c_p(T)$ with Θ_E between 70K and 105K is detected. Full potential band structure calculations for $\text{NaFe}_4\text{Sb}_{12}$ suggest an energetically driven off-center motion of the Na in its cage by about 0.1 Å. From temperature-dependent atomic displacement factors determined by X-ray diffraction the Einstein temperature and the heat capacity are calculated and compared with our structural data.

- [1] A. Leithe-Jasper et al. Phys. Rev. Lett. 91, 037208 (2003).
 [2] A. Leithe-Jasper et al. Phys. Rev. B, in print (1 Dec 2004).

TT 12.6 Sa 12:00 TU H2053

Observation of Successive Phase Transitions and Orbital Ordering in Ca_2RuO_4 with Resonant X-ray Scattering — •IOANNIS ZEGKINOGLU¹, JOERG STREMPFER¹, CHRISTIE S. NELSON², JOHN P. HILL³, JONATHAN C. LANG⁴, GEORGE SRAJER⁴, HIDETO FUKAZAWA⁵, YOSHITERU MAENO⁵, and BERNHARD KEIMER¹ — ¹Max-Planck-Institut fuer Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — ²NLSL, Brookhaven National Laboratory, Upton, NY 11973-5000, USA — ³Department of Physics, Brookhaven National Laboratory, Upton, NY 11973-5000, USA — ⁴Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA — ⁵Department of Physics, Kyoto University, Kyoto 606-8502, Japan

Resonant x-ray scattering (RXS) performed at the L_{II} and L_{III} absorption edges of Ru has been used to investigate the magnetic properties and orbital ordering of Ca_2RuO_4 single crystals. A very large resonance enhancement of the magnetic signal due to $2p \rightarrow 4d$ dipole electronic transitions is observed at the antiferromagnetic wave-vector (100). Besides the well-known antiferromagnetic phase transition at $T_N = 110\text{K}$, an additional phase transition is observed around 260K. The polariza-

tion dependence of the corresponding scattering intensity indicates the absence of any charge scattering contribution. No scattering is observed at several reciprocal space positions where orbital ordering has been theoretically predicted. Instead, a resonant peak is observed at the magnetically forbidden (110) position, which has not been reported by previous experiments.

TT 12.7 Sa 12:15 TU H2053

Temperature dependent bulk sensitive valence band XPS measurements on LaCoO_3 single crystals — •T. KOETHE¹, M.W. HAVERKORT¹, Z. HU¹, M. REUTHER¹, T. LORENZ¹, N.B. BROOKES², J.C. CEZAR², and L.H. TJENG¹ — ¹II. Physikalisches Institut der Universität zu Köln, Germany — ²ESRF, Grenoble, France

The transition metal oxide compound LaCoO_3 displays a series of gradual spin state transitions from a diamagnetic state to a paramagnetic state with a maximum in the susceptibility at 100K and from semiconductor to metal above $\approx 500\text{K}$. The Co^{3+} ions have a $3d^6$ configuration and can take a low spin state (LS) $S = 0$, high spin state (HS) $S = 2$ or even an intermediate spin state (IS) $S = 1$. There is general agreement about the LS nature of the low temperature phase, whereas the spin state in the intermediate and high temperature phases is much debated in the literature concerning the amount of contribution from IS or HS . We address this question with photoelectron spectroscopy using high photon energies on high quality single crystals in order to enhance bulk sensitivity. Our spectra show for temperatures below 300K clearly more LS contribution than previous experimental results. However, we observe a considerable HS component even at 100K. We infer that this HS spectral weight originates from the surface since the crystal field at the surface is strongly reduced due to the smaller coordination number.

TT 12.8 Sa 12:30 TU H2053

Co- $L_{2,3}$ XMCD study on one-dimensional $\text{Ca}_3\text{Co}_2\text{O}_6$ single crystals — •Z. HU¹, M.W. HAVERKORT¹, J. GEGNER¹, A. MAIGNAN², N.B. BROOKES³, J.C. CEZAR³, and L.H. TJENG¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Laboratoire CRISMAT, Caen, France — ³European Synchrotron Radiation Facility, Grenoble, France

We have carried out x-ray magnetic circular dichroism (XMCD) measurements at the Co- $L_{2,3}$ edges on single crystals of $\text{Ca}_3\text{Co}_2\text{O}_6$, in which $\text{Co}(1)\text{O}_6$ octahedron alternates with $\text{Co}(2)\text{O}_5$ trigonal prism along the chain. We found that the dichroism in the L_3 edge mainly occurs in the lower part of the spectrum and that the dichroism in the L_2 edge is negligible. In combination with cluster model simulations, we deduce that the dichroism originates from the trigonal prism $\text{Co}^{3+}(2)$ ions which are in the high spin state and that the octahedron $\text{Co}^{3+}(1)$ ions are nonmagnetic, i.e. in the low spin state. From the orbital sum rule we obtain an orbital moment of $1.2 \mu_B$ for the $\text{Co}^{3+}(2)$.

TT 13 Transport - Quantum Coherence and Quantum Information Systems

Zeit: Samstag 08:45–12:45

Raum: TU H3027

TT 13.1 Sa 08:45 TU H3027

Relation between high- and low-frequency noise — •ALEXANDER SHNIRMAN¹, GERD SCHÖN¹, IVAR MARTIN², and YURIY MAKHLIN³ — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe — ²Los Alamos National Laboratory, Los Alamos, NM, USA — ³Landau Institute for Theoretical Physics, Moscow, Russia

Low-frequency (1/f) noise dominates the decoherence in most superconducting qubits. Thus it is very important to understand its origin and properties. Recently, coherent two-level systems have been observed in Josephson junctions [1]. These systems influence strongly qubits' dynamics at high ($\approx 10\text{GHz}$) frequencies. In addition, recent experiments [2] indicate a connection between the high- and low-frequency noise. In this work we note that an ensemble of coherent two-level systems produces simultaneously high- and low-frequency noise. The relation between these two contributions depends on the statistical properties of the ensemble. We analyze several possible distribution functions and relate the results to the known experimental facts. We also note that a similar relation holds for ensembles of many-level fluctuators with discrete spectrum.

- [1] R.W. Simmonds et al., Phys. Rev. Lett. 93, 035301 (2004)
 [2] O. Astafiev et al., cond-mat/0411216 (2004)

TT 13.2 Sa 09:00 TU H3027

Fermionic Mach-Zehnder interferometer subject to a Quantum Bath — •FLORIAN MARQUARDT — Department of Physics, Yale University, New Haven, USA

The Mach-Zehnder interferometer represents the simplest possible two-way interference setup, and its recent experimental realization in an electronic system [1] has raised many intriguing questions. The loss of interference contrast with rising voltage or temperature and the shot noise of the output current have been measured. In this talk I will present a theoretical analysis of decoherence in a fermionic Mach-Zehnder interferometer coupled to any quantum mechanical environment [2]. I will discuss the energy-resolved dephasing rate, the connections to the theory of dephasing in weak localization, the importance of Pauli blocking, and the shot noise correction due to the environment. The results will be compared with simpler models of dephasing, including classical noise sources [3].

- [1] Y. Ji et al., Nature 422, 415 (2003)
 [2] F. Marquardt, cond-mat/0410333 (2004)
 [3] F. Marquardt and C. Bruder, Phys. Rev. Lett. 92, 056805 (2004)

TT 13.3 Sa 09:15 TU H3027

Perfect state transfer through dispersive quantum chains — •DANIEL BURGARTH and SOUGATO BOSE — Department of Physics & Astronomy, University College London, UK

Quantum chains are very promising for the transfer of quantum states along short distances. However, in many cases the transfer is strongly dispersive and its fidelity is in general very small. I will present a simple and experimentally feasible scheme that can achieve perfect state transfer even in the presence of dispersion. It is applicable to a large variety of systems, including Heisenberg spin chains. Furthermore, it has a built-in stability to imperfections, decoherence and dissipation.

TT 13.4 Sa 09:30 TU H3027

Cluster States From Heisenberg Interaction — •MASSOUD BORHANI — Department of Physics - University of Basel - Switzerland

We show that a special type of entangled states, cluster states, can be created with Heisenberg interactions and local rotations in 2d steps where d is the dimension of the lattice. We find that, by tuning the coupling strengths, anisotropic exchange interactions can also be employed to create cluster states. Finally, we propose electron spins in quantum dots as a possible realization of a one-way quantum computer based on cluster states.

TT 13.5 Sa 09:45 TU H3027

Entanglement measures for multipartite qubit systems and beyond — •ANDREAS OSTERLOH¹ and JENS SIEWERT² — ¹Institut für Theoretische Physik, Universität Hannover — ²DMFCI, Università di Catania, Catania, Italy

We propose an approach to construct entanglement measures for multipartite systems of qubits, which can be extended to an arbitrary number of half-integer spins. The essential step is the construction of an operator that we call *comb* in reference to the *hairy ball theorem*. These combs necessarily have to be antilinear operators. A particularly nice feature of this approach is that for qubits (or spin 1/2) the combs are automatically invariant under $SL(2, \mathbb{C})$, which implies that the constructed measures are entanglement monotones by construction. The central idea provides a key to formulate (multipartite) entanglement measures for entanglement of arbitrary subsystems. In order to illustrate our approach, we construct operators for the N -tangle ($N = 3, \dots, 6$) Candidates for maximally entangled states are presented and their tangles are evaluated. An extension towards general half-integer spin is discussed.

TT 13.6 Sa 10:00 TU H3027

Single Electron Spin Dynamics due to Interaction with Nuclear Spins investigated with Time-dependent DMRG — •ANDREAS FRIEDRICH¹, ALEXANDER V. KHAETSKII², and ULRICH SCHOLLWÖCK¹ — ¹Institut für theoretische Physik C, RWTH Aachen — ²Physics Department, LMU München

We investigate the dynamics of a single electron spin due to its interaction with the underlying spin-1/2 carrying nuclei motivated by decoherence effects in spin-based quantum-bits, like a single electron in a quantum dot which became of central interest in recent years. We study the dependence of characteristic timescales on different initial states and analyze the effects of magnetic fields by means of a special type of time-dependent density-matrix renormalization-group method that allows to prepare different kinds of initial states and let them evolve in time.

TT 13.7 Sa 10:15 TU H3027

Quantum-Error-Correction in spatially correlated quantum-noise — •ROCHUS KLESSE and SANDRA FRANK — Universität Köln

We study the performance of quantum error-correcting codes in a model that admits error-correlations. The model consists of n spins (qubits) coupled to a common bosonic bath. The amount of error-correlation is determined by the spatial distance d between the spins. We find that the performance of error correcting Calderbank-Shor-Steane codes is very sensitive to error-correlations: while independent errors ($d \rightarrow \infty$) can be effectively corrected, error correlations that are present at vanishing distances d lead to a complete failure of the error correction in the limit of large n . We also discuss the case of intermediate error correlations at finite distances d .

TT 13.8 Sa 10:30 TU H3027

Quantum Frustration in the damped harmonic Oscillator — •HEINERICH KOHLER¹ and FERNANDO SOLS² — ¹Institut für theoretische Physik, Universität Heidelberg — ²Universidad Complutense Madrid

We study the dissipative properties of a harmonic oscillator subjected to two independent heat baths which couple linearly to its position and to its momentum respectively. We find that the effects of the two heat baths partially cancel each other, due to the noncommutativity of position and momentum (quantum frustration). This leads to unexpected effects as underdamped oscillations in the strong coupling regime. We compare this model with the scenario where only one bath couples linear to the position and the momentum of the central oscillator. In the latter case no quantum frustration effects occur.

Pause

TT 13.9 Sa 11:00 TU H3027

Multiphoton antiresonance and Rabi oscillations of ac driven quantum oscillators — •M. V. FISTUL¹ and M. I. DYKMAN² — ¹Theoretische Physik III, Ruhr-Universität Bochum — ²Department of Physics and Astronomy, Michigan State University, East Lansing, USA

We report a theoretical analysis of coherent multiphoton quantum transitions of ac driven nonlinear oscillators. We show that these transitions are accompanied by a novel effect, an *antiresonance* of the response. The nonlinear response of a quantum oscillator displays antiresonant dips and resonant peaks with varying frequency of the driving field. The effect is a consequence of special symmetry and is related to resonant multiphoton mixing of several pairs of oscillator states at a time. The shape and magnitude of the dips (peaks) strongly depend on the field. We calculate the multiphoton Rabi frequency and discuss the possibility to observe the antiresonance and the associated multiphoton Rabi oscillations in various mesoscopic systems, e.g. Josephson junctions, nanomechanical resonators and molecular magnets. The role of a specific source of decoherence, i.e. a low frequency noise is discussed.

TT 13.10 Sa 11:15 TU H3027

Charge Qubits for Quantum Computation: Chances and Limitations — •MARTINA HENTSCHEL^{1,2}, EDUARDO R. MUCCILO³, and HAROLD U. BARANGER¹ — ¹Duke University, Durham, NC, USA — ²Universität Regensburg — ³University of Central Florida, Orlando, FL, USA

Charge qubits realized in lateral quantum dot systems allow one to combine well-established semiconductor technologies with using the electron's classical charge, rather than its spin, to define the computational basis. The charge qubit we consider is a ring of three identical quantum dots joined by controllable tunneling barriers with one (extra) unpaired electron in the system. A magnetic flux through the ring allows one to define the working point of the qubit such that the two lowest eigenstates are degenerate in energy and have a homogeneous charge distribution which is hoped to reduce the decoherence due to coupling to piezoelectric phonons that is of importance in a double-dot charge qubit. We demonstrate the possibility to carry out one and two qubit operations and find that one qubit operations do not require the varying of magnetic fields locally. Performing a Schrieffer-Wolf transformation we show that the swap two qubit operation can be implemented using a single pulse of appropriate length. Based on a microscopic model and a Markov approximation, we solve the resulting Redfield equation and compare the energy and phase relaxation time with the respective times of a double-dot charge qubit. Interpreting the counterintuitive result, we extend the understanding of charge qubits.

Supported in part by ARO Contract No. DAAD19-02-1-0079.

TT 13.11 Sa 11:30 TU H3027

Inductively coupled charge qubits with asymmetric SQUIDS — •CARSTEN HUTTER¹, YURIY MAKHLIN², ALEXANDER SHNIRMAN¹, and GERD SCHÖN¹ — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe — ²Landau Institute for Theoretical Physics, Moscow, Russia

We investigate various methods of inductive coupling of SQUIDS used as charge qubits. For symmetric SQUIDS, this coupling produces $\sigma_y \sigma_y$ [1] or $\sigma_x \sigma_x$ [2,3] terms in the charge basis. In the latter case the interaction term commutes with the single-qubit Hamiltonian at the degeneracy point, $\propto E_J \sigma_x$. We analyze the stability of the interaction with respect to asymmetries of the parameters of junctions in SQUIDS and find, that the interaction term ceases to commute with the single-qubit Josephson

terms, when the symmetry is lifted.

- [1] Yu. Makhlin *et al.*, Nature 398, 305 (1999).
 [2] J.Q. You *et al.*, Phys. Rev. Lett. 89, 197902 (2002).
 [3] J. Lantz *et al.*, Phys. Rev. B 70, 140507(R) (2004).

TT 13.12 Sa 11:45 TU H3027

Coherence stabilization of a driven two-qubit gate by AC fields — ●SIGMUND KOHLER, KAREN M. FONSECA ROMERO, and PETER HÄNGGI — Institut für Physik, Universität Augsburg

In order to perform logical operations, a quantum computer requires tunable nonlinear interactions between two qubits. In particular, a spin-spin interaction of the Heisenberg type has been proposed for the construction of a CNOT gate. The quality of a gate operation is affected by decoherence which results from the coupling of the qubits to external degrees of freedom. In this talk, we propose a coherence stabilization scheme which reduces the influence of bit-flip noise in two-qubit gate operations. As a microscopic model, we consider a pair of driven qubits coupled to a harmonic oscillator bath with an ohmic spectral density. The bath is eliminated within a Floquet-Bloch-Redfield formalism. This allows on the one hand to derive an approximate analytical solution for the dephasing and relaxation times and, on the other hand, provides a physical explanation of the observed coherence stabilization. Our analytical estimates are in good agreement with numerical results.

- [1] K. M. Fonseca Romero, S. Kohler, and P. Hänggi, cond-mat/0409774.

TT 13.13 Sa 12:00 TU H3027

Spectroscopy of a driven solid-state qubit and its detector — ●M. THORWART¹, M.C. GOORDEN², and M. GRIFONI³ — ¹Universität Düsseldorf — ²Universiteit Leiden, The Netherlands — ³Universität Regensburg

We study the asymptotic dynamics of a driven quantum two-level system coupled via a quantum detector to the environment [1]. We find multi-photon resonances which are due to the entanglement of the qubit and the detector. Different regimes are studied by employing a perturbative Floquet-Born-Markov approach for the qubit+detector system, as well as non-perturbative real-time path integral schemes for the driven spin-boson system. We find analytical results for the resonances, including the red and the blue sidebands which have been observed in superconducting flux-qubit-SQUID systems [2]. The analytical results agree well with those of exact ab-initio real-time path-integral calculations.

- [1] M.C. Goorden, M. Thorwart, and M. Grifoni, Phys. Rev. Lett., in press.
 [2] I. Chiorescu, P. Bertet, K. Semba, Y. Nakamura, C.J.P.M. Harmans, and J.E. Mooij, Nature **431**, 159 (2004).

TT 14 Symposium Superconducting Quantum Systems

Zeit: Samstag 13:45–16:45

Raum: TU H104

Hauptvortrag

TT 14.1 Sa 13:45 TU H104

Flux Qubits — ●HANS MOOIJ — Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands

We investigate superconducting flux quantum bits. The qubits are fabricated of aluminum and consist of a loop with three junctions. The basic quantum states have persistent currents of opposite sign. Measurements are performed with a SQUID. Quantum operations are performed by applying microwave pulses with a frequency that is resonant with the energy splitting of the qubit. We have studied the coherence of the systems and have measured relaxation and dephasing times. The best decoherence times are of the order of 1 microsecond, while qubit operations can be performed in a few nanoseconds. We have coupled a qubit to a harmonic oscillator and we have been able to transfer a single photon. We have coupled two qubits and are able to perform conditional two-qubit operations. In the talk the general status and the latest results will be discussed.

Hauptvortrag

TT 14.2 Sa 14:15 TU H104

Single-Shot State Measurement of Coupled Phase Qubits — ●JOHN MARTINIS — Physics Department, University of California, Santa Barbara, CA 93106, USA

The Josephson junction is an ideal solid-state system for building

TT 13.14 Sa 12:15 TU H3027

Theoretical Description of Cavity-QED with Superconducting Flux Qubits — ●MARKUS J. STORCZ¹, MATTEO MARIANTONI², RUDOLF GROSS², and FRANK K. WILHELM¹ — ¹Physics Department and CeNS, Ludwig-Maximilians-Universität München — ²Walther-Meißner-Institute Garching

The symbiosis of cavity-quantum-electrodynamics (cQED) and superconducting quantum bit (qubit) circuits has gained great interest lately. This scheme can drastically improve the decoherence properties of superconducting qubits and allows for the manipulation and read-out of qubits more easily than existing architectures. We point out the special design requirements for placing a superconducting qubit circuit inside an e.m. cavity. In particular we explore one possible realization, which is to embed a three Josephson-junction flux qubit into a high quality factor microstrip resonator that can serve as the cavity. Moreover, we investigate the control and read-out of flux qubits in the cavity, and propose a scheme for coupling several qubits by way of cavity modes. We explore the limits of the Jaynes-Cummings model that is commonly used to describe the strongly coupled cavity-qubit system and compare this to a Spin-Boson model. We derive a description of the dissipative cavity-qubit system and its interaction with a photon field (i.e. in the case of flux qubits a microwave field) to analyze the characteristic decay rates of the system.

TT 13.15 Sa 12:30 TU H3027

Spectroscopic Investigation of Dynamic Features of a Ring-Type Charge Qubit — ●THOMAS WAGNER¹, DETLEF BORN², VLADIMIR SHNYRKOV², WOLFRAM KRECH², EVGENI IL'ICHEV¹, and HANS-GEORG MEYER¹ — ¹IPHT Jena — ²Institut für Festkörperphysik, FSU Jena

We investigated dynamic properties of a special Josephson charge qubit consisting of a single-Cooper-pair transistor (with capacitive gate) closed by a superconductive loop. First, focussing the considerations on the term of the effective Josephson inductance, we sketch theoretically some quantum-dynamic features of the qubit depending on gate charge and total phase of the transistor within a two-level model. Second, we report on the experimental implementation of the ring-type charge qubit conception. For readout purposes, the interferometer loop is inductively coupled to a radio frequency tank circuit (e.g. in flip-chip configuration). In this arrangement, the tank serves as inductance detector or spectrometer, respectively. Applying external microwaves to the device, we obtained inductance alterations connected with redistributions of the energy level occupation. This way using methods of nonresonant and resonant spectroscopy, we demonstrated Landau-Zener transitions between ground and excited bands, single-photon and multiphoton absorptions, and measured the energy gap etc.

electrical "atoms" that can function as quantum bits for a quantum computer. I will discuss experimental work based on large-area "phase" qubits, where experiments have demonstrated qubit state preparation and measurement with good fidelity, as well as manipulation of the qubit state via the observation of Rabi oscillations.

A more advanced measurement technique, based on a fast pulse in the current bias, has reduced the measurement time for our phase qubits from 100 ns to less than 2 ns. With this improvement, we have recently been able to perform experiments on capacitively-coupled qubits, demonstrating coherent oscillations corresponding to the i-swap operation $01 \leftrightarrow 10$. This is the first experiment with Josephson qubits to achieve simultaneous single-shot state measurements of both qubit states. During the oscillations, the states 01 and 10 are found to be anti-correlated, as expected for an entangled quantum state.

Detailed measurements show that the two measurement pulses have to be timed within about 1 ns of each other in order for large crosstalk in the state probabilities not to appear in the measurement data. A semi-classical theory explaining this phenomenon will be presented.

With these developments, we will shortly be able to demonstrate CNOT gates with full state analysis using process tomography. I will present the simple theory describing these future experiments.

Fachvortrag

TT 14.3 Sa 14:45 TU H104

Quantum Electrometry using the Radio-Frequency Single-Electron Transistor — ●TIM DUTY, KEVIN BLADH, JONAS BYLANDER, DAVID GUNNARSSON, and PER DELSING — Chalmers University of Technology, Göteborg, Sweden

The fastest and most sensitive way to measure charge is based upon the radio-frequency single-electron transistor (RF-SET). We have employed RF-SET electrometers both as a read-out device for Josephson charge qubits, and to count individual electron and Cooper-pair charge solitons passing through an 1-D array of tunnel junctions.

Our experimental studies of Josephson charge qubits demonstrate how to mitigate the effects of non-equilibrium quasiparticles and produce Cooper-pair boxes with robust even-parity ground states. Coherent free-precession with a large visibility has been observed, and measurements of dephasing indicate the presence of low-frequency background charge fluctuations. Measured relaxation times are generally shorter than expected and not yet fully understood.

The quantum mechanical tunnelling of single charges in a one-dimensional array is time correlated and consequently the detected signal exhibits the frequency $f=I/e$, where I is the current and e is the electron charge. For Cooper-pairs, one observes $f=I/2e$. We present the first direct observation of time-correlated single-electron and Cooper-pair tunnelling oscillations.

Fachvortrag

TT 14.4 Sa 15:15 TU H104

Circuit Quantum Electrodynamics: Doing Quantum Optics with Superconductors — ●ANDREAS WALLRAFF — Department of Applied Physics, Yale University, New Haven, CT 06520, USA

I will describe recent experiments in which the strong coupling limit of cavity quantum electrodynamics has been realized for the first time using superconducting circuits [1]. In our approach, we use a Cooper-pair box as an artificial atom, which is coupled to a one-dimensional cavity formed by a transmission line resonator. In the case when the Cooper-pair box qubit is tuned into resonance with the cavity, we observe the vacuum Rabi splitting of the cavity mode, indicating that the strong coupling regime is attained, and coherent superpositions between the qubit and a single photon are generated. When the qubit is detuned from the cavity resonance frequency, we perform high-fidelity dispersive quantum non-demolition readout of the qubit state. Using this readout technique, we have characterized the qubit properties spectroscopically, performed Rabi oscillations of the qubit, and attained coherence times greater than 500 ns, indicating that this architecture is extremely attractive for quantum computing and control [2].

[1] A. Wallraff, D. I. Schuster, A. Blais, L. Frunzio, R.-S. Huang, J. Majer, S. Kumar, S. M. Girvin and R. J. Schoelkopf, *Nature* (London) 431, 162 (2004)

[2] A. Blais, R.-S. Huang, A. Wallraff, S. M. Girvin and R. J. Schoelkopf, *Phys. Rev. A* 69, 062320 (2004)

Fachvortrag

TT 14.5 Sa 15:45 TU H104

Quantum communication with Josephson arrays — ●ROSARIO FAZIO¹, ALESSANDRO ROMITO¹, and CHRISTOPH BRUDER² — ¹NEST-INFM & Scuola Normale Superiore, 56126 Pisa, Italy — ²Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Josephson junction arrays can behave as a quantum channels and used to transfer quantum information between distant sites. We discuss simple protocols to realize, without external control, state transfer [1] and cloning [2] with high fidelity in Josephson chains. The great advantage of these schemes is that they not require complicate gating but they simply use the natural dynamics of a properly designed array. We propose an experiment, realizable with present day technology, that may allow to implement these protocols. Communication is only mildly affected by the presence of unavoidable defects in the Josephson array.

[1] A. Romito, R. Fazio and C. Bruder, *cond-mat/0408057*.

[2] G. De Chiara et al. *quant-ph/0402071*.

Fachvortrag

TT 14.6 Sa 16:15 TU H104

Optimizing two-qubit quantum logic gates for superconducting systems — ●FRANK WILHELM — Department Physik and CeNS, LMU, Theresienstr. 37, 80333 München

With the maturation of superconducting qubits it is now possible to implement two-qubit quantum logic operations such as the controlled-not (CNOT) gate [1]. We describe the necessary ingredients: i) An suitable interaction. I will describe a scheme for coupling flux qubits controlled by an external current [2]. ii) An appropriate pulse sequence. We will use optimum control theory, well known in nuclear magnetic resonance, to derive optimum smooth pulses. For untunable interaction [3], a substantial improvement of gate fidelity (to 0.99) and time (50 ps) compared to [1] can be achieved by pulse shaping. In the tunable case, the optimum pulse is much simpler [2]. iii) Sufficient coherence. We will discuss the sensitivity of the gate performance to decoherence and the benefit of encoding into decoherence-free subspaces (DFSs) [4].

[1] T. Yamamoto, Y.A. Pashkin, O. Astafiev, Y. Nakamura, and J.S. Tsai, *Nature* 425, 941 (2003).

[2] B.L.T. Plourde, J.Zhang, K.B. Whaley, F.K. Wilhelm, T.L. Robertson, T. Hime, S. Linzen, P.A. Reichardt, C.-E. Wu, and John Clarke, *Phys. Rev. B*(R) 70, 140501 (2004).

[3] V. Bergholm, A. Spoerl, T. Schulte-Herbrueggen, S.J. Glaser, M.J. Storcz, and F.K. Wilhelm, in preparation.

[4] M.J. Storcz, J. Vala, K.R. Brown, J. Kempe, F.K. Wilhelm, and K.B. Whaley, *cond-mat/0407780*.

TT 15 Superconductivity - Properties, Electronic Structure, Order Parameter I

Zeit: Samstag 14:00–16:45

Raum: TU H2053

TT 15.1 Sa 14:00 TU H2053

Collision-limited Raman response in normal metals and superconductors — ●DIRK MANSKE¹ and DIETRICH EINZEL² — ¹Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — ²Walther-Meissner-Institut, 85748 Garching

We formulate a theory for describing the electronic Raman response in metals and superconductors with anisotropic scattering rates due to (a) elastic scattering of quasiparticles on impurities and (b) due to inelastic electron-electron scattering. Our approach is based on the Landau-Boltzmann equation for anisotropic metals at finite wavenumbers and takes into account (within RPA) the Coulomb repulsion as well as the relevant scattering processes. We employ our theory to the high- T_c cuprates for which the inelastic part of the scattering rates is taken from the solution of generalized Eliashberg equations based on a spin fluctuation-mediated Cooper-pairing. Numerical results for different scattering rates are presented.

TT 15.2 Sa 14:15 TU H2053

Electric fields above the surface of superconductors — P. LIPAVSKÝ¹, ●K. MORAWETZ^{2,3}, JAN KOLÁČEK¹, J.J. MARES¹, E.H. BRANDT⁴, and M. SCHREIBER² — ¹Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16258 Praha 6, Czech Republic — ²Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ³Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — ⁴Max-Planck-Institute for Metal Research, D-70506 Stuttgart, Germany

The electrostatic potential above the Abrikosov vortex lattice, discussed earlier by Blatter *et al.* [*Phys. Rev. Lett.* 77, 566 (1996)], is evaluated within the Ginzburg-Landau theory [1]. Unlike previous studies we include the surface dipole [2,3]. 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. Within the extension of the Landau-Ginzburg theory towards lower temperatures the electric fields above the superconducting surface are calculated for different experimental situations.

[1] P. Lipavský, K. Morawetz, J. Kolacek, J. J. Mares, E. H. Brandt, M. Schreiber, *Phys. Rev. B* in press, *cond-mat/0409397*

[2] P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, M.

Schreiber, Phys. Rev. B 69 (2004) 024524-1-7

[3] P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, M. Schreiber, Phys. Rev. B 70 (2004) 104518-1-7

TT 15.3 Sa 14:30 TU H2053

Superconductivity related core level shift in HTSC — ●JÖRG VOIGT^{1,2}, RAFFAELE GILARDI¹, HENRIK RONNOW¹, JOEL MESOT¹, LUC PATTHEY¹, MING SHI¹, OSCAR TJERNBERG³, and THOMAS CLAESON³ — ¹Paul Scherrer Institut, 5232 Villigen-PSI, Schweiz — ²Forschungszentrum Jülich, 52425 Jülich — ³Royal Institute of Technology, Electrum 229, S-164 40 Kista, Sweden

We have studied the energy of the core levels in different families of cuprate superconductors as a function of temperature and doping. We confirm earlier results that showed a shift towards lower binding energy with increased hole doping. As a new result, we find a shift to lower binding energy on crossing the superconducting phase transition. We discuss, how the screening can be related to the electronic gap present in the superconducting state.

TT 15.4 Sa 14:45 TU H2053

Splitting of the CuO-band — ●B. MÜLLER¹, L. DUDY¹, H. DWELK¹, A. KRAPP¹, C. JANOWITZ¹, H. HÖCHST² und R. MANZKE¹ — ¹Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — ²Synchrotron Radiation Center (SRC), Madison/Wisconsin (USA)

Polarization dependent ARPES measurements revealed a double-peak structure close to the Fermi surface in Bi2201 at a specific polarization of the incident light [1,2]. There are strong hints that this phenomenon displays charge-spin separation expected to occur in one-dimensional systems [2,3]. It is not yet clear, if this charge-spin separation stems from an actual one-dimensionality in the electronic structure of the CuO_2 -plane or if it is a feature persisting also in two-dimensional systems. Now the same double-peak structure could be confirmed in Bi2212. In both materials this double-peak structure shows similar properties regarding dispersion of the peaks and dependence on temperature. The double-peak structure vanishes at a temperature which seems to coincide with T^* , the temperature of the closing of the pseudogap.

[1] R. Manzke, R. Müller, C. Janowitz, C. Ast, H. Höchst, Phys. Rev. B **63** (2001) R 100504 [2] C. Janowitz, R. Müller, L. Dudy, A. Krapp, R. Manzke, C. Ast, H. Höchst, Europhys. Lett. **60** (2002) 615 [3] K. Byczuk, C. Janowitz, R. Manzke, J. Spalek, W. Wojcik, Europhys. Lett. **67** (2004) 1011

TT 15.5 Sa 15:00 TU H2053

Determination of the hole density of $(Bi, Pb)_2(Sr, La)_2CuO_{6+\delta}$ superconductors — ●L. LASOGGA¹, R. MITDANK¹, A. KRAPP¹, H. DWELK¹, S. ROGASCHEWSKI¹, C. JANOWITZ¹, R. MANZKE¹, K. SCHEURELL², and I. MURWANI² — ¹Humboldt University Berlin, Department of Physics, Newtonstrasse 15, 12489 Berlin — ²Humboldt University Berlin, Department of Chemistry, Brook-Taylor-Strasse 2, 12489 Berlin

The hole concentration of the CuO_2 planes of $Bi_{2-y}Pb_ySr_{2-x}La_xCuO_{6+\delta}$ cuprates has been investigated in great detail by two techniques, x-ray absorption spectroscopy (XAS) at the $Cu - L_3$ edge and iodometric titration. The XAS measurements were performed at the BESSY II beamline PM3. Our investigations include both ceramics and single crystals containing no lead ($y = 0$) and larger amounts of lead ($y = 0,16 \dots 0,45$). For each case we studied series of variable content of lanthanum ($x = 0,0 \dots 0,8$). Finally we compare ceramics and single crystals, discuss the dependence between hole density, critical temperature and content of lead and lanthanum. Moreover we show the dependence of the x-ray absorption from the angle of incidence.

Pause

TT 15.6 Sa 15:30 TU H2053

STM structure analysis of Pb-doped Bi-2212 depending on the Pb-content — ●HENDRIK GLOWATZKI, ALICA KRAPP, CHRISTOPH JANOWITZ, and RECARDO MANZKE — Institut f. Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

Scanning Tunneling Microscopy (STM) was used to analyse the surface modification of double layered bismuth single crystals (BSCCO) due to partial substitution of Bi by Pb resulting in $Bi_{2-x}Pb_xSr_2CaCu_2O_{8+\delta}$. A typical structure found on Pb-free BSCCO is the well known (4.7×1)

superstructure modulation, which can be clearly seen along the ab -(001) plane. The increasing substitution of Bi by Pb was reported to lead to a weakening of the modulation structure, thus increasing the modulated wavelength and finally disappearing at $x = 0,5$ [1]. Depending on the Pb-content x we were able to verify the increasing wavelength, but not a complete disappearance of the modulation. We found the modulation structure not covering the whole surface but building an arrangement of domains at $x \geq 0,3$. Our observations show an alternation of domains, parts of which seem to be flat while others reveal the modulated structure. The structural features will be discussed in terms of the crystal composition.

[1] Lei Shi *et al.*, J. Phys.: Condens. Matter **13**, 5195 (2001)

TT 15.7 Sa 15:45 TU H2053

Scanning tunneling spectroscopy on (100) plane of $NdBa_2Cu_3O_{7-\delta}$ — ●PINTU DAS¹, MICHAEL R. KOBLISCHKA¹, THOMAS WOLF², UWE HARTMANN¹, and IDURU SHIGETA³ — ¹Institute of Experimental physics, University of Saarbruecken, P.O.Box-151150, D-66041 Saarbruecken, Germany — ²Forschungszentrum Karlsruhe GmbH, Institute of Solid State Physics, D-76021, Karlsruhe Germany — ³Department of General Education, Kumamoto National College of Technology, Kumamoto 861-1102, Japan

We report the results of STS experiments performed on the (100) plane of $NdBa_2Cu_3O_{7-\delta}$ (NdBCO) single crystals ($T_c = 95,5$ K) at 4.2 K. From the dI/dV curves, which represents the local density of states (LDOS), we find a V-shaped curve with a very high conductance at the zero bias in the gap region which is typical in case of d-wave symmetry of the order parameter. In a region of 200 Å, we also observed other curves with very low coherence peaks or even with no peak structure, which is possible if the oxygen content is inhomogeneously distributed across the surface. A third type of curve, which is not frequently observed, has a peak at the zero bias conductance (ZBCP). We consider that the ZBCP is due to the Andreev reflection at the impurity potential (geometrically rough surface) and can be explained with the theory of roughness effect on the density of states of d-wave superconductor [1]. We can explain the data considering the symmetry order parameter to be $d_{x^2-y^2}$ wave, but at this moment we can not confirm if there is a mixing of any other component.

[1] Tanuma *et al.*, Phys. Rev. B **57**, 7997 (1998).

TT 15.8 Sa 16:00 TU H2053

Two length scales in the crystalline electronic state of underdoped cuprate superconductors — ●JÜRGEN RÖHLER — Universität zu Köln, D-50937 Köln, Germany

Spatial- and energy-resolved differential tunneling measurements from STM have shown evidence for a crystalline electronic structure in the pseudogap regime of lightly doped cuprate superconductors [1]. The conductance exhibits *minima* at the perimeter atoms of a four Cu_2O -unit-cell square "checkerboard". The internal electronic structure of the $4a \times 4a$ squares consists of 3×3 conductance *maxima*, incommensurate with the atomic lattice. We suggest to relate this electronic crystal structure with a "supersolid" of paired self-protecting singlets (PSPS) [2]. Hole pairs underlying not only a non-double-occupancy constraint for the copper sites, but also for the oxygen cages, extend over $4a$ (4 oxygen cages), and may cause a $4a \times 4a$ modulation of the electronic structure. Maxima in the local density of states, however, are expected to occur with a periodicity of $3a$ (4 copper sites). The interference between the $4a$ and $3a$ length scales yields a possible explanation for the atomic-scale electronic structure variations observed within the checkerboard.

[1] T. Hanaguri *et al.*, Nature **430**, 1001 (2004), cond-mat/0409102.

[2] J. Röhler, J. Supercond. **17**, 159 (2004), cond-mat/0307310.

TT 15.9 Sa 16:15 TU H2053

Unkonventionelle Supraleitung und starke Fluktuationen in $Na_{0,3}CoO_2 \cdot 1,3H_2O$ — ●NIELS OESCHLER¹, R.A. FISHER¹, N.E. PHILLIPS¹, J.E. GORDON², M.L. FOO³ und R.J. CAVA³ — ¹LNBL and Department of Chemistry, University of California, Berkeley, CA, USA — ²Physics Department, Amherst College, Amherst, MA, USA — ³Department of Chemistry, Princeton University, Princeton, NJ, USA

Seit Entdeckung der Hoch-Temperatur-Supraleiter 1986 sind viele Gruppen auf der Suche nach neuen Supraleitern, in denen die Kupferatome durch andere Übergangsmetalle ersetzt sind. Erst 2003 wurde die erste supraleitende Kobaltoxid-Verbindung $Na_{0,3}CoO_2 \cdot 1,3H_2O$ mit $T_c = 4,5$ K gefunden. In diesem System ordnen sich die Co-Atome nicht quadratisch in der Kobaltoxid-Schicht wie die Cu-Atome in den Kupraten, sondern trigonal an. Dies führt zu einer Frustration der Co-Spins,

die vermutlich entscheidend für die Supraleitung ist. Daher spekuliert man auf nicht-phononische Supraleitung, die über magnetische Fluktuationen vermittelt wird. Wir berichten über Messungen der spezifischen Wärme an $\text{Na}_{0.3}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$ im Bereich $0.8\text{K} \leq T \leq 12\text{K}$ und $B \leq 9\text{T}$. Die spezifische Wärme (C) von $\text{Na}_{0.3}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$ unterscheidet sich in der supraleitenden Phase deutlich von der eines konventionellen Supraleiters. Bei tiefen Temperaturen folgt die spezifische Wärme einem T^2 -Verhalten ($C \propto T^2$). Dies deutet auf Knoten der supraleitenden Energielücke auf der Fermi-Fläche hin. Weitere Hinweise auf unkonventionelle Supraleitung werden durch die Magnetfeldabhängigkeit des Sommerfeld-Koeffizienten erhalten. Starke Fluktuationen zeigen sich trotz relativ niedrigem T_c in einer feldunabhängigen Onset-Temperatur T_c^{onset} .

TT 15.10 Sa 16:30 TU H2053

Cooperative effect of phonons and electronic correlations for superconductivity in cobaltates — ●A. FOUSSATS¹, A. GRECO¹, M. BEJAS¹, and A. MURAMATSU² — ¹Facultad de Ciencias Exactas, Ingeniería y Agrimensura and Instituto de Física Rosario (UNR-CONICET). Av. Pellegrini 250-2000 Rosario, Argentina — ²Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany

TT 16 Posters Correlated Electrons, Measuring Devices, Cryotechnique

Zeit: Samstag 11:00–16:30

Raum: Poster TU C

TT 16.1 Sa 11:00 Poster TU C

Quantum Criticality in the frustrated Laves phase compound NbFe_2 — ●DENNIS MORONI-KLEMENTOWICZ, MANUEL BRANDO, and FRIEDRICH MALTE GROSCHE — Department of Physics, Royal Holloway, University of London, Egham, TW20 OEX, United Kingdom

Geometric frustration in nearly magnetic metals provides a promising and relatively little explored path to obtaining high electronic density of states - hatching condition of novel quantum order. Various compounds close to the border of magnetism can be found amongst intermetallic C14 and C15 Laves phases. We have focused on one of the most interesting examples: NbFe_2 . Depending on precise stoichiometry, pressure and applied magnetic field, NbFe_2 can be tuned between ferromagnetic, antiferromagnetic and enhanced paramagnetic low temperature states. Because stoichiometry and annealing are crucial in this compound we have put particular effort in making high quality samples using cold crucible RF heating techniques, extended annealing close to the melting point and zone refining, as well as detailed characterisation by heat capacity and magnetisation measurements. The complex phase diagram of NbFe_2 gives rise to several regions in which an ordering temperature is suppressed to low temperatures. We investigate the vicinity of these quantum critical points by high sensitivity measurements of the electrical resistivity under applied magnetic fields and high hydrostatic pressure, as well as ambient pressure heat capacity measurements, down to the sub-100 mK range.

TT 16.2 Sa 11:00 Poster TU C

Systematic Strong-Coupling Expansion of the $T \otimes T$ Jahn-Teller System — ●HEINZ BARENTZEN — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

Transition-metal oxides are notoriously difficult to describe because of a rather strong interplay between the spin, orbital and lattice degrees of freedom. This applies, in particular, to the recently investigated titanates with one t_{2g} electron per site, whose magnetic properties are surprising and controversial. Thus, e.g., while YTiO_3 shows a ferromagnetic ground state accompanied by a large Jahn-Teller (JT) distortion, LaTiO_3 exhibits an antiferromagnetic ground state with no detectable JT effect. To resolve the puzzling magnetic behavior of LaTiO_3 , the concept of an orbital liquid has been worked out by Khaliullin et al. (Phys. Rev. Lett. **85**, 3950 (2000)), while a perturbing crystal field of the GdFeO_3 -type has been proposed by Mochizuki and Imada (J. Phys. Soc. Jpn. **70**, 2872 (2001)).

To put these concepts on a quantitative basis we intend to elucidate the role of the $T \otimes T$ JT problem, relevant to these systems. So far, however, analytic results are available only for the limiting cases of weak and strong coupling. In an attempt to find the lowest eigenvalue of the $T \otimes T$ system over the whole coupling range, we have recently succeeded in obtaining systematic expansions for weak and strong coupling, the first steps on the way towards the complete solution of the problem. The reasoning behind these expansions will be explained and illustrated for the strong-coupling case.

We propose that unconventional superconductivity in hydrated sodium cobaltate Na_xCoO_2 results from an interplay of electronic correlations and electron-phonon interactions [1]. On the basis of the $t - V$ model plus phonons we found evidences for a) unconventional superconductivity, b) realistic values of T_c and c) the dome shape existing near $x \sim 0.35$. This picture is obtained for V close to the critical Coulomb repulsion V_c which separates the uniform Fermi liquid from $\sqrt{3} \times \sqrt{3}$ CDW ordered phase.

[1] A. Foussats, A. Greco, M. Bejas, A. Muramatsu, cond-mat/0410290

TT 16.3 Sa 11:00 Poster TU C

Antiferromagnetic Quantum Chain Systems with Competing nn and nnn Interaction — ●REINHARD K. KREMER — MPI für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Antiferromagnetic (afm) $S=1/2$ Heisenberg chain systems with uniform nearest-neighbour exchange coupling are best understood. The ground state and the excitation spectrum are well known and the experimental observations are in good agreement with theory. Additional next-nearest neighbour exchange along the chains which can be described by the Majumdar-Ghosh Hamiltonian $H = J_{nn} \sum_i (S_i S_{i+1} + \alpha S_i S_{i+2})$ with $\alpha = J_{nnn}/J_{nn}$ gives rise to a more complex behaviour, since next-nearest neighbour interaction may lead to magnetic frustration. I review the magnetic properties of the afm $S=1/2$ Cu^{2+} chain systems LiCuVO_4 and CuX_2 ($X=\text{Cl}, \text{Br}$) for which afm *incommensurate* long-range ordering has been observed by neutron diffraction at low temperatures. The appearance of *incommensurate* ordering is ascribed to competing nn and nnn exchange interaction which is also evidenced in the bulk magnetic properties.

TT 16.4 Sa 11:00 Poster TU C

$S=1$ ground state in a hexacopper(II) molecular complex — ●VOLODYMYR PASHCHENKO¹, MICHAEL LANG¹, BERND WOLF¹, BERNHARD BRENDEL¹, NORBERT AUNER², OLGA SHCHEGOLIKHINA³, and YULIA MOLODTSOVA³ — ¹Physikalisches Institut, J.W. Goethe-Universität, FOR 412, 60054 Frankfurt(M), Germany — ²Institut für Anorganische Chemie, J.W. Goethe-Universität, 60439 Frankfurt(M), Germany — ³A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS), 28 Vavilov Str., 117813 Moscow, Russia

We report on an experimental determination by ESR of the molecular ground state in a hexacopper(II) siloxanolate compound. This system is distinct in that the six Cu^{2+} ions within the molecule are arranged in two almost parallel, linear trimers. According to magnetic measurements, the individual trimers couple antiferromagnetically with the dominant intratrimer exchange of $J/k_B=85$ K, yielding a spin-1/2 ground state at low temperatures. The weak intertrimer interactions of $J'/k_B=-3$ K appear to favor a ferromagnetic ground state for the molecules, with weak antiferromagnetic interactions between the molecules. Our low temperature single crystal ESR study clearly demonstrates that the molecular ground state of the complex is a triplet-singlet state, which is typical for an effective $S=1$ spin state. The data have been fitted by using the solutions of the spin Hamiltonian $\hat{H} = DS_z^2 + E(S_x^2 - S_y^2) + \mu_B \hat{g}BS$ with the parameters $D=-0.30$ cm^{-1} , $E=-0.12$ cm^{-1} , $g_x=g_y=g_z=2.00 \pm 0.05$. It was found that the progressive formation of the molecular $S=1$ ground state occurs only below 40 K when the excited doublet and quartet states of individual trimers become completely thermally depopulated.

TT 16.5 Sa 11:00 Poster TU C

The Influence of Disorder and Thermal Fluctuations on 1d Density Waves and Luttinger Liquids — •THOMAS NATTERMANN und ANDREAS GLATZ — Institut für Theoretische Physik der Universität zu Köln, Zùlpicher Str. 77, 50937 Köln

The low temperature phase diagram of 1D weakly disordered quantum systems like charge or spin density waves and Luttinger liquids is studied by a full finite temperature renormalization group (RG) calculation. For vanishing quantum fluctuations this approach is amended by an exact solution in the case of strong disorder and by a mapping onto the Burgers equation with noise in the case of weak disorder, respectively. At zero temperature we reproduce the quantum phase transition between a pinned (localized) and an unpinned (delocalized) phase for weak and strong quantum fluctuations, respectively, as found previously by Fukuyama or Giamarchi and Schulz.

At finite temperatures the localization transition is suppressed: the random potential is wiped out by thermal fluctuations on length scales larger than the thermal de Broglie wave length of the phason excitations. The existence of a zero temperature transition is reflected in a rich cross-over phase diagram of the correlation functions. The results can be transferred directly to the discussion of the influence of disorder in superfluids. Finally we extend the RG calculation to the treatment of a commensurate lattice potential. Applications to related systems are discussed as well.

TT 16.6 Sa 11:00 Poster TU C

Tomonaga-Luttinger-liquid parameter from density-matrix renormalization group calculations — •SATOSHI EJIMA¹, FLORIAN GEBHARD¹, and SATOSHI NISHIMOTO² — ¹Fachbereich Physik, Philipps-Universität Marburg — ²Institut für Theoretische Physik, Universität Göttingen

In a Tomonaga-Luttinger-liquid the density of states vanishes algebraically at the Fermi energy. The corresponding exponent α can be observed experimentally in quasi one-dimensional systems, e.g., in single-walled carbon nanotubes and other organic conductors. Experimental results, $\alpha > 1$, deviate substantially from those for simple one-dimensional models such as the Hubbard model where $\alpha \leq 1/8$. More realistic models contain nearest-neighbor interactions which strongly modify the critical exponent. However, the calculation of α for the extended Hubbard model is very difficult because no exact solution exists.

We use the density-matrix renormalization group (DMRG) method to calculate numerically the density-density correlation function for large systems with open boundary conditions. We extract α from the large-distance behavior of the density-density correlation function. We test our approach against analytical results for the one-dimensional Hubbard model and the XXZ Heisenberg chain and find an excellent agreement. As an application we calculate α in the extended Hubbard model. We show that a lightly doped charge-density-wave insulator can exhibit $\alpha > 1$.

TT 16.7 Sa 11:00 Poster TU C

Influence of electronic correlations on the Drude response of two-dimensional organic conductors — •NATALIA DRICHKO¹, MARTIN DRESSEL¹, JAIME MERINO², and JOHN SCHLUETER³ — ¹Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — ²Universidad Autonoma de Madrid, Madrid, Spain — ³Materials Science Division, Argonne National Laboratory, Argonne, USA

We use organic conductors as model objects to investigate the effects of reduced dimensions and electronic correlations. Conductivity in BEDT-TTF crystals occurs in the planes of the organic molecules, the overlap of the molecular orbitals defines the bandwidth W , the electronic correlations depend on the BEDT-TTF molecule parameters.

For the compounds α -(BEDT-TTF)₂MHg(SCN)₄ (M =Rb, Tl, K, and NH₄) the structural parameters vary slightly, leading to an increase of ratio of electron-electron correlations to W on going from metallic Rb-salt to Tl, to K, and further to NH₄ (which becomes superconducting at $T_c \sim 1$ K). By measuring polarized reflection in the conducting plane of the crystals in the 8000-50 cm⁻¹ range from $T = 300$ K to 5 K, we investigate how the electronic parameters depend on temperature and electronic correlations. The intensity of a Drude-peak increases below 50 K. The width of the Drude-component decreases when going from the Rb to the NH₄-compound, which we relate to the increase of electronic correlations. In addition, in the K-salt a pseudogap is observed around 100 cm⁻¹ at T below 50 K, indicating charge-order fluctuations close to the superconducting state.

TT 16.8 Sa 11:00 Poster TU C

Tuning the Spin-State and Insulator-Metal Transition in LaCoO₃ by Eu-Doping — •J. BAIER, M. KRIENER, S. JODLAUK, A. REICHL, C. ZOBEL, H. KIERSPEL, A. FREIMUTH, and T. LORENZ — II. Physikalisches Institut, Universität zu Köln

We present a study of the structure, the electric resistivity, the magnetic susceptibility, and the thermal expansion of La_{1-x}Eu_xCoO₃ [1]. LaCoO₃ shows a temperature-induced spin-state transition around 100 K and a metal-insulator transition around 500 K. Partial substitution of La³⁺ by the smaller Eu³⁺ causes chemical pressure and leads to a drastic increase of the spin gap from about 190 K in LaCoO₃ to about 2000 K in EuCoO₃, so that the spin-state transition is shifted to much higher temperatures. A combined analysis of thermal expansion and susceptibility gives evidence that the spin-state transition has to be attributed to a population of a spin-triplet state, as is realized in the intermediate-spin state of Co³⁺. In contrast to the spin-state transition, the metal-insulator transition is shifted only moderately to higher temperatures with increasing Eu content, showing that the metal-insulator transition occurs independently from the spin-state distribution of the Co³⁺ ions. Around the metal-insulator transition the magnetic susceptibility shows a similar increase for all x and approaches a doping-independent value around 1000 K indicating that well above the metal-insulator transition the same spin state is approached for all x .

[1] Baier *et al.*, cond-mat 0405680, appears in Phys. Rev. B

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TT 16.9 Sa 11:00 Poster TU C

Possible resolution of a temperature profile: A spin-chain study — •MARKUS HENRICH, MICHAEL HARTMANN, and GÜNTER MAHLER — Institute of Theoretical Physics 1, University of Stuttgart

Possible spatial resolution of temperature profiles and their measurability have drawn increasing attention because of their relevance in recent experiments [1].

We investigate such a scenario in a simple quantum model: a spin-chain in contact with two heat baths at different temperatures. We study, under which conditions a local spin-temperature could exist in such spin-chains and how local a possible temperature measurement could be [2].

[1] P. Kim *et al.*, Phys. Rev. Lett. 87/21, 215502 (2001).[2] M. Hartmann *et al.*, Phys. Rev. Lett. 93, 080402 (2004).

TT 16.10 Sa 11:00 Poster TU C

The Holstein-Hubbard Model away from Half-Filling — •WINFRIED KOLLER, ALEX C. HEWSON, and DIETRICH MEYER — Department of Mathematics, Imperial College London

Recent experimental results in strongly correlated materials, such as fullerides, manganites and the high T_c compounds, have stimulated a renewed theoretical interest in the effects of electron-phonon interaction. The simplest model to examine the interplay of the electron-phonon and electron-electron interactions is Holstein-Hubbard model. This model has been predominantly studied under the assumption of particle-hole symmetry. Here we present results for the model away from half-filling using the dynamical mean-field theory in combination with the numerical renormalisation group. We calculate one-electron spectral densities and two-particle response functions. In particular, we examine the crossover from bipolaronic to polaronic behaviour, and compare our results with those derived from the many-body coherent-potential approximation (CPA).

TT 16.11 Sa 11:00 Poster TU C

Singular Dynamics of Underscreened Magnetic Impurity Models — •WINFRIED KOLLER, ALEX C. HEWSON, and DIETRICH MEYER — Department of Mathematics, Imperial College London

We give a comprehensive analysis of the singular dynamics and of the low-energy fixed point of one-channel impurity s-d models with ferromagnetic and underscreened antiferromagnetic couplings. We use the numerical renormalization group (NRG) to perform calculations at $T = 0$. The spectral densities of the one-electron Green's functions and t-matrices are found to have very sharp cusps at the Fermi level ($\omega = 0$), but do not diverge. The approach of the Fermi level is governed by terms proportional to $1/\ln 2(\omega/T_0)$ as $\omega \rightarrow 0$. The scaled NRG energy levels show a slow convergence as $1/(N+C)$ to their fixed point values, where N is the iteration number and C is a constant dependent on the coupling J from which the low energy scale T_0 can be deduced. We calculate also the dynamical spin susceptibility, and the elastic and inelastic scattering cross-sections as a function of ω . The inelastic scattering goes to zero

as $\omega \rightarrow 0$, as expected for a Fermi liquid, but anomalously slowly compared to the fully screened case. We obtain the asymptotic forms for the phase shifts for elastic scattering of the quasiparticles in the high-spin and low-spin channels.

TT 16.12 Sa 11:00 Poster TU C

Quantenphasenübergang im spinlosen Holstein-Modell — ●STEFFEN SYKORA¹, ARND HÜBSCH^{1,2} und KLAUS W. BECKER¹ — ¹Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden — ²Department of Physics, University of California, Davis, CA 95616, USA

Mit Hilfe des Projektor-basierten Renormierungsverfahrens (PRM) wird der Metall-Nichtmetall-Quantenphasenübergang im eindimensionalen Holstein-Modell bei Halbfillung untersucht. In dem PRM-Verfahren werden sukzessiv hochenergetische Anregungsoperatoren der Elektron-Phonon-Wechselwirkung herausintegriert. Als Ergebnis erhält man einen effektiven Hamiltonoperator für ein quasifreies System aus renormierten ungekoppelten Elektronen und Phononen. Für Werte der Elektron-Phonon-Kopplung g oberhalb eines kritischen Wertes g_c befindet sich das System in einem geordneten Zustand entsprechend einer isolierenden Peierls-Phase. In dieser Arbeit wird das Verhalten der renormierten Ordnungsparameter für die Peierls-Gitterverzerrung Δ^b und die Ladungsdichtewelle $\hat{\Delta}_k^c$ in Abhängigkeit von g für beide Phasen untersucht. Desweiteren wird für den gesamten Parameterbereich von g die renormierte Phononenfrequenz $\tilde{\omega}_q$ und die elektronische Einteilchenenergie $\tilde{\varepsilon}_k$ berechnet. Wird der quantenkritische Punkt g_c überschritten, so öffnet sich eine Lücke an der Fermikante im elektronischen Anregungsspektrum, was dem Übergang von der metallischen in die isolierende Phase entspricht.

TT 16.13 Sa 11:00 Poster TU C

Dynamic charge and spin susceptibility of the Hubbard model — ●SEBASTIAN SCHMITT and NORBERT GREWE — Institut für Festkörperphysik, Hochschulstraße 6, 64289 Darmstadt

We present Bethe-Salpeter equations, derived via a cumulant expansion in terms of the transfer between lattice sites, which are valid for models with large local Coulomb matrix elements. Employing a RPA-like decoupling scheme, susceptibilities of a Stoner form are obtained, in which the local parts and their dynamic interactions are explicitly known.

For the Hubbard model the dynamic charge and spin susceptibility is presented and discussed. In particular the spectra of charge and spin fluctuations are analyzed as well as tendencies towards the formation of a charge or magnetically ordered state for various wave vectors, temperatures, and doping.

TT 16.14 Sa 11:00 Poster TU C

Electronic Phase Separation in $La_{1-x}Sr_xMnO_3$ films, $x \approx 1/8$. — ●PETER WOCHNER¹, U. GEBHARDT¹, A. VIGLIANTE², N. KASPER¹, J. GECK³, H.U. HABERMEIER⁴, and F. RAZAVI⁵ — ¹MPI f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Bruker AXS GmbH, Karlsruhe — ³Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden — ⁴MPI f. Festkörperforschung, Stuttgart — ⁵Brock University, St. Catharines, Ontario, Canada

Recently, it was shown by J. Geck et al. that the low temperature ferromagnetic and insulating phase of bulk $La_{7/8}Sr_{1/8}MnO_3$ can be explained by an ordering of orbitals and holes in form of an orbital polaron lattice. Films of the same material on $SrTiO_3 < 001 >$ oriented substrates show a metal-insulator transition for thicknesses smaller 500 Å. Thicker films are insulators at low temperature. By synchrotron X-ray diffraction we found in these films one of the signatures of the orbital polaron (OP) phase which indicates the presence of half doped charge stripes together with a structural modulation. This OP phase is only short-range ordered and coexists with the antiferro-orbital ordered matrix.

TT 16.15 Sa 11:00 Poster TU C

Anomalous high ordering temperature in $YbRu_2Ge_2$ — ●H. S. JEEVAN¹, Z. HOSSAIN^{1,2}, and C. GEIBEL¹ — ¹MPI-CPFS Nöthnitzer Str. 40, 01187 Dresden, Germany — ²Department 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 $YbRu_2Ge_2$, Yb is in a stable trivalent state and present some kind of ordering at a much higher

temperature $T_M = 10K$ 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 through 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 16.16 Sa 11:00 Poster TU C

Crossover from Single-Ion to Coherent Non-Fermi Liquid Behavior in $Ce_{1-x}La_xNi_9Ge_4$ — ●E.-W. SCHEIDT¹, U. KILLER¹, H. MICHOR², S. KEHREIN³, and W. SCHERER¹ — ¹CPM, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — ²Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria — ³TP III – EKM, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

We report specific heat, susceptibility and resistivity studies on the compound $Ce_{1-x}La_xNi_9Ge_4$ for various concentrations ranging from the stoichiometric system with $x = 0$ to the dilute limit $x = 0.95$ [1]. Our data reveal single-ion scaling with the Ce-concentration and the largest ever recorded value of the electronic specific heat $\Delta c/T \approx 5.5 JK^{-2}mol^{-1}$ at $T = 0.08K$ for the stoichiometric compound at $x = 0$ without any trace of magnetic order. While in the doped samples $\Delta c/T$ and ρ increase logarithmically in the range between 3K and 50mK and between 20K and 5K, respectively, their magnetic susceptibility behaves Fermi liquid like below 1K. $\Delta c/T$ in $CeNi_9Ge_4$ flattens out below 200mK and displays a pronounced maximum in the resistivity curve at 4K indicating a coherent heavy fermion groundstate [2]. These properties render the compound $Ce_{1-x}La_xNi_9Ge_4$ a unique system on the borderline between Fermi liquid and non-Fermi liquid physics. [1] U. Killer, E.-W. Scheidt, G. Eickerling, H. Michor, J. Sereni, Th. Pruschke, S. Kehrein, Phys. Rev. Let. (condmat/0402498), in print. [2] E.-W. Scheidt, U. Killer, H. Michor, E. Bauer, C.Dusec, S. Kehrein and W. Scherer, Physika B, in print.

TT 16.17 Sa 11:00 Poster TU C

Thermal transport properties of $YbRh_2(Si_{1-x}Ge_x)_2$ at low temperatures — ●STEFANIE HARTMANN, ADRIANA SANCHEZ, SILKE PASCHEN, OCTAVIO TROVARELLI, CHRISTOPH GEIBEL, and FRANK STEGLICH — MPI CPFS, Nöthnitzer Str. 40, 01187 Dresden

The heavy-fermion compound $YbRh_2Si_2$ orders antiferromagnetically at $T_N = 70$ mK and reveals non-Fermi liquid behavior in the vicinity of a (magnetic-field induced) quantum critical point [1,2]. Here we present thermal transport properties of pure and 5% Ge-doped samples. The previously reported logarithmic temperature dependence of the electronic specific heat coefficient C_{el}/T between 0.3 and 10 K [2] is reflected in the thermal conductivity over temperature ratio κ/T . The electronic contribution of κ shows deviations from the predictions of the Wiedemann-Franz law based on calculations from resistivity measurements. Thus, the applicability of the WF law seems to be questionable. The logarithmic behavior of $C_{el}(T)/T$ is also observed in the thermopower over temperature ratio $S(T)/T$ as theoretically predicted by Paul et al. [3]. But below 2 K S/T exhibits a stronger than logarithmic divergence ("upturn") with decreasing temperature.

[1] P. Gegenwart et al., PRL 89, 056402 (2002)

[2] J. Custers et al., Nature 424, 524 (2003)

[3] I. Paul and G. Kotliar, PRB 64, 184414 (2001)

TT 16.18 Sa 11:00 Poster TU C

Tetracritical point in $CeCu_2(Si_{1-x}Ge_x)_2$ investigated by neutron diffraction — ●ENRICO FAULHABER¹, OLIVER STOCKERT², BEATRICE GRENIER³, BACHIR OULADDIAF³, MICHA DEPPE², CHRISTOPH GEIBEL², FRANK STEGLICH², and MICHAEL LOEWENHAUPT¹ — ¹Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — ²Max-Planck-Institut für Chem. Physik fester Stoffe, D-01187 Dresden, Germany — ³Institut Laue-Langevin, F-38042 Grenoble, France

The heavy-fermion system $CeCu_2(Si_{1-x}Ge_x)_2$ attracts not only interest close to $x = 0$ with the interplay of antiferromagnetism and superconductivity in pure $CeCu_2Si_2$, but also in the vicinity of $x = 0.25$ where the antiferromagnetic order is suggested to change from a spin-density wave to a more localized type of magnetic order. Moreover, specific heat

as well as thermal expansion measurements indicate the possible existence of a tetracritical point at $x \approx 0.25$. For higher and lower Ge concentrations exists a first order transition below the Néel temperature, whereas for $x = 0.25$ both transitions seem to be degenerate. Furthermore, the anomalies in the thermal expansion have opposite signs below and above $x = 0.25$ suggesting a different magnetic structure. We performed extensive neutron diffraction on $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ single crystals with $x = 0.16$ and 0.45 , i.e. on either site of $x = 0.25$. Both samples show antiferromagnetic order with slightly different propagation vectors followed by a lock-in transition. This suggests a modified nesting of the Fermi surface. The magnetic structure will be discussed in comparison to macroscopic measurements.

TT 16.19 Sa 11:00 Poster TU C

Distribution of the Kondo temperature in strongly coupled two-level systems: an NRG study — ●CHRISTIAN KOLF — kolf@th.physik.uni-bonn.de

Conductance measurements on quantum point contacts show zero-bias anomalies in the differential conductance which are consistent with the presence of two-channel Kondo (2CK) impurities and which are difficult to explain by any other known microscopic mechanism. The 2CK effect has been proposed by degenerate two-level systems. As one of the unresolved problems within the two-channel Kondo scenario, however, the experimental results indicate a very narrow distribution of the Kondo temperature T_K , $P(T_K)$. We argue by general renormalization group arguments that a wide distribution of the Kondo coupling constant J – which is expected for a nanoscopic point contact – leads to a peaked distribution of the resulting T_K , if the distribution of J extends beyond the region $J \ll D$ where D is the characteristic high energy scale, i.e. the band width. We investigate the distribution $P(T_K)$ by means of explicit numerical renormalization group (NRG) calculations.

TT 16.20 Sa 11:00 Poster TU C

Multi-level Kondo effect in single-wall carbon nanotubes (SW-NT) — ●THERESA HECHT, MICHAEL SINDEL und JAN VON DELFT — Department of Physics and Center for NanoScience, LMU München, Theresienstr. 37, 80333 München

Recently Herrero et al. investigated the Kondo effect [1] in SWNTs. In absence of a magnetic field an (approximate) orbital as well as a spin degeneracy is present in those SWNT. Herrero et al. were able to identify two consequences of this degeneracy, namely the so-called SU(4) Kondo effect [2] and a purely orbital Kondo effect [3]. A finite magnetic field was found to remove both spin and orbital degeneracy, reflected by multiple splittings of the Kondo resonance. Moreover, a particular magnetic field might even result in a degeneracy between adjacent orbital levels, giving rise to a purely orbital Kondo effect [3]. In some samples, the Kondo resonance is split even in the complete absence of a magnetic field, suggesting that the orbital states are weakly coupled, lifting their degeneracy.

Motivated by these experiments, we study a two-level Anderson model by means of Wilson's numerical renormalization group method. We investigate both magnetic field and energy dependence of the spectral function and propose a mechanism that leads to the various types of splittings of the Kondo resonance.

[1] P. Jarillo-Herrero et al., submitted to Nature

[2] L. Borda et al., PRL 90, 026602, (2003)

[3] P. Jarillo-Herrero et al., to be published

TT 16.21 Sa 11:00 Poster TU C

Phase Transitions in the Pseudogap Anderson and Kondo models — ●LARS FRITZ, MARIJANA KIRCAN, and MATTHIAS VOJTA — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe

The Pseudogap Kondo problem, describing quantum impurities coupled to fermionic quasiparticles with a pseudogap density of states, $\rho(\omega) \propto |\omega|^r$, shows a rich zero-temperature phase diagram, with different screened and free moment phases and associated transitions. We analyze both the particle-hole symmetric and asymmetric cases using renormalization group techniques. In the vicinity of $r = 0$, which plays the role of a lower critical dimension, an expansion in the Kondo coupling is appropriate. In contrast, $r = 1$ is the upper-critical dimension in the absence of particle-hole symmetry, and here insight can be gained using an expansion in the hybridization strength of the Anderson model. As a by-product, we show that the particle-hole symmetric strong coupling fixed point for $r < 1$ is described by a resonant level model, and corresponds to an intermediate-coupling fixed point in the renormalization

group language. Interestingly, the value $r = \frac{1}{2}$ plays the role of a second lower-critical dimension in the particle-hole symmetric case, and there we can make progress by a novel expansion performed around a resonant level model. The different expansions allow a complete description of all critical fixed points of the models and can be used to compute a variety of properties near criticality, describing universal local-moment fluctuations at these impurity quantum phase transitions.

TT 16.22 Sa 11:00 Poster TU C

Magnetic field dependence of the electronic phase coherence length of diffusive nanowires with magnetic impurities — ●CHRISTIAN SCHIRM¹, ELKE SCHEER¹, CHRISTIAN PASCHKE², CHRISTOPH SÜRGER², and HILBERT v. LÖHNEYSSEN² — ¹Fachbereich Physik, Universität Konstanz, D-78464 Konstanz — ²Physikalisches Institut und DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe

For the study of the electronic phase coherence length l_φ of diffusive metal structures at very low temperatures, Mohanty et al. [1] propose to investigate the conductance fluctuations (CF) at high magnetic fields. The authors claim that the possible presence of small amounts of magnetic impurities should be detectable by analyzing the field dependence of the fluctuations. In [2] the CF of diffusive Cu nanowires, intentionally contaminated with Mn impurities in the ppm range, were investigated. We had observed a complex field and concentration dependence of l_φ . We re-evaluated the data of [2] with a refined numerical treatment. The influence of the signal to noise ratio (SNR) of the conductance measurements on the determination of l_φ is discussed. Although the SNR in [2] is of the same order or better than in [1] we obtain a wide range of possible values for l_φ depending on the treatment of the background and other numerical or physical parameters. Thus, the absence of a magnetic field dependence of l_φ cannot be taken as evidence against the presence of magnetic impurities limiting l_φ for $T \rightarrow 0$.

[1] P. Mohanty et al., Phys. Rev. Lett. 91, 066604 (2003)

[2] H. v. Löhneysen et al., Physica B 284-288, 1858 (2000)

TT 16.23 Sa 11:00 Poster TU C

Self-energy near Pomeranchuk instability — ●LUCA DELL'ANNA and WALTER METZNER — Max Planck Institut fuer FKF, D-70569 Stuttgart

Electron-electron interaction can induce Fermi surface deformations. We study the decay rate behavior for single particle excitations near d-wave Pomeranchuk instability in two dimensions.

TT 16.24 Sa 11:00 Poster TU C

Delocalization of electrons in disordered films induced by parallel magnetic field and film thickness — ●R.K. BROJEN SINGH, V.Z. CEROVSKI, and M. SCHREIBER — Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

We present results of the investigation of delocalization of non-interacting electrons in disordered thin films induced by parallel magnetic field B and film thickness b . We compare two procedures within the framework of self-consistent theory of localization for weak fields generalized to situations lacking time reversal invariance by (a) taking the diffusion constants, D^{pp} and D^{ph} corresponding to particle-particle and particle-hole channels respectively as equal, and (b) taking $D^{pp} \neq D^{ph}$. The two procedures give different results, the main one being that (a) gives the metal-insulator transition (MIT) at $T = 0$ induced by the magnetic field and film thickness, but (b) does not. In the insulating regime we find the localization length as a function of B , b and λ (disorder strength) and calculate critical values of B , b and λ . In the metallic regime we calculate conductivity as a function of these parameters. At $T > 0$ both procedures give an MIT.

TT 16.25 Sa 11:00 Poster TU C

Density of states of the three dimensional Bernoulli-Anderson model — ●P. KARMAN, V. Z. CEROVSKI, and M. SCHREIBER — Institut für Physik, Technische Universität Chemnitz, D-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 of Hamiltonians. In particular, we determine the band structure and the properties of the band tail states and compare the results with the Anderson model of disorder.

TT 16.26 Sa 11:00 Poster TU C

Metal-insulator transition in quasi-2D systems — ●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 conductivity in quasi two-dimensional systems is calculated using the quantum kinetic equation. 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 16.27 Sa 11:00 Poster TU C

Optical studies of the bandwidth controlled Mott-Hubbard transition in 2-dim organic charge transfer salts. — ●DANIEL FALTERMEIER, MICHAEL DUMM, and MARTIN DRESSSEL — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The quasi two-dimensional organic charge-transfer salts κ -(BEDT-TTF)₂Cu[N(CN)₂Br_xCl_{1-x}] have attracted lots of interest because of their unique physical properties: by applying moderate external pressure or by alloying with Br or Cl the ground state can be switched between an antiferromagnetic insulating and superconducting state. In contrast to the high-T_c cuprates the Mott-Hubbard-transition is achieved by bandwidth control and not by hole doping. We present polarization dependent reflection data of the κ -(BEDT-TTF)₂ salts in a spectral range from 50 to 8000 cm⁻¹ with different concentration x of Br and in a temperature range from 5 to 300 K. Starting from the pure Cl component, with increasing Br concentration and decreasing the temperature, the material becomes continuously more and more metallic, what is characterized by a strong Drude tail at low frequencies. Furthermore, we present detailed analysis of the optical conductivity in the vicinity of the insulator-to-metal transition including e.g. the broad absorption hump in the mid-infrared region.

TT 16.28 Sa 11:00 Poster TU C

Metal-insulator transition in the Hubbard Model at finite doping and temperature — ●ROLF HELMES, ACHIM ROSCH, and THEO COSTI — Institut für Theoretische Physik, Universität zu Köln

The dynamical mean field theory in combination with the numerical renormalization group is used to compute the phase diagram of the Hubbard model away from half-filling in the (T,U) plane. We find regions of coexistence of two solutions with the same doping at finite temperature, as for half filling. In addition we find regions of phase-separation. We discuss the effect of particle-hole asymmetry on the phase diagram at half-filling, and the influence of a small doping on the single-particle spectra of a Mott insulator.

TT 16.29 Sa 11:00 Poster TU C

The Role of Power-Law Correlated Disorder in the Anderson Metal-Insulator Transition — ●A. CROY, V. Z. CEROVSKI, and M. SCHREIBER — Institut für Physik, Technische Universität, 09107 Chemnitz, Germany

The effect of long-range correlations of the form $g(r) \propto r^{-\alpha}$ in classical systems, such as site or bond percolation problems, is well understood in terms of the *extended Harris criterion* [1]. It predicts a critical value $\alpha_c = 2/\nu_0$ for the correlation strength, below which the correlations become relevant and the critical exponent changes from ν_0 to $\nu = 2/\alpha$. The question whether this criterion still holds for quantum systems is still under investigation. Recent results for ν in the Anderson model of localization in 3d suggest such a behavior for fixed disorder strength W , but not for a fixed energy $E = 0$ at the band center [2]. We present results of the dependence of ν on α for both fixed W and fixed E , obtained using the finite size scaling of the largest inverse Lyapunov exponent of the transfer matrices of long quasi-1d systems.

[1] A. Weinrib, Phys. Rev. B29, 387 (1984)

[2] M. L. Ndawana, R. A. Römer and M. Schreiber, Europhys. Lett.,

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TT 16.30 Sa 11:00 Poster TU C

Hubbard model in a magnetic field at weak coupling — ●CARSTEN KNECHT and P.G.J. VAN DONGEN — Institut fuer Physik, Universitaet Mainz

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 16.31 Sa 11:00 Poster TU C

Exact diagonalization studies of hole-doped spin rings — ●FATIHA OUCHNI and JÜRGEN SCHNACK — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Motivated by the effect of holes on the electric and magnetic properties of the spin-chain and -ladder compound Sr₁₄Cu₂₄O₄₁, we study the influence of the Coulomb repulsion between different holes on the ring using exact diagonalization of an extended Hubbard model via a Lanczos procedure. The resulting correlation functions depend strongly on the strength and the range of the screened Coulomb potential. It is shown that strong Coulomb repulsion leads to well-localized holes and very likely to a dimerized ground state in the case of 60 % intrinsic hole doping.

TT 16.32 Sa 11:00 Poster TU C

Structural and magnetic investigations on new molecular quantum rings — ●VOLODYMYR PASHCHENKO¹, MICHAEL LANG¹, BERND WOLF¹, LARISA ZHERLITSINA², NORBERT AUNER², OLGA SHCHEGOLIKHINA³, and YULIA POZDNIKOVA³ — ¹Physikalisches Institut, J.W. Goethe-Universität, FOR 412, 60054 Frankfurt(M), Germany — ²Institut für Anorganische Chemie, J.W. Goethe-Universität, 60439 Frankfurt(M), Germany — ³A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS), 28 Vavilov Str., 117813 Moscow, Russia

Three oxygen-bridged polynuclear Cu(II) ($N=6,8,10$) cyclosiloxanolate complexes, [Cu₆(MeSiO₂)₁₂·6DMF], {[Cu₈(MeSiO₂)₁₆·8DMF}·EtOH and {[Cu₁₀(MeSiO₂)₂₀·10DMF}·6DMF, have been synthesized and characterized structurally and magnetically. All three molecule-based complexes exhibit a similar structure consisting of rings of $N=6, 8$ or 10 Cu(II) atoms sandwiched by two N -membered cyclomethylsiloxanolate ligands. Within the rings, adjacent Cu²⁺ ions are linked by pairs of siloxanolate oxygen atoms which provide the magnetic exchange path for the Cu(II) $S=1/2$ spins. A detailed analysis of the magnetic properties reveals a strong ferromagnetic Cu-Cu exchange interaction ($J/k_B=-62$ K) for the $N=6$ compound with an $S=3$ high-spin ground state, a moderately strong ferromagnetic interaction ($J/k_B=-27.6$ K) for $N=8$ and an antiferromagnetic interaction ($J/k_B=+17.2$ K) with a nonmagnetic $S=0$ ground state for $N=10$. These results together with structural investigations enable to correlate structural parameters such as the Cu-O-Cu bridging angle with the sign and strength of the magnetic exchange coupling J .

TT 16.33 Sa 11:00 Poster TU C

Charge Transport Through Quench-Condensed Hydrogen Films — ●JÖRG ANGRİK, PATRICK SCHWINZER, JÜRGEN KLIER, and PAUL LEIDERER — Fachbereich Physik, Universität Konstanz, Postfach M676, D-78457 Konstanz

The self-charging of quench-condensed tritium films prevents their use as a source in the next generation direct neutrino mass experiments. The KATRIN experiment, which is set up at the Forschungszentrum Karlsruhe, is the successor of the Mainz neutrino mass experiment, where such films were used. As the resolution of the KATRIN experiment will be in the sub-eV range, the self-charging effect cannot be tolerated. While the mobility of positive charges (³He⁺, originating from the β -decay) is well understood in terms of a thermal hopping model in a critical electric field ($E_c \approx 62$ MV/cm at 1.9 K), little is known about the transport of negative charges. Hence we place electrons on top of hydrogen films, which then form surface states, and investigate their transport through the films. Hereby hydrogen, and also deuterium, are used to model the tritium films. As the transport is supposed to be strongly dependent on the structure of the, e.g., quench-condensed, films, we focus on prepara-

tion procedures and treatments in order to increase the conductivity of the electrons or discharge of the films.

TT 16.34 Sa 11:00 Poster TU C

Optical studies on the two-leg ladder compounds $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ under pressure — ●S. FRANK¹, R. KLINGELER², B. BÜCHNER², and C. A. KUNTSCHER¹ — ¹Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²Leibniz-Institut für Festkörper- und Werkstofforschung Dresden, PF 27 01 16, 01171 Dresden, Germany

The low-dimensional quantum spin system $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$, composed of planes consisting of edge-sharing CuO_2 chains and planes of two-leg Cu_2O_3 ladders, has been studied extensively because of its interesting electronic and magnetic properties. Its electronic characteristics and the distribution of charges among the various structural entities are influenced by Ca-doping. The most interesting phenomenon in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ is a superconducting phase for high Ca-doping and under high pressure. Pressure-dependent resistivity measurements on $\text{Sr}_{2.5}\text{Ca}_{11.5}\text{Cu}_{24}\text{O}_{41}$ [1] suggest the occurrence of a dimensional crossover from one to two under pressure, and that the superconductivity in this system is essentially a 2D phenomenon.

We carried out polarization-dependent RT reflectivity measurements on $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ single crystals, with $x=4$ and 11.5, as a function of pressure (<20 GPa). The results are discussed in terms of changes in the charge dynamics along and perpendicular to the ladders and a possible pressure-induced dimensional crossover. *Supported by the DFG, Emmy Noether-program.*

[1] T. Nagata *et al.*, Phys. Rev. Lett. **81**, 1090 (1998).

TT 16.35 Sa 11:00 Poster TU C

NMR Untersuchungen der Spindiffusion in den Spinleitern von $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ — ●A. BOSSE¹, M.S. ROSE², L. SHU², D.E. MACLAUGHLIN², R. KLINGELER³, B. BÜCHNER³, F.J. LITTERST¹ und H.-H. KLAUSS¹ — ¹Institut für Metallphysik und Nukleare Festkörperphysik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig — ²Department of Physics, University of California Riverside, CA 92521, USA — ³Institut für Festkörperforschung, IFW Dresden, Helmholtzstr. 20, 01069 Dresden

In dem eindimensionalen $S = \frac{1}{2}$ Quantenspinsystem $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$, das Cu_2O_3 Spinleitern enthält, wurde eine außergewöhnlich hohe thermische Leitfähigkeit entlang der Kettenrichtung beobachtet, die auf Spinanregungen zurückgeführt wird [1]. Wir haben Messungen der longitudinalen NMR-Relaxationsrate an den ⁶³Cu-Kernen der Spinleiter als Funktion der Temperatur und des externen Magnetfelds durchgeführt. Es ergibt sich ein Anstieg der Spindiffusion im Temperaturregime der Spinanregungslücke. Die Ergebnisse werden im Hinblick auf einen Zusammenhang mit der thermischen Leitfähigkeit diskutiert.

[1] C. Hess, H. ElHaes, B. Büchner, U. Ammerahl, M. Hücker, A. Revcolevschi, PRL 93 (2004), 027005

TT 16.36 Sa 11:00 Poster TU C

Heat transport in $S=1/2$ spin ladders and chains — ●C. HESS¹, P. RIBEIRO¹, H. ELHAES², G. ROTH², C. SEKAR¹, G. KRABBES¹, B. BÜCHNER¹, F. HEIDRICH-MEISNER³, W. BREINIG³, M. HÜCKER⁴, U. AMMERHAHL⁴, and A. REVCOLEVSCHI⁴ — ¹IFW Dresden, Germany — ²RWTH Aachen, Germany — ³Institut für Theoretische Physik, TU-Braunschweig, Germany — ⁴Laboratoire de Physico-Chimie des Solides, Université Paris-Sud, France

We present experimental results for the magnon thermal conductivity κ_{mag} of several one-dimensional $S=1/2$ spin systems, like spin ladders and chains. We discuss in detail the different scattering mechanisms of magnons in the spin ladder system $(\text{Sr}, \text{Ca}, \text{La})_{14}\text{Cu}_{24}\text{O}_{41}$, i.e. scattering on static defects, phonons, magnons and holes. We compare these results with the magnetic heat transport in the anisotropic ladder compound CaCu_2O_3 and the spin chain material $(\text{Sr}, \text{Ca})\text{CuO}_2$.

TT 16.37 Sa 11:00 Poster TU C

Triplet excitations of bond-disordered spin-1/2 ladders — ●MARCELO ARLEGO^{1,2}, WOLFRAM BREINIG¹, DANIEL CABRA³, FABIAN HEIDRICH-MEISNER¹, ANDREAS HONECKER¹, and GERARDO ROSSINI^{3,2} — ¹Technische Universität Braunschweig, Institut für Theoretische Physik, Mendelssohnstraße 3, 38106 Braunschweig, Germany — ²Universidad Nacional de La Plata, Departamento de Física, C.C. 67, (1900) La Plata, Argentina — ³Université Louis Pasteur, Laboratoire de Physique Théorique, 3 Rue de l'Université, 67084 Strasbourg Cedex, France

We analyze the effect of weak bond disorder in two-leg spin ladders, focusing on the appearance of bound states in the spin gap. Performing a projection on the single-triplet subspace we analytically derive the position of bound states for single-impurity and small impurity clusters in the strong-coupling limit, i.e., strong dimerization. Both the case of modified exchange couplings on the rungs and on the legs of the ladder are studied. Numerically, we analyze the single-impurity problem in a spin ladder by the Lanczos method to obtain the low-lying excitations. The case of a finite concentration of impurities is treated to leading order in the inter-rung coupling within the single-triplet subspace by numerical impurity averaging of large systems. We compare the spectra obtained numerically with the results of diagrammatic techniques, particularly the coherent-potential approximation (CPA). Since the CPA does not account for the interference of impurities we discuss the contribution of small impurity clusters to the density of states.

TT 16.38 Sa 11:00 Poster TU C

Anisotropic thermal transport in one-dimensional spin systems — ●K. KORDONIS¹, T. LORENZ¹, A. FREIMUTH¹, Y. UEDA², M. ISOBE², A. VASIL'EV³, and S. CHEONG⁴ — ¹II. Phys. Inst., Universität zu Köln — ²Inst. Sol. St. Phys., University of Tokyo — ³Low Temp. Phys. Dep., Moscow State University — ⁴Dep. of Phys. & Astron., Rutgers University

One-dimensional spin systems show unusual and rich physical properties. Of particular interest are the dynamics of magnetic excitations and their coupling to the lattice. A valuable tool for their study is provided by measurements of the thermal conductivity κ . We present measurements of κ of the spin-ladder system $\alpha\text{-NaV}_2\text{O}_5$, of the spin-chain systems $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$, LiV_2O_5 and the Haldane system Y_2BaNiO_5 . A double-peak structure of κ versus T is obtained in both sodium vanadates along and perpendicular to the magnetic directions. The origin of these double peaks is ambiguous yet, but the isotropic behavior of κ concerning different lattice directions is evidence for a phononic thermal conductivity. The minimum of κ can be explained by damping close to the transition temperature. In LiV_2O_5 , κ shows only one low-temperature maximum along and perpendicular to the chains. Accordingly, κ of the vanadates is purely phononic. In contrast, κ of Y_2BaNiO_5 behaves strongly anisotropic; a double-peak of κ versus T is obtained only along the spin chains. This is a clear evidence for an additional magnetic contribution to the thermal conductivity of the Haldane system.

supported by the DFG through SFB 608

TT 16.39 Sa 11:00 Poster TU C

The use of hydroquinone-derived linkers for the design of low-d spin systems: from isolated dimers to Heisenberg chains — ●BERND WOLF¹, ANDREAS BRÜHL¹, JÖRG MAGERKURTH¹, VOLODYMYR PASHCHENKO¹, BERNHARD BREINDEL¹, MICHAEL LANG¹, GÜNTER MARGRAF², HANS-WERNER LERNER², TONIA KRETZ², and MATHIAS WAGNER² — ¹Physikalisches Institut, Universität Frankfurt, 60054 Frankfurt, FOR 412 (Germany) — ²Institut für Anorganische Chemie,

In the course of an interdisciplinary research program to synthesize new classes of molecule-based quantum magnets which enable their fundamental physical properties to be explored systematically upon variations of physical or chemical parameters, we have produced a series of low-dimensional quantum-spin systems. The materials are all based on hydroquinone-derived linkers connecting Cu^{2+} ions carrying a spin of $S = 1/2$. The measurements of magnetic, magnetothermal and magnetoelectric properties cover wide ranges of temperatures $0.06 \text{ K} < T < 320 \text{ K}$ and magnetic fields $B < 50 \text{ T}$. Especially for a 1-D Heisenberg antiferromagnet with a moderate magnetic coupling constant we have been able to perform experiments across the saturation field $g\mu_B B_S = 2|J|$ which marks, at $T = 0$, the endpoint of a quantum-critical line in the B-x plane. It has been found that crossing B_S is accompanied by a distinct magnetocaloric effect. In addition, a pronounced acoustic anomaly has been

observed close to B_S and identified as a generic property of the uniform antiferromagnetic Heisenberg chain with a finite spin-lattice coupling.

TT 16.40 Sa 11:00 Poster TU C

Bosonization of dimerized Hubbard chains — ●CARMEN MOCANU, PETER SCHWAB, MICHAEL DZIERZAWA, and ULRICH ECKERN — Institut für Physik, Universität Augsburg, 86135 Augsburg

The foundations of bosonization were laid more than 50 years ago in a seminal paper by Tomonaga. During the following decades the method has been worked out and successfully applied to one-dimensional electron and spin systems. Despite its long history there are still some subtle points in the bosonization formalism which are not taken into consideration in the majority of the literature. One of these issues is the proper treatment of the so-called Klein factors which have to be introduced in order to preserve the anticommuting property of the fermionic fields during the bosonization procedure.

In our approach we handle the Klein factors in a systematic way, both in the thermodynamic limit and for finite systems, using a variational method which treats the bosonic fields and the Klein factors on equal footing. As prototypical models we consider spinless fermions [1] and dimerized Hubbard chains [2].

[1] C. Mocanu, M. Dzierzawa, P. Schwab and U. Eckern, *J. Phys.: Condens. Matter* **16**, 6445 (2004).

[2] C. Mocanu, M. Dzierzawa, P. Schwab and U. Eckern, accepted for publication in *Physica Status Solidi* (b) (cond-mat/0411315).

TT 16.41 Sa 11:00 Poster TU C

Charge order in organic linear chain compounds investigated by ESR — ●BELAL SALAMEH, MICHAEL DUMM, and MARTIN DRESSEL — 1.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70555 Stuttgart.

We investigated the ferroelectric charge ordered state of the quasi one-dimensional organic charge-transfer salts $(\text{TMTCF})_2X$ ($C=\text{Se}, S$; $X=\text{PF}_6, \text{AsF}_6, \text{SbF}_6, \text{BF}_4$ and SCN) by performing comprehensive ESR experiments in the temperature range from 4 to 300 K. At high temperatures, all investigated compounds show a linear decrease of the linewidth with decreasing temperature. Below $T \approx 200$ K the linewidth starts to decrease more rapidly with lowering the temperature. We will discuss different models for this general behaviour of the ESR linewidth in the organic spin chain compounds investigated. For the sulfur salts the anisotropy and the temperature dependence of the ESR linewidth change below the charge ordering (CO) transition around 100 K. The characteristic changes of the angular dependence of the linewidth well below T_{CO} will be discussed in detail. Our findings in the charge ordered region might be due to the formation of two magnetically inequivalent TMTTF sites below the charge ordering transition temperature.

TT 16.42 Sa 11:00 Poster TU C

Optical spectroscopy of magnetic excitations — ●E. BENCKISER¹, M. GRÜNINGER¹, T. NUNNER², T. KOPP², C. SEKAR³, G. KRABBES³, and A. REVCOLEVSCHI⁴ — ¹II. Physikalisches Institut, Universität zu Köln — ²Experimentalphysik VI, Universität Augsburg — ³IFW Dresden — ⁴Laboratoire de Physico-Chimie de l'Etat Solides, Universite Paris-Sud, France

The magnetic excitations of several low-dimensional spin systems have been studied systematically by means of phonon-assisted infrared absorption. We present the optical conductivity $\sigma(\omega)$ of the 1D $S=1/2$ chain compound SrCuO_2 , of the $S=1/2$ pseudo-ladder compound CaCu_2O_3 and of the 2D system $\text{Ba}_2\text{Cu}_3\text{O}_4\text{Cl}_2$. CaCu_2O_3 has been discussed as a two-leg $S=1/2$ ladder with $J_\perp \ll J_\parallel$. A detailed analysis of the optical conductivity shows that CaCu_2O_3 is rather a 3D system of weakly coupled chains with $J_\parallel \approx 165$ meV, where the two couplings perpendicular to the chains are much weaker but comparable with each other. The compound SrCuO_2 contains antiferromagnetic double-chains with $J \approx 181$ meV, whereas the inter-chain coupling is weak ferromagnetic and frustrated. The 2D Cu_3O_4 layers in $\text{Ba}_2\text{Cu}_3\text{O}_4\text{Cl}_2$ contain a CuO_2 square lattice plus a second Cu square lattice with a much weaker coupling constant J_2 . For $\omega \gg J_2$ the compound represents a clean realization of an undoped CuO_2 layer. We find that the high-energy spectral weight above the 2-magnon peak is larger than assumed previously.

TT 16.43 Sa 11:00 Poster TU C

Interchain Coupling in Mixed-Spin Quantum-Ferrimagnets — ●SIMON GROSSJOHANN, ANDREAS HONECKER, and WOLFRAM BREINIG — Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

We present an analysis of the thermodynamic properties of 1D- and 2D-mixed-spin quantum-magnets. Using the *Stochastic Series Expansion* method for evaluating the partition function we provide results for the uniform susceptibility and the static structure factor. The relevance of the *Random Phase Approximation* to describe interchain-exchange is investigated by extracting effective interchain-coupling-constants from our numerical findings. Furthermore, we provide a finite-size-scaling analysis of the static structure factor for selected system-parameters to address the question of zero temperature long-range magnetic ordering. Finally we comment on the relation of our results to bulk thermodynamic data recently observed in the molecular ferrimagnet $\text{MnNi}(\text{NO}_2)_4(\text{en})_2$.

TT 16.44 Sa 11:00 Poster TU C

Interplay between structure, magnetism and ordering phenomena in $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ — ●M. CWIK¹, M. BENOMAR¹, M. HAIDER¹, T. LORENZ¹, Y. SIDIS², and M. BRADEN¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Laboratoire Léon Brillouin, C.E.A./C.N.R.S., France

La_2CoO_4 is an antiferromagnetic insulator with $T_N \sim 275$ K and Co^{2+} in the $S=3/2$ high-spin state [1]. Doping with Sr induces a $\text{Co}^{2+}/\text{Co}^{3+}$ mixed valency, destroys long-range antiferromagnetic order and removes the concomitant orthorhombic distortion of the K_2NiF_4 structure. In the half-doped compound $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ spin and charge order have been found [2,3]. However, the effective magnetic coupling and the role of the three possible Co^{3+} spin states are not yet clarified. So far, it is also unknown how variations of doping affect both types of order in the $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ series. We present a study of structure, spin order, charge order, magnetic fluctuations, resistivity, and susceptibility on high-quality single crystals for $0.2 \leq x \leq 1.0$. We find a drastic change in the tetragonal CoO_6 -octahedra distortion which is not consistent with a simple ionic picture and incommensurable spin order next to the half-doped compound. An analysis of the magnon dispersion suggests an effective three-dimensional magnetic coupling scheme away from a simple frustrated antiferromagnetic square lattice with competing nearest- and next-nearest-neighbor interaction.

[1] K. Yamada *et al.*, *Phys. Rev. B* **39**, 2236 (1989)

[2] I. A. Zaliznyak *et al.*, *Phys. Rev. Lett.* **85**, 4353 (2000)

[3] I. A. Zaliznyak *et al.*, *Phys. Rev. B* **64**, 195117 (2001)

TT 16.45 Sa 11:00 Poster TU C

Transport and Thermodynamic Properties of RCoO_3 , $\text{R} = \text{La}, \text{Pr}, \text{Nd}$ and Eu — ●M. KRIENER, K. BERGGOLD, J. BAIER, S. JODLAUK, H. KIERSPEL, T. LORENZ, M. REUTHER, C. ZOBEL, and A. FREIMUTH — II. Physikalisches Institut, Universität zu Köln, 50937 Köln

LaCoO_3 is an insulator with unusual magnetic properties. Around 100 K LaCoO_3 shows a temperature-induced spin-state transition from a nonmagnetic low-spin state (electronic configuration of the Co^{3+} -ions: $t_{2g}^6 e_g^0$ with $S=0$) to an intermediate-spin state ($t_{2g}^5 e_g^1$ with $S=1$) [1]. Around 500 K a metal-insulator transition occurs. The spin state of Co^{3+} is determined by the balance of crystal-field splitting and Hund's rule coupling. We have studied the influence of an enhanced crystal field by substituting the La^{3+} ions by smaller isovalent rare-earth ions. Our study of the magnetic susceptibility, the thermal expansion and the electrical resistivity shows that Eu-doping causes a strong shift of the spin-state transition to higher temperatures, whereas the metal-insulator transition temperature increases only moderately [2]. Moreover, at low temperatures the thermal conductivity is strongly suppressed due to the spin-state transition in LaCoO_3 . Replacing La completely by $\text{R} = \text{Pr}, \text{Nd}$ or Eu systematically increases the thermal conductivity with decreasing radius of R , because of the shift of the spin-state transition towards higher temperatures.

[1] C. Zobel *et al.*, *Phys. Rev. B* **66**, 020402(R) (2002)

[2] J. Baier *et al.*, appears in *Phys. Rev. B*, cond-mat 0405680 (2004)

Supported by the DFG through SFB 608.

TT 16.46 Sa 11:00 Poster TU C

The optical properties of charge ordered Fe_3O_4 — ●ALEXANDER YARESKO^{1,2}, IVAN LEONOV^{3,4}, VICTOR ANTONOV², MICHAEL KOROTIN⁴, and VLADIMIR ANISIMOV⁴ — ¹MPI PKS, Noethintzer Str. 38, 01187, Dresden, Germany — ²Institute of Metal Physics, Kiev, Ukraine — ³Theoretical Physics III, Institute for Physics, University of Augsburg, Germany — ⁴Institute of Metal Physics, Russian Academy of Science-Ural Division, Yekaterinburg, Russia

Charge and orbital ordering in the low-temperature monoclinic phase of magnetite (Fe_3O_4) and its optical and magneto-optical properties are investigated using the LSDA and LSDA+ U approaches. It is found that while the difference between t_{2g} minority occupancies of Fe_B^{2+} and Fe_B^{3+} cations is large and gives direct evidence for charge ordering, the screening is so effective that the total $3d$ charge disproportion is rather small. The calculated optical spectra agree well with the experimental ones. A band-by-band decomposition of the calculated optical conductivity allows to relate the experimentally observed peaks to particular interband transitions.

TT 16.47 Sa 11:00 Poster TU C

Electrostatically driven charge ordering in Fe_2OBO_3 — ●I. LEONOV¹, A. N. YARESKO², V. N. ANTONOV³, and V. I. ANISIMOV⁴ — ¹Theoretical Physics III, Institute for Physics, University of Augsburg — ²Max-Planck Institute for the Physics of Complex Systems, Dresden — ³Institute of Metal Physics, Vernadskii Street, 03142 Kiev, Ukraine — ⁴Institute of Metal Physics, Russian Academy of Science-Ural Division, 620219 Yekaterinburg GSP-170, Russia

Charge ordering in the low-temperature monoclinic structure of iron oxoborate (Fe_2OBO_3) is investigated using the local spin density approximation with Coulomb interaction correction (LSDA+ U) method. While the difference between t_{2g} minority occupancies of Fe^{2+} and Fe^{3+} cations is large and gives direct evidence for charge ordering, the screening is so effective that the total $3d$ charge disproportion is rather small. The occupied Fe^{2+} and Fe^{3+} cations are ordered alternately within the chain which is infinite along a -direction, resulting in ferromagnetic intrachain order due to $d^5 - d^6$ superexchange. The charge order obtained by LSDA+ U is consistent with observed enlargement of the β angle.

TT 16.48 Sa 11:00 Poster TU C

High-Energy Scattering Study of Charge and Orbital Order of $\text{Pr}_{0.7}(\text{Ca}_{0.9}\text{Sr}_{0.1})_{0.3}\text{MnO}_3$ under pressure — ●S. KIELE¹, J. GECK¹, M. VON ZIMMERMANN², N. WIZENT¹, B. BÜCHNER¹, and M.M. ABD-ELMEGUID³ — ¹Institut für Festkörperforschung, IFW Dresden, Helmholtzstr. 20, D-01171 Dresden — ²Hamburger Synchrotronstrahlungslabor am DESY, Notkestr. 85, D-22603 Hamburg — ³II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, D-50937 Köln

We present a high-energy scattering study of the superlattice reflections attributed to charge and orbital order in $\text{Pr}_{0.7}(\text{Ca}_{0.9}\text{Sr}_{0.1})_{0.3}\text{MnO}_3$ under hydrostatic pressure. Pure $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ shows an antiferromagnetic insulating ground state with a long-range charge and orbital order. Utilizing pressure it can be driven to a ferromagnetic metallic state, where the long-range charge order is destroyed. The Sr-substituted system can be understood in a phase separation scenario. Due to the different cation sizes, the double-exchange at the Sr-substituted sites changes, leading to the formation of ferromagnetic metallic non-charge ordered regions in the antiferromagnetic insulating charge ordered background. Under external pressure we found a drastic decrease of the onset of the charge/orbital ordering temperature and a thermal hysteresis of the order parameter. The measurements have been done at the HASYLAB beamline BW5 with a three-crystal setting utilizing a new implementation of a clamp-type piston-cylinder cell of a relatively small size and reduced wall thickness in a closed-cycle cryostat on a four-circle diffractometer.

TT 16.49 Sa 11:00 Poster TU C

Low temperature behaviour of Sr and Ca doped manganites — ●E. FORZANI, V. MOSHNYAGA, and K. WINZER — I. Physikalisches Institut Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Perovskite manganites show insulator (I) to metal (M) phase transition, accompanied with a long range ferromagnetic ordering for doping level $x \geq 0.175$. Recently it was argued [1] that electronic phase separation of IM-type can take place due to the competition of double- and superexchange interactions even for chemically homogeneous samples. To check for the possible phase separation and thus recovering of insulating behaviour ($d\rho/dT \leq 0$) at very low temperatures in the metallic sam-

ples, we studied single crystals and epitaxial films of Sr- and Ca-doped manganites. Measurements were carried out in a demagnetization cryostat for temperatures down to 40 mK and magnetic fields $B = 0-7$ T. As starting point, a $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x = 0.2$) single crystal exhibits metallic behaviour of the resistivity $\rho(T)$ for $4.2 \text{ K} \leq T \leq 300 \text{ K}$. The high residual resistivity ratio $\text{RRR} = 58$ and temperature coefficient of resistivity $\text{TCR} = 1/\rho(d\rho/dT) \approx 13\%/K$ by the IM-transition at 305 K confirm the high crystal quality.

Göttingen Graduate School of Physics and DFG (SFB 602, TP A2) are acknowledged.

[1] E.Dagotto, T.Hotta, A.Moreo, Physics Reports 344,1 (2001)

TT 16.50 Sa 11:00 Poster TU C

The electronic structure of $\text{La}_{1-x}\text{Sr}_x\text{TiO}_{3+\delta}$ — ●ALEXANDER GÖSSLING, REINHARD RÜCKAMP, HOLGER ROTH, THOMAS LORENZ, and MARKUS GRÜNINGER — II. Physikalisches Institut, Universität zu Köln

Transition-metal oxides with orbital degeneracy have attracted a lot of interest. Their optical conductivity shows multi-peak structures in the visible and ultraviolet energy range. These excitations have been attributed to interband transitions either into the upper Hubbard band or the charge-transfer band. The spectral weight of the transitions from the lower into the upper Hubbard band sensitively depends on orbital and magnetic correlations. In this way, the physics of high ($\sim \text{eV}$) and low ($\sim \text{meV}$) energies is intimately connected.

In this context we studied the effect of hole doping on the optical conductivity of the Mott-Hubbard insulator LaTiO_3 in the range of 0.7 to 6.4 eV across the metal-insulator transition by means of ellipsometry. Furthermore we compare the spectra with the data of YTiO_3 , having a reduced bandwidth. *Supported by the DFG through SFB 608.*

TT 16.51 Sa 11:00 Poster TU C

Comparison of X-ray absorption spectra of V_2O_3 at the O K edge to full multiple scattering calculations — ●P. PFALZER, J.-P. ÜRBACH, J. MOOSBURGER-WILL, A. NATEPROV, JR., M. KLEMM und S. HORN — Universität Augsburg, Lehrstuhl für Experimentalphysik II, Universitätsstr. 1, 86135 Augsburg

X-ray absorption measurements at the O K edge are compared to full multiple scattering (FMS) calculations for the paramagnetic metallic, paramagnetic insulating and antiferromagnetic insulating phases of V_2O_3 . The description of angular dependencies in experimentally recorded X-ray absorption near edge structure (XANES), even over an extended energy range, is possible with these calculations for the first time. Additionally, comparison of the experimental XANES with the FMS calculations corroborates the findings from EXAFS measurements, that V_2O_3 does not have local structure with trigonal symmetry in the metallic phase at room temperature. The observed large anisotropy of the XANES in the insulating phases is shown to be a direct consequence of the distorted physical structure. The calculations also suggest that the low energy part of the O 1s absorption edge is not rigorously split into a “ t_{2g} ”- and an “ e_g ”-part as suggested from bandstructure calculations.

TT 16.52 Sa 11:00 Poster TU C

Magnetic structure of $\text{DyBaCo}_2\text{O}_{5.5}$ — ●H. LUETKENS¹, H.-H. KLAUSS², A. BOSSE², D. CHEPTIAKOV³, S. STREULE³, E. POM-JAKUSHINA³, A. PODLESNYAK³, K. CONDER³, and P. LEMMENS⁴ — ¹Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut CH-5232 Villigen PSI, Switzerland — ²IMNF, TU Braunschweig, D-38106 Braunschweig, Germany — ³Laboratory for Neutron Scattering ETHZ & PSI, CH-5233 Villigen PSI, Switzerland — ⁴IHO, TU Braunschweig, D-38106 Braunschweig, Germany

The magnetic perovskite $\text{REBaCo}_2\text{O}_{5.5}$ system shows a rich magnetic and electronic phase diagram, with a MI transition at higher temperatures and magnetic ordering just below room temperature. Here, we report on neutron diffraction and muon spin rotation (μSR) measurements on a powder of $\text{DyBaCo}_2\text{O}_{5.5}$. From the neutron diffraction measurements an AFM (G-type) phase below 285 K is indicated by a doubling of the magnetic unit cell along both the crystallographic a and c axis. Further cooling below 260 K leads to a second magnetic phase which can be equally well described by two different spin-state ordered AFM structures. Microscopically, three magnetic transitions at 285 K, 260 K and 162 K have been observed by μSR . The high as well as the low temperature phase both show well defined muon spin precession characteristic for long range magnetic order. In the high temperature regime it was possible to independently measure the magnetic order parameter as well as the

magnetic volume fraction. Additionally, at low temperatures a slowing down of the fluctuating Dy moment is observed by a characteristic peak in the longitudinal relaxation rate.

TT 16.53 Sa 11:00 Poster TU C

A Raman study of the charge-density-wave system $A_{0.3}\text{MoO}_3$ ($A=\text{K,Rb}$) — ●D. M. SAGAR¹, D. FAUSTI¹, P. H. M. VAN LOOSDRECHT¹, S. YUE², C. A. KUNTSCHER², M. DRESSEL², and S. VAN SMAALEN³ — ¹Material Science Center, University of Groningen, 9747 AG Groningen, The Netherlands — ²1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ³Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany

The Peierls instability in (quasi)-one-dimensional metals leads to the formation of a charge-density-wave ground state at reduced temperatures. The fundamental excitations of this state, phasons and amplitudons, are strongly coupled charge-lattice excitations. While the infrared-active pinned phason mode is relatively well studied by various spectroscopic techniques, less is known on the low frequency Raman-active amplitudons. We present results of a Raman study of the well known bronzes $A_{0.3}\text{MoO}_3$ ($A = \text{K,Rb}$), focusing not only on the amplitudon mode but also on the so-called phase phonons in the charge-density-wave state, as well as on the observed pre-transitional Peierls fluctuations in the high temperature phase. *Supported by the NWO, DN-67-310, and DFG, SPP 1073.*

TT 16.54 Sa 11:00 Poster TU C

Doping effects on the electrical properties of blue bronze $\text{K}_{0.3}\text{MoO}_3$ — ●S YUE¹, C. A. KUNTSCHER¹, M. DRESSEL¹, S. VAN SMAALEN², F. RITTER³, and W. ASSMUS³ — ¹1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany — ³Physikalisches Institut, Universität Frankfurt, 60054 Frankfurt, Germany

The temperature dependence of the dc resistivity and the nonlinear transport properties in pure, rubidium-, and tungsten-doped blue bronze $\text{K}_{0.3}\text{MoO}_3$ single crystals are presented. In comparison with the rubidium doping, the tungsten doping has larger effects on the electrical transport properties and the Peierls transition. In particular, the peak in the threshold field for nonlinear transport, observed in the pure and rubidium-doped samples around 100 K, is absent in tungsten-doped $\text{K}_{0.3}\text{MoO}_3$. These results are discussed with respect to the proposed incommensurate-commensurate transition of the charge-density-wave and its interaction with impurities. *Supported by the DFG, SPP 1073.*

TT 16.55 Sa 11:00 Poster TU C

Doping and pressure dependence of the optical properties of quasi-one-dimensional $\text{LaTiO}_{3.4}$ — ●C. A. KUNTSCHER¹, K. THIRUNAVUKKUARASU¹, S. FRANK¹, I. LOA², K. SYASSEN², and F. LICHTENBERG³ — ¹1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — ³Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

The perovskite-related compound $\text{LaTiO}_{3.4}$ shows a quasi-one-dimensional metallic character, which can be explained by its crystal structure consisting of chains of TiO_6 octahedra [1,2]. Based on temperature-dependent optical studies, a conduction mechanism involving polaronic quasiparticles was recently suggested [2]. To clarify the importance of polarons in $\text{LaTiO}_{3.4}$ polarization-dependent infrared reflectivity measurements were carried out as a function of doping and pressure. Besides the conduction mechanism, the issues of pressure-induced dimensional crossover and pressure dependence of phonon modes will be discussed. *Supported by the DFG, Emmy Noether-program.*

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).

[2] C. A. Kuntscher et al., *Phys. Rev. B* **67**, 035105 (2003).

TT 16.56 Sa 11:00 Poster TU C

Electronic and vibrational properties of low-dimensional perovskite-related $(\text{Sr,L a})\text{NbO}_{3.5-x}$ — ●C. A. KUNTSCHER¹, P. HAAS¹, B. GORSHUNOV^{1,2}, M. DRESSEL¹, and F. LICHTENBERG³ — ¹1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²General Physics Institute, Russian Academy of Sciences, Moscow, Russia — ³Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

Polarization-dependent infrared reflectivity measurements on various $(\text{Sr,L a})\text{NbO}_{3.5-x}$ single crystals [1] were carried out as a function of temperature [2]. All compounds have highly anisotropic optical properties; in particular, $\text{SrNbO}_{3.41}$ and $\text{SrNbO}_{3.45}$ show a Drude-like behavior along the chain direction and a semiconducting behavior along the perpendicular direction. In contrast, for $\text{Sr}_{0.8}\text{La}_{0.2}\text{NbO}_{3.50}$ the Drude contribution is very small, and has vanished completely for the ferroelectric insulator $\text{SrNbO}_{3.50}$. With decreasing temperature, for $\text{SrNbO}_{3.41}$ and $\text{SrNbO}_{3.45}$ a suppression of spectral weight is observed in the low-frequency optical conductivity for $\mathbf{E}\parallel a$, with the development of a pronounced peak, which can be interpreted in terms of the opening of an energy gap of only a few meV. The gap opening most probably is due to a Peierls-type instability. In contrast, no energy gap is found for $\text{Sr}_{0.8}\text{La}_{0.2}\text{NbO}_{3.50}$, which can be related to differences in the crystal structure. *Supported by the DFG.*

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).

[2] C. A. Kuntscher et al., to appear in *Phys. Rev. B* (2004).

TT 16.57 Sa 11:00 Poster TU C

Optical and magnetic properties of low-dimensional perovskite-related $(\text{La,C a})\text{TiO}_{3.4\pm\delta}$ — ●K. THIRUNAVUKKUARASU¹, F. LICHTENBERG², and C. A. KUNTSCHER¹ — ¹1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

The perovskite-related titanium oxides $\text{LaTiO}_{3.5-x}$ with $0\leq x\leq 0.5$ show a rich phase diagram, including a Mott-Hubbard insulator with antiferromagnetic ordering ($x=0.5$), metallic phases, semiconductors, and a ferroelectric insulator ($x=0$) [1]. In particular, for $x\approx 0.1$ the dc resistivity is strongly anisotropic, with metal-like values along the a axis. The optical conductivity spectrum contains a Drude component only for the polarization $\mathbf{E}\parallel a$, indicating the quasi-one-dimensional metallic character of $\text{LaTiO}_{3.4}$ [2].

We carried out polarization-dependent infrared reflectivity measurements and magnetic susceptibility measurements on various $(\text{La,C a})\text{TiO}_{3.4\pm\delta}$ single crystals. For all studied crystals the optical conductivity along the chain direction consists of a Drude-like contribution superimposed by phonon modes, and a pronounced band in the midinfrared range centered at $2000\text{-}3000\text{ cm}^{-1}$ ($\approx 250\text{-}370\text{ meV}$). For increasing carrier doping or decreasing temperature a shift of the midinfrared band towards lower frequencies is observed. These findings are discussed in terms of polaronic models.

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).

[2] C. A. Kuntscher et al., *Phys. Rev. B* **67**, 035105 (2003).

TT 16.58 Sa 11:00 Poster TU C

Ab-initio Phonons for the layered compound TiOCl — ●LEONARDO PISANI and MARIA-ROSER VALENTI — Institute for Theoretical Physics, University of Frankfurt, 60054 Frankfurt, Germany

We present first-principles frozen-phonon calculations for the determination of the three Raman-active A_g modes in the spin-1/2 layered TiOCl system within two different well-known approaches: the generalized gradient approximation (GGA) and the so-called LDA+U approximation. We observe that the inclusion of electron correlation in a mean-field level as implemented in the LDA+U leads to a better overall agreement with experimental results. We also discuss the implications of the two approaches on the physics of TiOCl .

TT 16.59 Sa 11:00 Poster TU C

Quantenoszillationsexperimente an $\Theta\text{-(BEDT-TTF)}_2\text{I}_3$ — ●AXEL NOTHARDT¹, EDURART BALTHES¹, BELAL SALAMEH¹, WOLFGANG SCHMIDT¹, DIETER SCHWEITZER¹ und DUNCAN MAUDE² — ¹3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart — ²MPI/CNRS Hochmagnetfeldlabor Grenoble, Avenue des Martyrs 25, B.P. 166, F-38042 Grenoble Cedex 9, Frankreich

Es ist erstmals gelungen durch ausschließliches Verwenden von I_3^{-1} Anionen den organischen Supraleiter $\Theta\text{-(BEDT-TTF)}_2\text{I}_3$ ($\text{BEDT-TTF} = \text{Bisethylendithiotetrathiofulvalen}$) als reine Einkristalle auf elektrochemische Weise zu synthetisieren ($T_C=3.6\text{K}$). Die Fermifläche wurde winkelabhängig mit Quantenoszillationsmessungen, sowohl in Magnetisierung (dHvA) als auch in Leitfähigkeit (SdH), untersucht. Die Wellung der Fermifläche, die wegen der Quasi-Zweidimensionalität des elektronischen Systems nahezu ein Zylinder ist, konnte mit den Schwebungsfrequenzen für das α -Orbit ($F_\alpha=780\text{T}$) und das β -Orbit ($F_\beta=4200\text{T}$) mit $\Delta F_\alpha=6.5\text{T}$ und $\Delta F_\beta=16\text{T}$ bestimmt werden. Die Schwebungsknoten von F_β liegen an denen von Yamaji berechneten Positionen. Die Knoten von F_α liegen hingegen deutlich verschoben zu den erwarteten Positionen. Mit

diesen Knotenverschiebungen, die erstmals an β -(BEDT-TTF)₂IBr₂ und an (BEDT-TTF)₄[Ni(dto)₂] entdeckt wurden, können neueste Theorien bezüglich der Knotenverschiebung verifiziert werden. Die Größe eines weiteren Orbits, das dreidimensional ist, wurde winkelabhängig untersucht, wobei die zugehörigen Oszillationsfrequenzen von $F_\gamma(90^\circ)=1,8T$ bis $F_\gamma(0^\circ)=7,8T$ reichen.

TT 16.60 Sa 11:00 Poster TU C

Untersuchungen von Schwebungsknoten bei Quantenoszillationsmessungen (dHvA und SdH) am (BEDT-TTF)₄[Ni(dto)₂] — ●WOLFGANG SCHMIDT, AXEL NOTHARDT, EDUARD BALTHES und DIETER SCHWEITZER — 3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Mit Quantenoszillationsexperimenten sowohl in Leitfähigkeit (SdH) als auch in Magnetisierung (dHvA) wurde bei der Fermifläche von (BEDT-TTF)₄[Ni(dto)₂] das α -Orbit ($F_\alpha = 634T$) und das β -Orbit ($F_\beta = 4245T$) gefunden. Aufgrund der gewellten Fermifläche sind die Oszillationen mit einer Schwebung überlagert. Yamaji berechnete hierzu die Positionen der Schwebungsknoten. Überraschenderweise weichen die Knotenpositionen bei SdH-Messungen deutlich von diesen Berechnungen ab. Diese Verschiebung wurde in den organischen Metallen (BEDT-TTF)₄[Ni(dto)₂] [1] und β -(BEDT-TTF)₂IBr₂ [2] untersucht, die beide mehrere Schwebungsknoten zeigen. Mehrere Knoten sind nötig, um die Theorie von Yamaji und aktuell diskutierte Theorien über die Ursache der Phasenverschiebung der Schwebung zu verifizieren [3].

Hier werden winkelabhängige Messungen von bis zu vier Schwebungsknoten erörtert und mit den Theorien verglichen.

- [1] M. Schiller et al.: Europhys. Lett. 51, 82 (2000)
- [2] M.V. Kartsovnik et al.: Phys. Rev. Lett. 89, 126802 (2002)
- [3] P.D. Grigoriev: Phys. Rev. B 67, 144401 (2003)

TT 16.61 Sa 11:00 Poster TU C

Electron Spin Resonance and Transport Measurements on the neat Organic Superconductor Θ -(BEDT-TTF)₂I₃ — ●BELAL SALAMEH, AXEL NOTHARDT, ANJA MUCH, and DIETER SCHWEITZER — 3.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

On crystals of the neat organic superconductor Θ -(BEDT-TTF)₂I₃ transport and magnetic properties have been investigated by means of ESR, SQUID and dc measurements. From the dc resistivity and susceptibility measurements this material has a typical metallic behaviour from room temperature down to the superconducting transition temperature ($T_c = 3.6$ K). The room temperature resistivities parallel and perpendicular to the conduction plane are typically 0.04 and 20 Ω -cm respectively. The resistivities decrease about three orders of magnitude at 4.2 K. The ESR linewidth ranges from about 60 to 80 G at room temperature and decreases with decreasing temperature down to about 8 G at 20 K. Below 20 K the linewidth increases again slightly probably due to magnetic interactions. At room temperature our crystals exhibit Dysonian line shape when the microwave magnetic field is applied perpendicular to the conduction plane and a Lorentzian lineshape when the microwave magnetic field is parallel to the conduction plane. The Lorentzian line is gradually converted to a Dysonian shape with decreasing temperature below about 250 K due to a significant decrease in the skin depth.

TT 16.62 Sa 11:00 Poster TU C

Pressure-induced dimensional crossover in the quasi-one-dimensional Mott-Hubbard insulator (TMTTF)₂AsF₆ — ●A. PASHKIN, M. DRESSEL, and C. A. KUNTSCHER — 1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The organic (TMTTF)₂X salts consist of basically uncoupled molecular stacks (half-filled) and are prime examples of one-dimensional Mott-Hubbard insulators. With increasing interchain hopping the systems become more metallic, as can be realized in the metallic TMTSF analogs where the coupling between the chains is enhanced. This dimensional crossover can be best explored experimentally by tuning of the interstack interaction with external pressure. A complete theoretical description is still missing for the case of a strictly one-dimensional half-filled chain when going to a more two-dimensional system.

We have studied the pressure dependence (<10 GPa) of the reflectivity of (TMTTF)₂AsF₆ along the molecular stacking axis a and along the b -direction. The evolution of the reflectivity with increasing pressure demonstrates the gradual onset of a Drude-like conductivity along b' . At high enough pressure (>3 GPa) the infrared response along both directions becomes similar to that of the conducting TMTSF-analogs

in accordance with the generalized temperature-pressure phase diagram. We also discuss the behavior of the phonon modes with change of the pressure.

TT 16.63 Sa 11:00 Poster TU C

Dynamic phonons and charge order in a quarter-filled ladder — ●T. C. LANG, D. R. NEUBER, M. AICHHORN, and H. G. EVERTZ — Institute for Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

We investigate the charge order transition of a quarter-filled extended Hubbard-Holstein ladder at finite temperature as a model for sodium vanadate. Based on the canonical Lang-Firsov transformation of the Hamiltonian, a principle component representation of the phonon degrees of freedom allows us to sample phonon configurations in the framework of determinantal Quantum Monte Carlo much more efficiently than previously possible. The sign problem is moderate in a wide range of model parameters relevant for α' -NaV₂O₅. Experiments and previous calculations imply great relevance of the lattice coupling to the charge order transition. Low frequency lattice vibrations increase the charge order, accompanied by dynamically produced zig-zag lattice distortions. The single-particle spectral function, spin- and charge-spectra of the ladder in the presence/absence of dynamic phonons are obtained.

TT 16.64 Sa 11:00 Poster TU C

Spin gap and charge order in weakly coupled quarter-filled ladders — ●BERNHARD EDEGGER^{1,2}, HANS GERD EVERTZ², and REINHARD M. NOACK³ — ¹Theoretische Physik, Universität des Saarlandes — ²Institut für Theoretische Physik, Technische Universität Graz — ³Fachbereich Physik, Philipps Universität Marburg

We present DMRG (Density Matrix Renormalization Group) calculations in quarter-filled ladders with model parameters relevant for NaV₂O₅. The properties of the low temperature phase are well described by including the coupling of the electrons to static lattice distortions in the extended Hubbard model. Charge order, charge gap and the effective magnetic exchange constant are determined. In addition, we show that a spin gap is induced by super-anti-ferroelectric charge order in weakly coupled quarter-filled ladders.

TT 16.65 Sa 11:00 Poster TU C

Parent Hamiltonian for the SU(3) trimer chain — ●STEPHAN RACHEL, DIRK SCHURICHT, and MARTIN GREITER — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe (TH), Postfach 6980, D-76128 Karlsruhe

In analogy to the Majumdar-Gosh model, which describes a dimerized chain of SU(2) spins, we present a Hamiltonian for an SU(3) spin chain, the ground state of which consists of SU(3) singlets of triples of neighboring spins. This Hamiltonian is local, translationally invariant, and consists only of two-spin interactions. We use the model to show that the fractionally quantized elementary excitations of the SU(3) trimer chain, the colorons, transform under representation $\bar{3}$ under SU(3) transformations if the spins of the original model transform under representation 3. In other words, if a basis for the spins on the chain is spanned by the colors blue, red, and green, a basis for the coloron excitations is given by the complementary colors yellow, cyan, or magenta.

TT 16.66 Sa 11:00 Poster TU C

Microscopic theory of half-metallic double perovskites — ●NILS BLÜMER, CARSTEN KNECHT, KRUNOSLAV POŽGAJČIĆ und P. G. J. VAN DONGEN — Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz

Half-metallic double perovskites such as Sr₂FeReO₆ and Sr₂FeReO₆ are promising materials for spintronic applications. Due to the strong correlations associated with the Fe sites, conventional band structure calculations are not reliable for this class of systems. We review the present status of correlated-electron approaches for double perovskite materials and outline our strategy for microscopic calculations using an improved algorithm for quantum Monte Carlo simulations within the framework of dynamical mean-field theory (DMFT). Prospects for application of the recently developed self-energy functional theory in this context are also discussed. Funded by DFG: FOR 559/1.

TT 16.67 Sa 11:00 Poster TU C

Itinerant electron metamagnetism and weak ferromagnetism in LaCo_9Si_4 and YCo_9Si_4 — ●H. MICHOR¹, S. ÖZCAN¹, M. EL-HAGARY¹, E. BAUER¹, M. REISSNER¹, G. HILSCHER¹, S. KHMELEVSKIY², P. MOHN², P. ROGL³, and H. ROSNER⁴ — ¹Institut für Festkörperphysik, T.U. Wien, A-1040 Wien, Austria — ²Center for Computational Materials Science, T.U. Wien, Austria — ³Institut für Physikalische Chemie, Universität Wien, Austria — ⁴Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

LaCo_9Si_4 is a strongly exchange enhanced Pauli paramagnet with an instability towards weak ferromagnetism, i.e. exhibits itinerant electron metamagnetism at about 3.5 T for $H||c$ and 6 T for $H\perp c$, which is the lowest value ever found for rare earth intermetallic compounds [1]. Despite of the smaller unit cell volume isostructural and isoelectronic YCo_9Si_4 exhibits a weak itinerant ferromagnetic ground state ($T_C \simeq 25$ K) already in zero-field. The ground state properties of La- and YCo_9Si_4 are discussed on basis of magnetisation, specific heat, and resistivity measurements and via ab-initio electronic structure calculations. The band structure calculations result in a ferromagnetic groundstate for both compounds with moments substantially larger than the experimentally observed moments. The origin of these discrepancies is briefly discussed. [1] H. Michor et al., Phys.Rev. B **69** (2004) 081404(R).

TT 16.68 Sa 11:00 Poster TU C

Magnetic Ordering in Trigonal Chain Compounds — ●CHRISTIAN LASCHINGER¹, UDO SCHWINGENSCHLÖGL¹, VOLKER EYERT¹, THILO KOPP¹, RAYMOND FRÉSARD², and ULRICH ECKERN¹ — ¹University of Augsburg — ²Institut des Sciences de la Matière et du Rayonnement, Caen, France

We investigate the microscopic origin of the ferromagnetic and antiferromagnetic spin exchange couplings in the quasi-one-dimensional cobalt compounds Ca_3ABO_6 with $A = \text{Fe, Co}$ and $B = \text{Co, Rh}$. From electronic structure calculations we find A 3d low spin and high spin states alternating along the characteristic chains. In addition strong d-p hybridisation leads to the formation of extended localized magnetic moments centered at the high spin sites. Antiferromagnetic coupling along the chains is induced by a strong metal-metal overlap via the $d_{3z^2-r^2}$ orbitals of the low spin sites. It competes with ferromagnetic exchange, which originates in a cyclic exchange through the ligand atoms.

TT 16.69 Sa 11:00 Poster TU C

Dimerization pattern or two-dimensional spin systems with spin phonon coupling in the adiabatic limit — ●CARSTEN AITS¹, UTE LÖW¹, and ANDREAS KLÜMPER² — ¹Universität zu Köln, Institut für Theoretische Physik, Zùlpicher Str.77, D-50937 Köln — ²Bergische Universität Wuppertal, Theoretische Physik, D-42097 Wuppertal

Little is known about the ground state phase diagram of two-dimensional spin systems with spin phonon coupling. In the adiabatic limit, however, they correspond to spin models with inhomogeneous couplings. In contrast to the one-dimensional case, where the dimerization pattern is unique, it is not clear how the two-dimensional lattice responds to a non-vanishing spin phonon coupling. As far as the $S=1/2$ Heisenberg model is concerned, different choices of inhomogeneous patterns of couplings lead to rather different ground state properties with magnetic energy gain that may or may not compete with the energy loss of the phonon system.

We apply a loop algorithm in continuous Trotter time to clarify which distortion pattern is energetically favored. Our approach is twofold. First, we extrapolate the ground state energies and magnetizations for various patterns of alternating couplings and analyze whether a transition to a gapped state appears. Second, we consider an expansion of the free energy of the distorted models at the point of vanishing distortion. In the adiabatic limit, this corresponds to an analysis of spin layers coupled to three dimensional phonons at finite temperatures. We determine the coefficients of the leading order from the (Euclidean) dynamical dimer correlation functions, which are directly accessible within our method.

TT 16.70 Sa 11:00 Poster TU C

Incommensurate spin dynamics in underdoped cuprate perovskites — ●ALEXEI SHERMAN¹ and MICHAEL SCHREIBER² — ¹Institute of Physics, University of Tartu, Estonia — ²Institut für Physik, Technische Universität Chemnitz

The incommensurate magnetic response observed in normal-state cuprate perovskites is interpreted based on the memory function formalism and the t - J model of Cu-O planes. In agreement with experiment

the calculated dispersion of maxima in the susceptibility has the shape of two parabolas with upward and downward branches which converge at the antiferromagnetic wave vector. The maxima are located at the momenta $(\frac{1}{2}, \frac{1}{2} \pm \delta)$, $(\frac{1}{2} \pm \delta, \frac{1}{2})$ and at $(\frac{1}{2} \pm \delta, \frac{1}{2} \pm \delta)$, $(\frac{1}{2} \pm \delta, \frac{1}{2} \mp \delta)$ in the lower and upper parabolas, respectively. The upper parabola reflects the dispersion of magnetic excitations of the localized Cu spins, while the lower parabola arises due to a dip in the spin-excitation damping at the antiferromagnetic wave vector. For moderate doping this dip stems from the weakness of the interaction between the spin excitations and holes near the hot spots. The frequency dependence of the susceptibility is shown to depend strongly on the hole bandwidth and damping and varies from the shape observed in $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$ to that inherent in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

TT 16.71 Sa 11:00 Poster TU C

Structural properties of RETiO_3 and $\text{Y}_{1-x}\text{Ca}_x\text{TiO}_3$ — ●A. KOMAREK¹, H. ROTH¹, T. LORENZ¹, W.D. STEIN¹, M. CWIK¹, F. BOURÉE², A. FREIMUTH¹, and M. BRADEN¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Laboratoire Léon Brillouin

We have studied the crystal structure of the RETiO_3 by different diffraction techniques as function of temperature. In all compounds we find significant distortions of the TiO_6 -octahedra which lead to a lifting of the t_{2g} -orbital degeneracy. A comparison with literature data on isostructural compounds with a $3d^0$ or a $4d^0$ -configuration shows that such distortions not necessarily are caused by orbital physics. In the RETiO_3 -series, however, the temperature dependence clearly points to a direct coupling. The octahedron distortions depend more sensitively on temperature than the tilt and rotation angles; and, in particular, we find strong anomalies at the Néel-temperatures in all antiferromagnetic RETiO_3 compounds.

Neutron diffraction on a sample of $\text{Y}_{0.62}\text{Ca}_{0.38}\text{TiO}_3$ yields strong evidence for charge ordering, which may be the key element to understand, why Ca-doped YTiO_3 stays non-metallic till rather high doping.

TT 16.72 Sa 11:00 Poster TU C

Orbital excitations in transition-metal compounds — ●R. RÜCKAMP¹, A. GÖSSLING¹, M. GRÜNINGER¹, H. ROTH¹, A. FREIMUTH¹, L. JONGEN², A. MÖLLER², G. MEYER², T.T.M. PALSTRA³, A. NUGROHO³, and S.-W. CHEONG⁴ — ¹II. Physikalisches Institut, Universität zu Köln — ²Institut für Anorganische Chemie, Universität zu Köln — ³Materials Science Centre, University of Groningen — ⁴Department of Physics & Astronomy, Rutgers University, New Jersey

In recent years orbital physics has attracted much interest since novel phenomena - such as an orbital liquid state or new elementary excitations in an orbitally ordered state - have been predicted. In order to observe these phenomena, one has to look for a system in which the orbital (electron-electron) coupling dominates over the coupling to the lattice (Jahn-Teller effect). We have studied orbital excitations in the optical conductivity spectra of several transition-metal compounds such as RTiO_3 , RVO_3 , TiOX or Y_2BaNiO_5 by measuring both transmittance and reflectance of single crystals. The energies of the orbital (d-d) transitions are compared with the results of a point-charge model including the hybridisation with the ligand ions. We find good agreement between experiment and theory, which suggests that the coupling to the lattice is dominant in the studied compounds.

TT 16.73 Sa 11:00 Poster TU C

Structural properties of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ — ●O. SCHUMANN¹, P. STEFFENS¹, R. MÜLLER¹, G. ANDRE², P.G. RADAELLI³, P. ADELMANN⁴, S. NAKATSUJI⁵, Y. MAENO⁵, and M. BRADEN¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Laboratoire Léon Brillouin — ³ISIS Facility, Rutherford Appleton Laboratory — ⁴Forschungszentrum Karlsruhe, IFP — ⁵Department of Physics, Kyoto University

We present our x-ray- and neutron diffraction work on $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ which shows an astonishing rich phase diagram, even though the substitution of Sr^{2+} by Ca^{2+} is an isovalent one [1]. Pure Sr_2RuO_4 ($x=2$) exhibits no structural distortions. Upon Ca-doping a rotation of the RuO_6 -octahedron sets in. This phase transition is strongly discontinuous, although a continuous one is allowed by symmetry. At rather higher Ca-content ($x\sim 0.2$) a metamagnetic transition is observed. The temperature and magnetic field dependence of small structural changes are an indication of an electron transfer between in- and out-of-plane t_{2g} -orbitals. This transfer is driven by a van-Hove singularity in one of the concerned bands [2]. At even higher Ca-content the rotational distortion changes its

stacking sequence. While for $x > 0.2$ the octahedrons in neighboring layers rotate out of phase, for $x < 0.2$ the rotation between neighboring layers is in-phase. This rather subtle change is in coincidence with a change of the ground state properties of the samples (metallic vs. af insulating).

[1] O.Friedt *et al.*, Phys. Rev. B **63** 174432 (2001)

[2] M.Kriener *et al.*, condmat/0408015

TT 16.74 Sa 11:00 Poster TU C

Magnetic Field Dependence of Thermodynamic Properties of $(\text{Ca,Sr})_2\text{RuO}_4$ — ●J. BAIER¹, T. ZABEL¹, M. KRIENER¹, P. STEFFENS¹, O. SCHUMANN¹, O. HEYER¹, T. LORENZ¹, A. FREIMUTH¹, O. FRIEDT¹, M. BRADEN¹, A. REVCOLEVSKI², S. NAKATSUJI³, and Y. MAENO³ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Lab. de Physico-Chimie de l'État Solide, Université Paris-Sud, France — ³Dep. of Physics, Kyoto University, Japan

We present a study of thermal expansion α and specific heat c_p of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ in magnetic fields. This series with the spin-triplet superconductor Sr_2RuO_4 and the antiferromagnetic Mott-insulator Ca_2RuO_4 as end members presents a rich spectrum of structural distortions accompanied by drastic changes of the magnetic and electronic properties [1]. We focus on $0.2 \leq x \leq 0.5$ where the compound is still metallic but close to localization. We find an anisotropic anomalous thermal expansion. The anomaly is suppressed by a magnetic field [2]. Below $T \simeq 20$ K, α , c_p and the magnetization show an anisotropic field dependence. The $x = 0.2$ sample shows a metamagnetic transition (MMT) accompanied by a large magnetostriction. Furthermore, c_p/T shows a non-monotonic field dependence with a maximum at the MMT. For $x = 0.5$, c_p/T reaches an unusually large value in zero field and 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] Friedt *et al.*, Phys.Rev.B **63** (2001)

[2] Kriener *et al.*, cond-mat 0408015, submitted to Phys. Rev. Lett.

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TT 16.75 Sa 11:00 Poster TU C

Low temperature mixed spin state of Co^{3+} in LaCoO_3 evidenced from local lattice distortions — ●V. GNEZDILOV¹, P. LEMMENS^{2,3}, YU.G. PASHKEVICH⁴, K.-Y. CHOI⁵, S. SHIRYAEV⁶, G. BYCHKOV⁶, and S. BARILO⁶ — ¹B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — ²Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — ³MPI-FKF, D-70569 Stuttgart, Germany — ⁴A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — ⁵Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — ⁶Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

Single- and multi-phonon excitations of the single crystalline LaCoO_3 were studied using Raman spectroscopy in the temperature region of 5 K - 300 K. First-order Raman spectra show a larger number of phonon modes than allowed for the rhombohedral (D_{3d}^5) structure. Additional phonon modes are interpreted in terms of activated modes due to local lattice distortions arising from the Jahn-Teller (JT) activity of the intermediate-spin (IS) state of Co^{3+} ions. The temperature dependence of the breathing- and stretching-type phonon modes on cooling suggests the presence of Co^{3+} ions in the intermediate spin state, even at lowest temperatures. The anomalous temperature dependence of the second-order phonon excitations spectra is in accordance with the Franck-Condon mechanism that is characteristic for a JT orbital order.

TT 16.76 Sa 11:00 Poster TU C

Co^{3+} spin state transition detected by phonon Raman scattering in $\text{GdBaCo}_2\text{O}_{5.5}$ — ●YU.G. PASHKEVICH¹, V.P. GNEZDILOV², P. LEMMENS^{3,4}, B. KEIMER⁴, C. AMBROSCH-D RAXL⁵, K.V. LAMONOVA¹, A.A. GUSEV¹, K.-Y. CHOI⁶, S.N. BARILO⁷, S.-V. SHIRYAEV⁷, and G.-L. BYCHKOV⁷ — ¹A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — ²B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — ³Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — ⁴MPI-FKF, D-70569 Stuttgart, Germany — ⁵Inst. für Theoretische Physik, Universität Graz, A-8010 Graz, Austria — ⁶Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — ⁷Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

The change of the spin state of Co^{3+} as function of temperature or pressure is an intriguing feature of cobalt-based perovskite compounds. In the layered cobaltites $\text{RBaCo}_2\text{O}_{5.5}$ this problem is rather compli-

cated due to the octahedral and opened square pyramidal coordinations of Co with oxygen. Raman spectroscopy can provide information about subtle changes in spin state through detecting changes of the phonon spectra, which are sensitive to the O-Co-O bonding length and angles. Raman spectra of single crystal $\text{GdBaCo}_2\text{O}_{5.5}$ were measured in the temperature range 5 - 400 K and remarkable changes of frequencies and intensities were observed. Frequencies and eigenvectors of Raman active phonon modes have been defined using frozen phonon ab initio band structure calculations and structural data at 300 K in Pmmm setting.

TT 16.77 Sa 11:00 Poster TU C

Finite Temperature Properties of the 2D Kondo-Necklace — ●WOLFRAM BRENG — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

We analyze several thermodynamic properties of the two-dimensional $\text{SU}(2)$ Kondo-necklace. Using a quantum Monte-Carlo approach based on the stochastic series expansion method we provide results for the staggered structure factor as well as the uniform and staggered susceptibilities as a function of the temperature and 'Kondo'-exchange in the vicinity of the quantum critical point, which separates long-range antiferromagnetic order from dimerization in this system. We study the local susceptibility at criticality and find evidence for a power-law temperature dependence. Finally we investigate the crossover from classical to renormalized classical behavior via the quantum critical regime. Work supported in part by the DFG through SPP 1073.

TT 16.78 Sa 11:00 Poster TU C

Orbital ordering in manganites in the band approach. — ●DMITRI EFREMOV¹ and DANIL KHOMSKII² — ¹TU Dresden, 01062 Dresden — ²University of Cologne, 50937 Cologne

We consider the orbital ordering in LaMnO_3 and similar systems, proceeding from the band picture. For the realistic magnetic structure of A-type there exist the nesting between two e_g -bands and the nesting inside the bands. We show that the interband nesting is more effective. It results in an orbital ordering - orbital density wave (ODW), the type of which coincides with those existing in LaMnO_3 .

TT 16.79 Sa 11:00 Poster TU C

Single hole dynamics across magnetic order-disorder quantum phase transitions. — ●CHRISTIAN BRÜNGER and FAKHER ASSAAD — Universität Würzburg

We consider a bi-layer Heisenberg model with interplanar (intraplanar) exchange J_{\perp} (J). It is known that as a function of J_{\perp}/J the model shows an order-disorder quantum phase transition. Our aim is to understand the behavior of the single particle spectral function of a doped hole in this magnetic background. In particular, the question of the vanishing of the quasiparticle weight in the vicinity of the quantum phase transition will be addressed. Our calculations are done within a self-consistent Born approximation as well as with the quantum Monte Carlo loop algorithm.

TT 16.80 Sa 11:00 Poster TU C

The Kimball-Overhauser approach to the pair density of the 3D electron gas and Friedel-like phase-shift sum rules — ●PAUL ZIESCHE — Max-Planck-Institut fuer Physik komplexer Systeme, D-01187 Dresden

Kimball-Overhauser geminals follow from a 2-body Schroedinger equation with an appropriately screened Coulomb repulsion. They parametrize the pair density together with geminal occupancies, which follow from the non-idempotent momentum distribution [1]. The neutrality sum rule for the pair density leads to sum rules for the geminal phase shifts, which resemble the Friedel sum rule of solid-state physics [2]. Friedel-like oscillations originate from the singularities of the geminal weight [3]. [1] P. Gori-Giorgi and P. Ziesche, Phys. Rev. B **66**, 235116 (2002) [2] P. Ziesche, Phys. Rev. B **67**, 233102 (2003) [3] P. Ziesche, phys. stat. sol. (b), in press.

TT 16.81 Sa 11:00 Poster TU C

Quasiparticle bands of the ionic Hubbard model — ●TORBEN JABBEN and NORBERT GREWE — Institut für Festkörperphysik, Tu-Darmstadt, D-64289 Darmstadt

The ionic Hubbard model on a simple cubic lattice is investigated using analytical approximations and Wilson's renormalization group for the charge excitation spectrum near the Mott insulating regime. The corresponding partial spectral weights and local densities of states show

characteristic features, which compare well with a hybridized-band picture appropriate for the regime at small U , which at half-filling is known as a band insulator. In particular, a narrow charge gap is obtained at half-filling in the ABR, and the distribution of spectral quasi-particle weight reflects the fundamental hybridization mechanism of the model.

TT 16.82 Sa 11:00 Poster TU C

Checkerboard Order in the projected $SO(5)$ model — ●MARTIN JÖSTINGMEIER¹, STEPHAN HOCHKEPPEL¹, WERNER HANKE¹, and SHOU-CHENG ZANG² — ¹Theoretische Physik, Am Hubland, D-97074 Würzburg, Germany — ²Department of Physics, Stanford University, Stanford, 94305 California

Based on Contractor renormalization group calculations, it was recently proposed [1] to extend the projected $SO(5)$ model by onsite Coulomb repulsions. We study this model, using numerically essentially exact Quantum-Monte Carlo calculations, in order to clarify the ($T = 0$) phase diagram. We find antiferromagnetism, superconductivity as well different types of charge-ordered phases. In particular, we determine the type of the phase transition at a multicritical point, that is a possible candidate for $SO(5)$ symmetry restoration. Motivated by scanning tunneling microscopy experiments on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ and $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ [2,3,4], that observe charge ordering patterns, we also study in detail checkerboard order as function of doping as well as temperature.

[1] H.-D. Chen, S. Capponi, F. Alet, and S.-C. Zhang, Phys. Rev. B (2004).

[2] J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, H. Eisaki, S. Uchida, and J. C. Davis, Science **295**, 466 (2002).

[3] C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B **67**, 014533 (2003).

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TT 16.83 Sa 11:00 Poster TU C

Generalization of Luttinger-Ward Functional and the Extended Variational Cluster Approach — ●NINGHUA TONG¹ and RALF BULLA² — ¹Institute for Theory of Condensed Matter, University of Karlsruhe — ²Theoretical Physics III, Institute for Physics, University of Augsburg

The Luttinger-Ward functional is generalized to a functional of more than one variable. Our generalization is based on the Legendre transformation to the grand potential functional, and therefore does not rely on the perturbative diagram analysis. Combining it with the idea of variational cluster approach (VCA), we obtain an extended VCA theory. In this theory, both non-interacting and interacting part of the reference Hamiltonian can be varied to approach the stationary point of a generalized self-energy functional. In the limit of continuous bath degrees of freedom, it can recover the extended dynamical mean-field theory for non-local density-density interaction as well as the dynamical mean-field theory for correlated hopping. We also propose a VCA realization of the dynamical cluster approximation.

TT 16.84 Sa 11:00 Poster TU C

Dynamical local fields for quasiparticles — ●KLAUS 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 shift and relaxation time. The latter one describes disorder or collisional effects. This parameterization of correlations includes local density functionals as a special case and is therefore applicable for density functional theories. 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. Consequently, solely local density functionals without taking into account effective masses cannot fulfill both sum rules simultaneously with a static local field. The comparison to the Monte-Carlo data seems to support such quasiparticle picture.

[1] K. Morawetz, Phys. Rev. B **66** (2002) 07512

TT 16.85 Sa 11:00 Poster TU C

Time-Dependent Density Functional Theory of Disordered Metals — ●V. G. VALEYEV^{1,2} and O. PANKRATOV¹ — ¹Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany — ²A. I. Alikhanov Institute for Theoretical and Experimental Physics, Bolshaya Chermushkinskaya, 25, 117218 Moscow, Russia

Time-dependent density functional theory for the interacting electron system with disorder is developed using the Keldysh dynamical formulation, [1,2]. Allowing for the averaging of the partition function over the realizations of the disorder potential, this approach circumvents the averaging of the highly non-linear Kohn-Sham equation. Our main result is the novel formulation of TD DFT, where the electron and the current density, as well as the one-particle density of states are determined by the distribution function of the Kohn-Sham particles, naturally emerging from the Keldysh formalism. Introduction of the exchange-correlation potential in fact is an alternative method to solve the appropriate saddle-point equation, which has now a structure of the Vlasov-type kinetic equation for the Kohn-Sham distribution function with the exchange-correlation potential as a self-consistent field. The time-dependent OEP-approximation for the latter is derived, accounting for the diffusive motion of electrons in the system. It describes the low-temperature quantum interference phenomena in a disordered conductor with the long-ranged Coulomb interaction. References: [1] L.V. Keldysh, Zh. Eksp. Theor. Fiz. **47**, 1515 (1964) [Sov. Phys. JETP **20**, 1018 (1965)]. [2] A. Kamenev and A. Andreev, Phys. Rev. B **60**, 2218 (1999).

TT 16.86 Sa 11:00 Poster TU C

Full orbital LDA+DMFT scheme and its application to strongly correlated materials — ●G. KELLER¹, V. I. ANISIMOV², D. E. KONDAKOV², A. V. KOZHEVNIKOV², I. A. NEKRASOV², Z. V. PCHELKINA², I. LEONOV¹, X. REN¹, and D. VOLLHARDT¹ — ¹Theoretische Physik III, Universität Augsburg, 86135 Augsburg — ²Institut für Metallphysik, Ekaterinburg GSP-170, Russland

We discuss a recently developed full orbital LDA+DMFT scheme [1] in Wannier basis. The Hamiltonian \hat{H}^{WF} for the partially filled bands of interest and the Coulomb interaction term between Wannier orbitals are obtained as *ab-initio* input to the correlation problem, which is then solved in DMFT(QMC). The interaction parameters for the DMFT(QMC) computations are calculated by constrained LDA. Subsequently, the self-energy matrix in Wannier basis, $\hat{\Sigma}(\epsilon)$, can be converted back into full-orbital Hilbert space, and thus can be used to calculate the full-orbital interacting Green function $G(r, r', \epsilon)$. The Green function can be also employed for the calculation of spectral, magnetic and electronic properties of the system. The results obtained with this method for SrVO_3 and V_2O_3 are compared with our previous results obtained with the LDA+DMFT with DOS input and with new bulk-sensitive experimental photoemission spectroscopy data [2,3,4].

[1] V.I. Anisimov *et al.*, cond-mat/0407359

[2] A. Sekiyama *et al.*, Phys. Rev. Lett. **93**, 156402 (2004)

[3] S.-K. Mo *et al.*, Phys. Rev. Lett. **90**, 186403 (2003)

[4] G. Keller *et al.*, Phys. Rev. B **70**, 205116 (2004)

TT 16.87 Sa 11:00 Poster TU C

Self-consistent LDA+DMFT investigation of NiO — ●X. REN¹, I. LEONOV¹, V. I. ANISIMOV², I. A. NEKRASOV², G. KELLER¹, and D. VOLLHARDT¹ — ¹Theoretische Physik III, Universität Augsburg, 86135 Augsburg — ²Institut für Metallphysik, Ekaterinburg GSP-170, Russland

A recently proposed self-consistent LDA+DMFT scheme [1] is implemented. In this new scheme the feedback from DMFT to LDA which is absent in the conventional LDA+DMFT scheme, is made possible by employing the basis of Wannier functions (WFs) in the DMFT calculation. This improvement is desirable because the electron density on which the LDA band structure depends may be changed by the correlation effect introduced by DMFT. The electronic spectrum of NiO in the non-magnetic phase is calculated by both the new scheme and the conventional one, and a comparison is made.

TT 16.88 Sa 11:00 Poster TU C

A hydrostatic pressure cell for precise resistivity measurement above 7 GPa at low temperatures in magnetic fields — ●TAKESHI NAKANISHI — Kompetenzgruppe Hohe Drücke, Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden

We report recent developments in a new type of hydrostatic pressure

cell [1] designed to measure the absolute value of the electrical resistivity in magnetic fields at low temperatures. This pressure cell, based on a technique using modified Bridgman anvils with a Teflon capsule that contains a liquid pressure transmitting medium, can generate nearly hydrostatic pressure at least up to $P \simeq 7.1$ GPa. The performance of this pressure cell was demonstrated by the electrical resistivity measurement on a single crystal of heavy fermion superconductor $\text{CeCu}_2(\text{Si}_{0.9}\text{Ge}_{0.1})_2$ at low temperatures down to $T = 50$ mK [2]. Pressure is controlled with high accuracy ($0 \leq P \leq 7$ GPa). Very recently, we have succeeded in generating a hydrostatic pressure of 7.7 GPa when a load of 74 kN ($\simeq 7.5$ ton) was applied. This implies a possibility that one can generate hydrostatic pressures above 10 GPa in the more compact size of this pressure cell. We present a modified design of the present pressure cell, which can be fitted to a commercial PPMS (Physical Property Measurement System, Quantum Design). [1] T. Nakanishi, N. Takeshita and N. Mōri, *Rev. Sci. Instrum.* **73**, 1828 (2002). [2] T. Nakanishi, G. Sparr, H.S. Jeevan, M. Deppe, C. Geibel and F. Steglich, to be published in *Proceedings of the International Conference on Strongly Correlated Electron Systems*, Karlsruhe, Germany, July 26-30, 2004.

TT 16.89 Sa 11:00 Poster TU C

Resonant soft x-ray diffraction to study electronic order — ●C. SCHÜSSLER-LANGEHEINE¹, J. SCHLAPPA¹, A. TANAKA², C.-F. CHANG¹, Z. HU¹, M. BENOMAR¹, H. OTT¹, E. SCHIERLE³, E. WESCHKE³, G. KAINDL³, M. BRADEN¹, and L. H. TJENG¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²ADSM, Hiroshima University, Japan — ³Institut für Experimentalphysik, Freie Universität Berlin

Resonant diffraction in the soft x-ray range (RSXS) is a new tool, which is particularly suited to study superstructures formed by modulations of the electronic state, like differences in the valence or in the orbital occupation. Such kind of order can be found in various correlated-electron systems. RSXS as a combination of spectroscopy and diffraction is based on the strong sensitivity of resonances in the soft x-ray range, namely the transition-metal $2p \rightarrow 3d$, oxygen $1s \rightarrow 2p$ and lanthanide $3d \rightarrow 4f$ excitations, on details of the electronic state. This sensitivity leads to different scattering cross sections for sites with different electronic configurations and creates a photon-energy dependent contrast for the diffraction process. Already on a qualitative level by comparison between the x-ray absorption spectrum and the energy dependence of the diffracted intensity, signatures of electronic order can be detected. Furthermore, since resonances in the soft x-ray range are well understood, a detailed microscopic modeling of the resonant diffraction is feasible, providing direct spectroscopic information about the ordered part of the system.

TT 16.90 Sa 11:00 Poster TU C

Status of the WERA Soft X-Ray Beamline at ANKA — ●ERIC PELLEGRIN, PETER NAGEL, BERND SCHEERER, and STEFAN SCHUPPLER — Forschungszentrum Karlsruhe, IFP, Postfach 3640, 76021 Karlsruhe, Germany

After its commissioning in early 2005, the WERA beamline at the 2.5 GeV ANKA synchrotron radiation facility within the Forschungszentrum Karlsruhe is to be used for classical as well as for advanced electron spectroscopy in the photon energy range between 80 and 1400 eV (with a later extension down to about 15 eV photon energy). The main objective of WERA is to provide the user with most of the presently available electron spectroscopy tools in situ in order to allow a complete characterization of the electronic as well as the magnetic structure of the sample under investigation. Thus, versatility (instead of specialization) is the primary goal for WERA.

The following experimental stations will be available (incl. an in situ

sample transfer between the individual experimental setups) together with the corresponding sample preparation chambers:

- photoemission electron microscopy
 - photoemission spectroscopy, resonant photoemission spectroscopy, near-edge x-ray absorption spectroscopy
 - soft x-ray magnetic circular dichroism (planned)
 - pulsed laser deposition of epitaxial thin film samples
- The technical specifications, the status and the future developments of the WERA soft x-ray beamline project will be presented.

TT 16.91 Sa 11:00 Poster TU C

Struktur- und thermisches Rauschen von optischen Komponenten für Gravitationswellendetektoren — ●ANJA ZIMMER, RONNY NAWRODT, SANDOR NIETZSCHE, RALF NEUBERT, MATTHIAS THUERK, WOLFGANG VODEL und PAUL SEIDEL — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena

Zur direkten Messung der von Einstein vorausgesagten Gravitationswellen mittels interferometrischer Gravitationswellendetektoren ist es erforderlich, das thermische Rauschen optischer Komponenten wie Endspiegel und Strahlteiler zu senken. Wurden die Interferometer bisher bei Raumtemperatur betrieben, so könnte die Anwendung von Kryotechniken entscheidende Fortschritte bringen und somit die "Gravitationswellenastronomie" ermöglichen.

Die Arbeiten im Teilprojekt des gleichnamigen von der DFG geförderten Sonderforschungsbereiches TR7 zielen insbesondere auf die experimentelle Untersuchung der in den optischen Komponenten zu Dämpfungsverlusten (und damit zu thermischem Rauschen) führenden Prozesse. Eine entscheidende Rolle dabei spielt die numerische Simulation der Struktur- und thermischen Rauschen optischer Komponenten, mit deren Hilfe sich das Schwingungsverhalten der Testkörper hinsichtlich Substratmaterial, Beschichtung und Strukturierung optimieren lässt. Neben den aktuellen Ergebnissen dieser FEM-basierten Simulationen werden wesentliche kryotechnische Aspekte eines speziellen Messaufbaus zur experimentellen Bestimmung der mechanischen Güte von optischen Komponenten im Temperaturbereich von 300 K bis zu 5 K diskutiert.

TT 16.92 Sa 11:00 Poster TU C

Neuartige Blei-Regeneratormaterialien für Kleinkältemaschinen im Temperaturbereich unterhalb 60 K — ●TORSTEN KOETTIG, STEFAN MOLDENHAUER, MATTHIAS THUERK und PAUL SEIDEL — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

Traditionelle Regeneratormaterialien wie Edelstahl- und Bronzedrahtsieb- und -gewebe erreichen in ein- und zweistufigen Kleinkältemaschinen unterhalb von 30 K ihre Leistungsgrenze. Wegen seiner höheren Wärmekapazität wird in diesem Temperaturbereich Blei eingesetzt. Die bisher übliche Kugelform des Regeneratormaterials begrenzt Regeneratorkenngrößen wie Porosität und Druckverlust auf thermodynamisch nicht optimale Bereiche. Die notwendige Fixierung des Bleipulvers im Festbett erfordert zusätzlichen technologischen Aufwand. Es ist gelungen ein Bleisieb- und -gewebe mit variablen Dimensionen herzustellen. Dadurch können auch Bleiregeneratoren hinsichtlich ihrer inneren Parameter wie mesh-Zahl, Drahtdurchmesser oder Oberflächenrauigkeit thermodynamisch optimiert werden. Die Möglichkeiten zur Verbesserung der Regeneratoreigenschaften des Bleidrahtgewebes gegenüber traditionellen Bleipulverregeneratoren werden diskutiert. Das Leistungspotenzial des Materials wird am Beispiel eines einstufigen Pulsationsröhrenkühlers demonstriert. Insbesondere erreicht dieser stark verbesserte Kälteleistungen unterhalb von 30 K ohne die üblichen Leistungsverminderungen bei höheren Kühltemperaturen über 60 K aufzuweisen.

TT 17 Symposium Quantum Magnetism in Molecule-based Materials

Zeit: Montag 10:15–13:00

Raum: TU H104

Hauptvortrag

TT 17.1 Mo 10:15 TU H104

From Spin to Quantum Order in Coordination Polymer Magnets — ●COLLIN BROHOLM — Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Coordination polymer magnets feature transition metals such as Cu and Ni on a range of different lattices and offer opportunities for exploring qualitatively different cooperative phases of quantum many

body systems. This talk will present an overview of neutron scattering experiments that have been performed to understand spin dynamics in systems ranging from spin-chains (copper pyrazine dinitrate, $\text{CuCl}_2 \cdot 2\text{dimethylsulfoxide}$, NENP, and NDMAP) through a spin-ladder ($\text{Cu}(\text{Quinoxaline})\text{Br}_2$) to frustrated two and three dimensional systems (PHCC and CuHpCl). While the isolated spin-1/2 chain systems are quantum critical and can develop spin order due to weak inter-chain in-

interactions at sufficiently low temperatures, cooperative singlet ground states are in fact more common in these low symmetry antiferromagnetic spin systems. The qualitatively different excitations spectra of gapless and gap-full systems will be described as well as their different responses to applied magnetic fields.

Hauptvortrag

TT 17.2 Mo 10:50 TU H104

Design, Synthesis and Study of Model Quantum Magnets — ●ANDREW HARRISON — School of Chemistry, The University of Edinburgh, Edinburgh, EH9 3JJ, UK

A major constraint on experimental studies of model magnets is the availability of suitable samples that provide tangible models to inspire or test theory. Some degree of rationalisation or even control may be introduced to synthetic strategies through consideration of bonding models: close-packing of spheres may be used to rationalise structures of ionic systems, while the linking of co-ordination polyhedra or vertices with a particular point group has some predictive power for systems where covalent bonding is prevalent. These strategies will be illustrated through the consideration of model frustrated systems such as triangular and kagome lattices, and specific examples will be given of model systems with $S = \frac{1}{2}$ on such lattices, one of which shows evidence for a quantum ground state. We will also consider the possibility of tuning systems strongly through accessible magnetic fields and diamagnetic doping to access quantum phases. What is required here are low-spin, low-dimensional (and perhaps also frustrated) antiferromagnets with relatively weak magnetic exchange and diamagnetic analogues that either isostructural, or close to being so. Examples of copper salts that act as model $S = \frac{1}{2}$ square Heisenberg antiferromagnets are presented

Fachvortrag

TT 17.3 Mo 11:30 TU H104

Molecular solids - model systems for exploring quantum magnetism in reduced dimensions — ●MICHAEL LANG¹, BERNHARD BRENDL¹, ANDREAS BRÜHL¹, JÖRG MAGERKURTH¹, VOLODYMYR PASHCHENKO¹, BERND WOLF¹, LARISA ZHERLITSINA², NORBERT AUNER², GÜNTER MARGRAF², HANS LERNER², and MATTHIAS WAGNER² — ¹Physikalisches Institut, J.W. Goethe-Universität Frankfurt, FOR 412, 60054 Frankfurt — ²Institut für Anorganische Chemie, J.W. Goethe-Universität, Frankfurt, FOR 412, 60439 Frankfurt

By combining open-shell transition metal ions with suitable organic linkers flexible building block systems may be produced for generating novel classes of materials, especially quantum magnets with distinct exchange-coupling topologies. A particularly interesting feature of these molecule-based magnets is their small exchange coupling constants J , weak enough for laboratory magnets to drive the systems into the interesting high-field regime where $g\mu_B B > J$. In this contribution we will discuss various realizations of molecule-based low-dimensional quantum magnets such as Cu(II) cyclosiloxanolate complexes or a Cu(II) coordination polymer. The latter system can be used to study generic magnetocaloric and magnetoelastic properties of the antiferromagnetic $S = 1/2$ Heisenberg chain near the saturation field.

Fachvortrag

TT 17.4 Mo 12:00 TU H104

Magnetocaloric effect in frustrated and molecular magnets — ●ANDREAS HONECKER — Technische Universität Braunschweig, Institut für Theoretische Physik, 38106 Braunschweig, Germany

Due to the magnetocaloric effect, adiabatic changes of the field applied

to a magnet yield a change of temperature. Adiabatic demagnetization of a paramagnetic salt was the first method to achieve temperatures below 1K. Recently, there has been renewed interest in cooling by adiabatic demagnetization for room-temperature applications. Also low-temperature records are still established by this method.

We discuss recent theoretical results for the magnetocaloric effect in the vicinity of field-induced quantum phase transitions in correlated and molecular magnets. Geometrically frustrated magnets are of special interest since they exhibit large entropies at low temperatures, promising a large magnetocaloric effect. In particular a comparative study of different one-dimensional quantum magnets shows that lower temperatures can indeed be achieved by adiabatic (de)magnetization of a frustrated system as compared to a non-frustrated one. Finally, we discuss potential applications of frustrated quantum magnets for efficient low-temperature magnetic refrigeration.

TT 17.5 Mo 12:30 TU H104

Quantum sine-Gordon behaviour in copper pyrimidine dinitrate — ●R. FEYERHERM¹, S. A. ZVYAGIN², and A. U. B. WOLTER³ — ¹Hahn-Meitner-Institut, 14109 Berlin, Germany — ²NHFL, Florida State University, Tallahassee, FL 32310, U.S.A. — ³IMNF, TU Braunschweig, 38106 Braunschweig, Germany

Copper pyrimidine dinitrate has been recently identified as $S = 1/2$ antiferromagnetic chain with a field-induced spin gap [1], and turned out to be one of the best realizations of the quantum sine-Gordon spin chain model known to date. The field-induced gap arises from a perturbation from the isotropic Heisenberg chain by an alternating g -tensor and the Dzyaloshinskii-Moriya (DM) interaction. Other consequences of this perturbation are an intrinsic Curie-like contribution to the magnetic susceptibility [1], a large field-induced staggered magnetization perpendicular to the applied field [2], and a T^{-2} contribution to the ESR-linewidth [3]. Most interestingly, in recent high-field submillimeter wave ESR studies of the gapped state signatures of three breather branches and a soliton, besides several multi-particle excitations, have been identified and allowed for a detailed comparison with predictions from the quantum-sine Gordon field theory [4].

[1] R. Feyerherm *et al.*, J. Phys.: Condens. Matter. 39 (2000) 8495

[2] A.U.B. Wolter *et al.*, Phys. Rev. B 68 (2003) 220406(R)

[3] T. Asaono *et al.*, Physica B 329-333 (2003) 1006

[4] S. A. Zvyagin *et al.*, Phys. Rev. Lett. 93 (2004) 027201

TT 17.6 Mo 12:45 TU H104

Magnetic properties of a molecular based antiferromagnet on a honeycomb lattice — ●IVAN SPREMO and PETER KOPIETZ — Institut für Theoretische Physik, Universität Frankfurt, Robert-Mayer-Str. 8, 60054 Frankfurt am Main

Using a modified spin-wave approach and exact diagonalizations we have calculated the finite-temperature magnetization curve $M(H)$ of a two-dimensional quantum Heisenberg antiferromagnet on a honeycomb-lattice in a uniform magnetic field H . Our theoretical curve for $M(H)$ agrees reasonably well with recent experimental data obtained for a molecular based antiferromagnet with stoichiometric formula $C_{22}H_{18}MnO_8$. We also discuss the nature of the spin-excitations of quantum antiferromagnets in a uniform magnetic field at zero temperature. We show that below three dimensions the coupling between transverse and longitudinal spin fluctuations leads to a breakdown of the quasi-particle concept for magnons.

TT 18 Superconductivity - Properties, Electronic Structure, Order Parameter II

Zeit: Montag 10:00–13:00

Raum: TU H2053

Hauptvortrag

TT 18.1 Mo 10:00 TU H2053

Two-Gap Superconductivity in MgB₂ — ●THOMAS DAHM — Universität Tübingen, Institut für Theoretische Physik

It is by now generally accepted that the recently discovered superconductor MgB₂ is a superconductor with two energy gaps. In this talk we discuss how this happens and address some of its unusual implications. Measurements of the microwave conductivity on MgB₂ thin films have shown an anomalous coherence peak appearing at significantly lower temperatures than in conventional superconductors [1] and the anisotropy ratio of the upper critical field in MgB₂ single crystals shows an unusual strong temperature dependence. We argue that both of these observations are natural consequences of the existence of the two gaps, if the

special Fermi surface structure of MgB₂ is taken into account [1,2]. We also examine consequences for the expected intrinsic nonlinear microwave response in MgB₂ [3].

[1] B.B.Jin, T.Dahm *et al.*, Phys. Rev. Lett. **91**, 127006 (2003).

[2] T.Dahm and N.Schopohl, Phys. Rev. Lett. **91**, 017001 (2003).

[3] T.Dahm and D.J.Scalapino, Appl. Phys. Lett. **85**, 4436 (2004).

TT 18.2 Mo 10:30 TU H2053

Interband Pairing Interaction in the Two-Band Superconductor MgB₂ Observed by Tunneling — ●J. GEERK¹, R. SCHNEIDER¹, G. LINKER¹, A. ZAITSEV¹, R. HEID¹, K.-P. BOHNEN¹, and H. V. LÖHNEYSEN^{1,2} — ¹Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe — ²Physikalisches Institut, Universität Karlsruhe

The anisotropic superconductor MgB₂ was studied by tunneling spectroscopy of tunnel junctions of the sandwich type prepared on as deposited thin films with T_c values near 32 K. The tunnel junctions revealed an energy gap between 2.5 and 3 meV and phonon induced structures in the tunnelling density of states. The inversion of the tunnel data using the standard single-band Eliashberg equations yielded a so-called effective Eliashberg function with three distinct peaks at 38,58 and 85 meV which is compared to a theoretical calculated counterpart obtained by inversion of superconducting density of states data from two-band Eliashberg equations where electron-phonon spectral functions extracted from ab-initio LDA calculations were inserted. Convincing agreement is found between the experimental and calculated effective Eliashberg functions. Further evaluation reveals that the central peak a 58 meV mainly reflects the shape of the π - σ interband pairing interaction which appears in the gap function of the π -sheet in an amplified way due to the large gap of the σ -sheet. It is concluded that the superconductivity on the π -sheet is essentially generated by interband electron-phonon coupling.

TT 18.3 Mo 10:45 TU H2053

Mixing between ballistic and diffusive motion in superconducting MgB₂ — ●MATTHIAS ESCHRIC¹, KAORI TANAKA^{2,3}, DANIEL AGTERBERG⁴, and JUHA KOPU⁵ — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, SK, Canada S7N 5E2 — ³Argonne National Laboratory, Argonne, IL 60439, U.S.A. — ⁴Department of Physics, University of Wisconsin-Milwaukee, P.O. Box 413, Milwaukee, WI 53211, U.S.A — ⁵Low Temperature Laboratory, Helsinki University of Technology, PO Box 2200, FIN-02015 HUT

We introduce a model for the two-band superconductor MgB₂ in which the motion of quasiparticles is diffuse in one band (the π -band) and ballistic in the other band (the σ -band). Diffusive and ballistic quasiparticles are coupled by the pairing interaction. We apply this model to examine the electronic structure of vortex cores in MgB₂. In particular, we study the effects of impurities on the ballistic motion of quasiparticles in the σ -band in the vortex core region under the presence of the hybridization with the diffusive π -band. We find that the induced superconductivity in the π band results in a core size larger than estimated by H_{C2} and in weakly bound states, and that those bound states are removed easily by impurities.

TT 18.4 Mo 11:00 TU H2053

Band filling and interband scattering effects in MgB₂: C vs Al doping — ●JENS KORTUS¹, O.V. DOLGOV², R.K. KREMER², and A.A. GOLUBOV³ — ¹Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, F-67034 Strasbourg Cedex 2, France — ²MPI-FKF, Heisenbergstr. 1, 70569 Stuttgart — ³MESA+ Research Institute and Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands

We argue, based on band structure calculations and Eliashberg theory, that the observed decrease of T_c of Al and C doped MgB₂ samples can be understood mainly in terms of a band filling effect due to the electron doping by Al and C. A simple scaling of the electron-phonon coupling constant λ by the variation of the density of states as function of electron doping is sufficient to capture the experimentally observed behavior. Further, we also explain the long standing open question of the experimental observation of a nearly constant π gap as function of doping by a compensation of the effect of band filling and interband scattering. Both effects together generate a nearly constant π gap and shift the merging point of both gaps to higher doping concentrations, resolving the discrepancy between experiment and theoretical predictions based on interband scattering only.

TT 18.5 Mo 11:15 TU H2053

Density functional theory for superconductors: Applications to MgB₂ and solids under pressure — ●ANDREA FLORIS¹, CESARE FRANCHINI², NEKTARIOS LATHIOTAKIS¹, GIANNI PROFETA³, SANDRO MASSIDDA², and E. K. U. GROSS¹ — ¹Institut für Theoretische Physik, Freie Universität Berlin, Germany — ²INFN SLACS, Sardinian Laboratory for Computational Materials Science and Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari, Italy — ³C. A. S. T. I. - Istituto Nazionale Fisica della Materia (INFN) and Dipartimento di Fisica, Università degli studi dell' Aquila, Italy

Understanding and predicting the properties of superconductors is of both fundamental and technological importance. The discovery of superconductivity in MgB₂, of its rather high critical temperature (T_c = 39.5K), and the appearance of multiple gaps, has renewed the interest in conventional superconductivity. Here we present several applications of a novel approach to superconductivity that allows one to calculate material-specific properties, such as the gap and the T_c, in a truly ab-initio fashion without using any adjustable parameters. Within this approach, we obtained the T_c and the two gaps of MgB₂ in good agreement with experiment, taking into account the strong anisotropy of both the electron-phonon and the Coulomb interactions. As a further application, we studied the behaviour of T_c in Li and Al as a function of pressure. Despite their common simple metal structure, these materials show different behaviour upon pressure. While Li undergoes several transitions favouring superconductivity, in Al the electron-phonon coupling decreases with pressure leading to a complete suppression of T_c around 8GPa.

TT 18.6 Mo 11:30 TU H2053

Multi-band influence on superconductivity in HoNi₂B₂C — ●A. WÄLTE¹, G. FUCHS¹, YU.G. NAIDYUK², K. NENKOV¹, S.-L. DRECHSLER¹, D. SOUPEL¹, H. ROSNER³, J. FREUDENBERGER¹, K.-H. MÜLLER¹, G. BEHR¹, and L. SCHULTZ¹ — ¹Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstr. 20, D-01171 Dresden — ²B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Lenin Ave., 61103 Kharkiv, Ukraine — ³MPI CPFS Dresden, Nöthnitzer Str. 40, D-01187 Dresden

Rare-earth nickel borocarbides RNi₂B₂C reveal, depending on the rare-earth R, superconductivity, magnetism or even a mixture of these competing phenomena [1]. The reduction of the superconducting ordering temperature T_c by magnetic pair-breaking fairly follows the Abrikosov-Gorkov model. However, details of the influence of magnetism on the electron system are not yet well understood. From specific heat measurements and point-contact spectroscopy on HoNi₂B₂C the phonon density of states F(ω) and the spectral function $\alpha^2F(\omega)$ have been extracted. The characteristic phonon frequency $\omega_{in} \approx 180$ K is similar to ω_{in} of non-magnetic LuNi₂B₂C. Comparing the specific heat jumps of both compounds, an unexpectedly strong deviation from the Abrikosov-Gorkov expectation for HoNi₂B₂C is found. A possible explanation is the different influence of pair-breaking on different electron bands.

[1] R.J. Cava et al., Nature 367, January 1994.

TT 18.7 Mo 11:45 TU H2053

Are intercalated metallochloronitrides electron-phonon mediated superconductors? — ●ROLF HEID and KLAUS-PETER BOHNEN — Institut für Festkörperphysik, Forschungszentrum Karlsruhe

The layered metallochloronitrides XNCl, X=Zr,Hf, have surprised with rather high superconducting transition temperatures of up to 25.5 K after intercalation with Li or Na [1], raising the question to what extent the conventional electron-phonon coupling mechanism is at work. Here we present results of an ab initio investigation of the lattice dynamics and electron-phonon coupling of undoped and Li-intercalated ZrNCl applying a density-functional perturbation approach, which allows a calculation of the full momentum dependency of these quantities. The theoretical phonon spectra are found to be in very good agreement with those obtained by neutron scattering experiments [2]. On intercalation, small Fermi surface pockets develop around the K points. This topology gives rise to strongly momentum dependent electron-phonon coupling, which is carried predominantly by two in-plane vibrations of Zr and N. We find that the integrated coupling constant is ≈ 0.5 , a value significantly larger than estimated before [3], but still rather small in view of the high T_c values observed. Implications for the superconducting mechanism will be discussed.

[1] S. Yamanaka et al., Nature 392, 580 (1998)

[2] P. Adelmann et al., J. Low Temp. Phys. 117, 449 (1999)

[3] R. Weht et al., Europhys. Lett. 48, 320 (1999)

Hauptvortrag

TT 18.8 Mo 12:00 TU H2053

Point-Contact Spectroscopy on Conventional and Unconventional Superconductors — ●GERNOT GOLL — Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

A growing number of metals is found to exhibit exotic types of superconductivity as manifested by their thermodynamic and transport properties. Unconventional superconductivity is observed in many U- and Ce-based heavy-fermion superconductors and oxide superconductors. Point-contact spectroscopy is one of the tools to study the symmetry and nodal structure of the energy gap Δ . Andreev reflection of charge carriers at the normal metal/superconductor interface leads to minima at $V \approx \pm\Delta/e$ in the differential resistance dV/dI as a function of applied bias V . In addition, Andreev reflection causes an excess current through the metallic point contact which can be analyzed with respect to the order-parameter symmetry. The talk will review recent developments in this field and focuses on investigations of Sr_2RuO_4 as a candidate for p -wave superconductivity, and of the heavy-fermion superconductor CeCoIn_5 as a possible d -wave superconductor.

TT 18.9 Mo 12:30 TU H2053

In-plane angular dependence of the upper critical field of the unconventional superconductor CeCoIn_5 - Implications for the order parameter symmetry — ●F. WEICKERT¹, P. GEGENWART¹, S. HAAS², H. WON³, and K. MAKI² — ¹Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany — ²Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089-0484, USA — ³Department of Physics, Hallym University, Chunchon 200-702, South Korea

CeCoIn_5 is a tetragonal heavy fermion system that shows unconventional superconductivity below $T_c = 2.3\text{K}$ with upper critical fields of about 5T ($B\parallel c$) and 11.5T ($B\perp c$). Below a temperature of 0.7K, the superconducting to normal transition is of first order and at lower tempera-

tures indications for an inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov state in close vicinity to $B_{c2}(T)$ have been discovered.

Here we use resistivity measurements to study the in-plane angular dependence of the upper critical field $B_{c2}(\theta)$ at 0.1K. A fourfold oscillation with 2% amplitude is observed. Since B_{c2} for fields parallel to the [110] direction is larger than along the [100] direction, our results would be compatible with a d_{xy} superconducting order parameter.

TT 18.10 Mo 12:45 TU H2053

Thermoelectric power of V_3Si single crystal near the structural transition — ●JUN SUNG KIM and REINHARD K. KREMER — MPI-FKF, 70569 Stuttgart

V_3Si , one of the A -15 superconductors, has attracted a lot of interest in experimental and theoretical studies because of the relatively high superconducting transition temperature and the unclear role of the lattice instability. The structural phase transition from cubic to tetragonal occurs at $T_M \sim 23\text{K}$, just above the superconducting transition $T_C = 16.7\text{K}$. To study the implication of the structural phase transition on the electronic properties, we have carried out highly temperature resolved thermoelectric power measurements in the regime of the structural transition on a single crystal which according to heat capacity measurements shows a clear transition at T_M . Above T_M , the thermoelectric power (S) shows a nonlinear temperature dependence with a knee structure near $T \sim 100\text{K}$, which is consistent with previous measurements on polycrystalline samples.[1] However, it is found that there is a clear slope change in $S(T)$ near T_M on the single crystal, and $S(T)$ rapidly decreases below T_M . These results indicate that the scattering asymmetry between hole and electron is reduced due to the structural phase transition. The change of the density of states near the Fermi level and electron-phonon coupling will be discussed as an origin of temperature dependence of $S(T)$.

[1] M. P. Sarachik, *et al.* Can. J. Phys. 41, 1542 (1963).

TT 19 Transport - Nanoelectronics I: Spintronics and Magnetotransport

Zeit: Montag 10:00–12:15

Raum: TU H3027

TT 19.1 Mo 10:00 TU H3027

Dielectric function of 2DEG with Rashba spin-orbit interaction — ●MIKHAIL PLETYUKHOV¹ and VLADIMIR GRITSEV² — ¹Institute for Theoretical Solid State Physics, University of Karlsruhe, Germany — ²Department of Physics, University of Fribourg, Switzerland

We study how the dielectric function of two-dimensional electron gas is modified due to Rashba spin-orbit interaction. We present the results of our calculations for finite momenta and frequencies. We discuss the modification of plasmon spectrum due to spin-orbit coupling, and make estimates for quasiparticle lifetime for different values of Rashba coupling parameter.

TT 19.2 Mo 10:15 TU H3027

Andreev magnetotransport in low-dimensional semiconductors: Application to spin detection — ●GRIGORY TKACHOV and KLAUS RICHTER — Institute for Theoretical Physics, Regensburg University, 93040 Regensburg, Germany

We investigate a possibility of using the superconducting proximity effect for detecting spin of transport carriers in two-dimensional electron systems (2DES), a problem closely related to the ongoing work on spin injection in semiconductors. The proximity effect is described within a ballistic approach taking into account the formation of an induced minigap in the excitation spectrum of a 2DES in planar superconductor/2DES contacts, which leads to enhanced Andreev reflection and the excess conductance at low bias voltages in agreement with experiments [1]. We show that in a 2DES subject to an in-plane magnetic field the Zeeman splitting of the proximity-modified states gives rise to spin-selective Andreev transport as opposed to conventional tunnel junctions where the spin splitting affects only the quasiparticle current [2]. Our model of spin-dependent Andreev reflection also accounts for a diamagnetic effect of the screening supercurrent induced by the magnetic field.

[1] C. Nguyen, H. Kroemer, and E.L. Hu, Phys. Rev. Lett. **69**, 2847 (1992); F. Rahman and T. J. Thornton, Superlat. Microstr., **25** 767 (1999); J. Eroms, M. Tolkiehn, D. Weiss, U. Rössler, J. DeBoeck, S. Borghs, Europhys. Lett. **58**, 569 (2002).

[2] R. Meservey, P. M. Tedrow, and P. Fulde, Phys. Rev. Lett. **25**, 1270

(1970); R. Meservey and P. M. Tedrow, Phys. Reports **238**, 173 (1994).

TT 19.3 Mo 10:30 TU H3027

Zero-bias anomaly in cotunneling transport through quantum-dot spin valves — IRENEUSZ WEYMANN¹, JÓZEF BARNAS^{1,2}, ●JÜRGEN KÖNIG³, JAN MARTINEK^{2,4}, and GERD SCHÖN⁴ — ¹Department of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland — ²Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland — ³Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — ⁴Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Quantum dots attached to ferromagnetic leads define quantum-dot spin valves. The interplay of spin-dependent transport due to finite spin polarization in the leads and strong Coulomb interaction gives rise to complex transport behavior. In the limit of weak dot-lead coupling, and deep in the Coulomb-blockade regime, sequential tunneling [1,2] is suppressed, and transport is dominated by cotunneling [3].

We analyze cotunneling transport through a quantum-dot spin valve with antiparallel alignment of the leads' magnetic moments. We find a zero-bias anomaly in the differential conductance for Coulomb-blockade valleys with an unpaired dot electron. It is a consequence of the interplay of single- and double-barrier cotunneling processes and their effect on the spin accumulation in the dot. The anomaly becomes significantly modified when an external magnetic field is applied.

[1] J. König and J. Martinek, Phys. Rev. Lett. **90**, 166602 (2003).

[2] M. Braun, J. König, and J. Martinek, cond-mat/0404455.

[3] I. Weymann, J. Barnas, J. König, J. Martinek, and G. Schön, preprint.

TT 19.4 Mo 10:45 TU H3027

Investigation of a mesoscopic spin-ratchet — ●ANDREAS PFUND and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, Germany

We consider the possibility to generalize the well known ratchet-mechanism to generate a spin-polarized current between electronic reservoirs. The effect of spin-orbit interaction is in particular considered. As a starting point, transport through a confined 2DEG in presence of a

'ratchet-potential', magnetic field and spin-orbit interaction is studied in a coherent and ballistic picture. The next step is to investigate the general non-equilibrium situation in contact with a heat-bath, introducing dissipation and thermal noise.

Hauptvortrag

TT 19.5 Mo 11:00 TU H3027

Spin Pumping in a Mesoscopic Spin Battery — ●BART VAN WEES — Department of Applied Physics and Materials Science Center, University of Groningen, The Netherlands

In the field of spintronics it has become possible to generate, study, and employ phenomena like spin currents and spin accumulation. A very new and exciting development is to use the fact that a spin current represents a flow of angular momentum. A new prediction [1] concerns a ferromagnetic island of which the magnetization direction is made to precess using ferromagnetic resonance, by driving it with a RF magnetic field with frequencies in the gigahertz range. It is predicted that as a result a spin current can be emitted into the non-magnetic metal or semiconductor which is attached to this ferromagnet. The ferromagnet will therefore act as a "spin battery", which can supply energy, not by an electronic charge current, but by a spin current. In this talk I will give an introduction into the relevant concepts for this phenomenon, including spin injection, spin mixing, spin transport and spin pumping. I will then discuss some of our recent experiments which show how spin accumulation can be created and studied in mesoscopic devices [2], and experiments [3] which show that spin currents are created by a "mesoscopic spin battery" by driving a micrometer sized ferromagnet with a strong RF field, generated by an "on-chip" microwave circuit close to the mesoscopic device structure. [1] Y. Tserkovnyak et al., Phys. Rev. Lett. 88, 117601 (2002) [2] M. Zaffalon, and B.J. van Wees, Phys. Rev. Lett. 91, 186601 (2003) [3] M. Costache et al., in preparation

Hauptvortrag

TT 19.6 Mo 11:30 TU H3027

Intrinsic Spin Hall Effect — ●SHUICHI MURAKAMI — Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

We theoretically predict that the electric field can induce a substantial amount of spin current at room temperature, in p-type semiconductors such as GaAs [1,2]. This spin current is even under time reversal, and can

flow without dissipation. It is caused by the topological Berry phase felt by a hole when it traverses the momentum space, and all the filled states below the Fermi level contribute to the spin current. On the other hand, in some band insulators such as PbTe, the charge conductivity vanishes, and the spin Hall current flows without any dissipation; we can call it a spin Hall insulator [3]. We discuss recent experimental observations of this effect. This effect leads to efficient spin injection into semiconductors without the need for metallic ferromagnets, opening up a new possibility for spintronic devices with low power consumption.

This work was done in collaboration with N. Nagaosa and S.-C. Zhang. References: S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003); Phys. Rev. B69, 235206 (2004); Phys. Rev. Lett. 93, 156804 (2004).

TT 19.7 Mo 12:00 TU H3027

Spin Hall conductivity of a two dimensional electron gas — ●PETER SCHWAB¹ and ROBERTO RAIMONDI² — ¹Institut für Physik, Universität Augsburg, 86135 Augsburg — ²Dipartimento di Fisica, Università di Roma Tre, 00146 Roma, Italy

In a two-dimensional electron gas with spin orbit coupling an electric field applied in the x -direction in the plane induces a spin current in the y -direction with the spins polarized perpendicular to the plane. Over the last year this so-called spin Hall effect has attracted a lot of attention due to possible applications in spintronics.

We calculate the spin Hall conductivity $\sigma_{xy}(\omega)$ for a weakly disordered two-dimensional electron gas, varying both the strength and type of disorder. In the static limit, i.e. for frequencies that are below the elastic scattering rate, we find a vanishing spin Hall conductivity, independent of the type of disorder. The spin Hall conductivity vanishes due to a cancellation between a reactive contribution to the conductivity $\sigma_{\text{react}} = e/8\pi$ whose universal value is related to a Berry phase, and a dissipative contribution $\sigma_{\text{diss}} = -e/8\pi$.

[1] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003); J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsy, T. Jungwirth, and A. H. MacDonald, Phys. Rev. Lett. 92, 126603 (2004).

[2] R. Raimondi and P. Schwab, cond-mat/0408233.

TT 20 Schottky Award Lecture

Zeit: Montag 12:30–13:15

Raum: TU P270

Hauptvortrag

TT 20.1 Mo 12:30 TU P270

Quantum Correlations in Mesoscopic Systems — ●WOLFGANG BELZIG — Department of Physics and Astronomy, University of Basel, Klingelbergstr. 82, 4056 Basel, Schweiz

Full counting statistics aims at a complete characterization of the distribution of measurement outcomes. In my talk I will demonstrate how this concept allows to investigate quantum correlations in a variety of mesoscopic systems. Three examples will be discussed:

a) In analogy to Schottky's work on the current fluctuations in a vacuum diode, shot noise in superconducting contacts allows to identify the nature of the elementary charge transfer events.

b) The Coulomb interaction in complex quantum dots or molecules leads to a strongly correlated current statistics.

c) The density fluctuation statistics in a fermionic quantum gas reflects the crossover from a superfluid state to a molecular Bose-Einstein condensate.

TT 21 Symposium Frustrated Systems

Zeit: Montag 14:00–18:00

Raum: TU H104

Fachvortrag

TT 21.1 Mo 14:00 TU H104

Competing Electronic Interactions and Complex Topology — ●WOLFRAM BRENIG — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

The interplay between competing interactions and complex topology is an emerging common theme in many condensed matter systems. On the one hand geometrically frustrated lattice topologies may hinder a physical system to minimize all of its two-particle interactions simultaneously, leading to novel elementary excitations, very low energy scales and even to macroscopically degenerate ground states. On the other hand, competing interactions can induce complex electronic topologies, like intrinsic superstructures, inhomogeneities or micro-phase-separation. This talk will survey some of these phenomenon, with a focus on systems with magnetic and electronic degrees of freedom. Work supported in part by the DFG through SPP 1073.

Hauptvortrag

TT 21.2 Mo 14:25 TU H104

2D Quantum Antiferromagnets from Néel-Ordered Phases to Spin Liquids — ●CLAIRE LHUILLIER — Laboratoire de Physique Théorique des Liquides, Université P. et M. Curie and UMR 7600 of CNRS, Case 121, 4 Place Jussieu, 75252 Paris Cédex, France

2D quantum magnets display a large variety of low energy phases. The spin-1/2 next neighbor 2-dimensional Heisenberg model on Bravais lattices (square, triangular) is Néel ordered. Frustration, small coordination number, competition between interactions can lead directly, or step by step, to various gapful quantum phases without magnetic long range order. The variety of long ranged ordered gapless phases is larger than usually expected: some examples will be given of exotic phases (nematic order) or "paradoxical" effects ($T \neq 0$ phase transitions in 2D magnets with SU(2) invariant interactions). In 2D the spin-gapped phases may be Valence Bond Crystals (VBC) with long range order in singlets or Spin Liquids (SL). There are major physical differences between these two kinds of spin-gapped phases. Propagating modes of integer spin can

describe 99 SL excitations are much more exotic: there are both fractionalized and topological ones (these last excitations being good candidates for quantum bits, with very low rate of quantum decoherence).

Fachvortrag TT 21.3 Mo 14:50 TU H104
Charge degrees of freedom in frustrated lattices — ●PETER FULDE — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 011787 Dresden

We consider electrons with strong short-range correlations in a pyrochlore lattice and its two-dimensional analogue, the checkerboard lattice. There are strong indications that at quarter filling (or half-filling in the case of spinless fermions) excitations exist with a charge $e/2$. For the checkerboard lattice extensive numerical calculations have been done which support that conjecture [1]. This, as well as the role of the spin and of statistics will be discussed. Some of the findings should also hold for a number of other frustrated lattices.

[1] E. Runge and P. Fulde, Phys. Rev. (in print)

Fachvortrag TT 21.4 Mo 15:15 TU H104
Frustration in ice, spin ice and elsewhere — ●RODERICH MOESSNER — CNRS and ENS Paris

Geometrically frustrated magnets are distinguished from more conventional ones by their large ground-state degeneracy, as the ground-state constraint does not lead to a unique low-energy configuration. Thus, even at very low temperatures, strong fluctuations can be present as the magnet explores the space of all ground states. In this talk, we discuss the properties of this low-temperature regime. In particular, we propose two schemes which capture its thermodynamics as well as its correlation functions very accurately. One of them is based on a gauge theory and leads to a magnetostatic effective energy functional. This leads to unusual algebraic correlations which are not indicative of a critical point.

This theory can be applied to ordinary (water) ice as well as its magnetic analogues, the spin ice compounds $\{Ho, Dy\}_2Ti_2O_7$. In the latter system, one can observe interesting effects, including ‘missing entropy’, as well as a field-induced tuning of the effective dimensionality from $d = 3$ to $d = 2$.

Fachvortrag TT 21.5 Mo 15:40 TU H104
Das ALPS-Projekt: Open Source Algorithmen für stark korrelierte Systeme — ●MATTHIAS TROYER und SIMON TREBST — ETH Zürich

Wir präsentieren das ALPS-Projekt, ein Projekt in welchem Algorithmen für die numerische Simulation von stark korrelierten Quantengittermodellen implementiert und als “open source” frei zur Verfügung gestellt werden. Die Programme sollen es insbesondere Nicht-Experten ermöglichen, numerische Simulationen schnell und effizient auszuführen. Hierbei wenden wir uns sowohl an Theoretiker, die neue Ideen testen möchten, als auch an Experimentalphysiker, denen wir ein neuartiges Werkzeug zur Datenanalyse zur Verfügung stellen. Bisher stehen erste Versionen von Implementierungen aller wichtigen Algorithmen für die numerische Simulation von Quantengittermodellen bereit: klassische und Quanten-Monte Carlo Programme, exakte und vollständige Diagonalisierung sowie die Dichtematrixrenormierungsgruppe (DMRG). Anhand einiger Anwendungen aus den letzten Monaten, unter anderem auf Quantenmagnete, ultrakalten Atome in optischen Gittern sowie stark korrelierte Fermionen, zeigen wir, wie die ALPS-Programme produktiv in der Forschung eingesetzt werden können. Die vollständige Software, einführende Anleitungen sowie eine Liste aller Beitragenden zum ALPS-Projekt finden sich auf unserer Webseite unter <http://alps.comp-phys.org/>

Hauptvortrag TT 21.6 Mo 16:20 TU H104
Geometrical Frustration as Paradigm for Low Temperature Physics — ●ARTHUR RAMIREZ — Bell Laboratories, Lucent Technologies, Murray Hill, USA

The study of geometrical frustration in triangle-based magnets continues to yield surprises. Phases such as spin liquid and spin ice are manifestations of low energy anharmonicity in full and as such, pose significant challenges for theory. The key ingredient for geometrical frustration, namely underconstraint from order parameter/space group incompatibility, leads to large spectral weight downshift. When these degrees of freedom continue to fluctuate, novel liquid-like magnetic states emerge. The notion of geometrical frustration is broadly applicable in magnetism and

can be used to understand selected orbital ordering and heavy fermion systems. These ideas are also portable to non-magnetic systems and I'll describe one example, the frustrated soft mode in the negative thermal expansion material, ZrW₂O₈. Thus a different view of low-temperature phenomena emerges, namely strong coupling at temperatures well below the mean field energy scale.

Fachvortrag TT 21.7 Mo 16:45 TU H104
Geometric Frustration in Thiospinels — ●J. HEMBERGER, R. FICHTL, P. LUNKENHEIMER, V. TSURKAN, H.-A. KRUG VON NIDDA, V. FRITSCH, E.-W. SCHEIDT, N. BÜTTGEN, A. KRIMMEL und A. LOIDL — Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg

The normal cubic spinel systems AB_2S_4 ($A = \text{Cd, Fe, Mn}$ and $B = \text{Sc, Cr}$) exhibit a wide range of exceptional ground state properties, depending on the appropriate choice of A- and B-site ions. The different scenarios reach from spin- and spin-orbital liquid behavior in the case of nonmagnetic B-sites (Sc) to ferrimagnetic and orbitally ordered or glassy states in the Cr-systems. Finally, even multiferroic behavior, namely the coexistence of ferromagnetism and relaxor ferroelectricity can be detected for the CdCr_2S_4 . In all compounds frustration in the magnetic, orbital, and as well in the structural sector dominates the interplay of the microscopic degrees of freedom and the corresponding order phenomena.

Fachvortrag TT 21.8 Mo 17:10 TU H104
Raman spectroscopy on frustrated spin systems — ●PETER LEMMENS — Inst. for Solid State Physics, TU Braunschweig, D-38106 Braunschweig, Germany and MPI for Solid State Research, D-70569 Stuttgart, Germany

Many transition metal oxides realize competing interactions based on spin, charge or orbital degrees of freedom (1). Raman scattering has contributed to the understanding of this interplay and the effect of frustration to a great extent due to its unprecedented sensitivity, resolution and additional symmetry information that may be gained considering selection rules. It will be discussed how ground state degeneracy and / or suppressed long range magnetic ordering due to novel spin topologies effect the excitation spectrum of a quantum spin system. Respective model systems are the tetrahedral cluster compound $\text{Cu}_2\text{Te}_2\text{O}_5\text{Br}_2$ and the frustrated dimer system $\text{SrCu}_2(\text{BO}_3)_2$. These compounds demonstrate a cross over from low energy singlet bound states to longitudinal magnons. In addition, multiband effects and polarons will be addressed in the hydrated superconductor $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$. This work was supported by DFG SPP1073 and INTAS 01-278.

[1] Spin - Orbit - Topology, a triptych, P. Lemmens and P. Millet, in “Quantum Magnetism”, Ed. U. Schollwöck, J. Richter, B.J.J. Farrell, R.F. Bishop, Springer, Heidelberg (2004).

Fachvortrag TT 21.9 Mo 17:35 TU H104
Spectroscopic studies on geometrically frustrated $\text{Na}_{1-x}\text{CoO}_2$ — ●J. GECK¹, T. KROLL¹, S.V. BORISENKO¹, J. FINK¹, A.A. KOR DYUK¹, M. KNUPFER¹, C. HESS¹, C. SEKAR¹, G. KRABBES¹, C. LIN², H. BERGER³, and B. BÜCHNER¹ — ¹Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — ²Max Planck Institute for Solid State Research in Stuttgart, Germany — ³Institute of Physics of Complex Matter Lausanne, Suisse

The investigation of strongly correlated electrons in geometrically frustrated lattices is one of the hot topics in current condensed matter research. For instance, the startling discovery of superconductivity in water-intercalated $\text{Na}_{1-x}\text{CoO}_2$ attracted a great deal of attention. The sodium cobaltites contain triangular CoO_2 sheets, leading to a topological frustration which favors unconventional electronic ground states. In addition to this, there is evidence that the spin-orbit and the crystal-field splitting in these materials are comparable, i.e. unusual coupled spin-orbital excitations might be relevant. Since low energy excitations still remain unclear, it is essential to characterize the electronic system in detail. We have performed angle resolved photoemission, as well as x-ray absorption and photoemission studies on $\text{Na}_{1-x}\text{CoO}_2$ single crystals with $x=0.3, 0.5$, and 0.7 . Our data reveal a low spin configuration of cobalt at all temperatures, a strongly temperature dependent narrow quasiparticle band as well as an anisotropic Fermi-velocity. The spectral weight transfer of the XAS spectra as a function of x is interpreted in terms of a Hubbard model.

TT 22 Transport - Nanoelectronics II: Quantum Dots and Wires, Point Contacts

Zeit: Montag 14:00–17:30

Raum: TU H2053

TT 22.1 Mo 14:00 TU H2053

Elektron-Elektron Wechselwirkung in nanostrukturierten, ferromagnetischen Leiterbahnen unterschiedlicher Dimension — ●MARIO BRANDS, AXEL CARL und GÜNTER DUMPICH — Fachbereich Physik, Experimentalphysik, AG Farle, Universität Duisburg-Essen (Campus Duisburg), Lotharstr. 1, 47048 Duisburg

Es wurden Magnetowiderstandsmessungen an einzelnen, nanostrukturierten Kobalt-Leiterbahnen bei tiefen Temperaturen durchgeführt. Die Leiterbahnen wurden zum Schutz vor Oxidation in-situ mit isolierendem Kohlenstoff abgedeckt. Die Kontaktierung erfolgt über nicht-magnetische Gold- bzw. Platinkontaktpads unter Zuhilfenahme eines aufwendigen Drei-Schritt-Elektronenstrahlithografie-Prozesses. Der Magnetowiderstand der Leiterbahnen kann, für beliebig orientierte Magnetfelder, mit Hilfe des AMR-Effektes erklärt werden. Hingegen zeigt sich in der Temperaturabhängigkeit des Widerstandes ein logarithmischer Beitrag aufgrund von erhöhter Elektron-Elektron-Wechselwirkung. Durch Reduzierung der Leiterbahnbreite kann ein Übergang von zweidimensionalem zu eindimensionalem Verhalten beobachtet werden. Beiträge aufgrund von schwacher Lokalisierung werden nicht beobachtet. Die Arbeit wird gefördert von der DFG im Rahmen des SFB 491.

TT 22.2 Mo 14:15 TU H2053

Giant super-poissonian Fano factors in shuttle devices — ●ANDREA DONARINI^{1,2}, TOMAŠ NOVOTNÝ², CHRISTIAN FLINDT², and ANTTI-PEKKA JAUHO² — ¹Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — ²MIC - Department of Micro and Nanotechnology, Technical University of Denmark

Shuttle devices are a particular kind of NEMS characterized by a nanometer scale oscillating quantum dot that transfers electrons one-by-one from the source to the drain lead. We study the dynamics of an archetypal model device in the density matrix formalism and represent the numerical results by means of phase space distribution (Wigner function), current and current noise (Fano factor). The device presents tunnelling and shuttling as limiting operating regimes for respectively high and low mechanical damping conditions. In the transition region between the tunnelling and shuttling regime the system is characterized by a giant super-poissonian Fano factor ($F \approx 100$).

This feature is the signature of a coexistence regime: i.e. a slow switching dichotomous process between the tunnelling and the shuttling current modes. For this regime we propose a simplified description in terms of a bistable effective potential. This description captures the main features of the coexistence regime (confirmed by the quantitative agreement with the numerical results) and gives also a more transparent physical insight of the device dynamics.

TT 22.3 Mo 14:30 TU H2053

Quantized Conductance in Atomic-Scale Point Contacts Formed by Local Electrochemical Deposition of Silver — ●STEFAN BRENDELBERGER¹, CHRISTIAN OBERMAIR¹, ROBERT KNIESE¹, FANGQING XIE¹, and THOMAS SCHIMMEL^{1,2} — ¹Institute for Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

We report on conductance quantization at room temperature in atomic-scale silver point contacts electrochemically fabricated within a nanoscale gap between two gold electrodes on a glass substrate. The formation of stable contacts exhibiting quantized conductance at integer multiples of the conductance quantum $G_0 = 2e^2/h$ ($\approx 1/12.9k\Omega$) was observed. While transient contacts with other conductance values were also found, a clear preference for values close to integer multiples of G_0 was observed for contacts stable for up to several hours. When applying electrochemical deposition or dissolution potentials, sharp transitions were induced between different quantized conductance levels while between these transitions, horizontal plateaus of constant conductance were found.

[1] Ch. Obermair et al. In: A. S. Alexandrov et al. (eds.) *Molecular Nanowires and Other Quantum Objects*, NATO Science Series II, Kluwer, Dordrecht, The Netherlands, 233-242, 2004.

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

TT 22.4 Mo 14:45 TU H2053

Conduction Channels of One-Atom Zinc Contacts — ●MICHAEL HÄFNER¹, PATRICK KONRAD², FABIAN PAULY¹, JUAN-CARLOS CUEVAS^{1,3}, and ELKE SCHEER² — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — ³Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, 28049 Madrid, Spain

We have determined the transmission coefficients of atomic-sized Zn contacts using a new type of breakjunction which contains a whisker as a central bridge. We find that in the last conductance plateau the transport is unexpectedly dominated by a well-transmitting single conduction channel. We explain the experimental findings with the help of a tight-binding model which shows that in an one-atom Zn contact the current proceeds through the 4s and 4p orbitals of the central atom.

TT 22.5 Mo 15:00 TU H2053

Transport properties of single channel quantum wires with an impurity: Influence of finite length and temperature on average current and noise — ●FABRIZIO DOLCINI¹, BJÖRN TRAUZZETTEL², INÈS SAFI³, and HERMANN GRABERT¹ — ¹Albert-Ludwigs-Universität, Freiburg — ²Leiden University, The Netherlands — ³Université Paris-Sud, France

The inhomogeneous Tomonaga Luttinger liquid model describing an interacting quantum wire adiabatically coupled to non-interacting leads is analyzed in the presence of a weak impurity within the wire. Due to strong electronic correlations in the wire, the effects of impurity backscattering, finite bias, finite temperature, and finite length lead to characteristic non-monotonic parameter dependencies of the average current [1]. We discuss oscillations of the non-linear current voltage characteristics that arise due to reflections of plasmon modes at the impurity and quasi Andreev reflections at the contacts. The finite frequency current noise is also investigated in detail. We find that the effective charge extracted in the shot noise regime in the weak backscattering limit depends on the noise frequency ω relative to v_F/gL , where v_F is the Fermi velocity, g the Tomonaga Luttinger interaction parameter, and L the length of the wire [2]. The excess noise is finite even for frequencies larger than the applied voltage, which is a signature of correlation effects.

[1] F. Dolcini, H. Grabert, I. Safi, and B. Trauzettel, *Phys. Rev. Lett.* 91, 266402 (2003).

[2] B. Trauzettel, I. Safi, F. Dolcini, and H. Grabert, *Phys. Rev. Lett.* 92, 226405 (2004).

TT 22.6 Mo 15:15 TU H2053

Co-tunneling current and shot noise in quantum dots and molecules — ●AXEL THIELMANN¹, MATTHIAS H. HETTLER¹, JÜRGEN KÖNIG² und GERD SCHÖN^{1,3} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — ²Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — ³Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

We study current and shot noise up to second-order perturbation theory in the coupling of a mesoscopic object (e.g. quantum dot or molecule) to metallic electrodes. In particular, we discuss the influence of co-tunneling processes for the Anderson-impurity model with finite spin splitting. We show that spin-flip co-tunneling leads to a super-Poissonian Fano factor at a different energy scale than expected from first-order calculations. Furthermore, we find the Fano factor in the Coulomb-blockade regime to be very sensitive to the tunnel-coupling strength, which may serve as a spectroscopic tool for the latter.

TT 22.7 Mo 15:30 TU H2053

Anomalous conductance of a spin-1 quantum dot — ●ANNA POSAZHENNIKOVA¹ and PIERS COLEMAN² — ¹TKM, Universität Karlsruhe, 76128, Germany — ²Center for Materials Theory, Rutgers University, Piscataway, NJ 08855, USA

We interpret the recent observation of a zero-bias anomaly in spin-1 quantum dots in terms of an underscreened Kondo effect. Although a spin-1 quantum dots are expected to undergo a two-stage quenching effect, in practice the log normal distribution of Kondo temperatures leads to a broad temperature region dominated by underscreened Kondo

physics. General arguments, based on the asymptotic decoupling between the partially screened moment and the leads, predict a singular temperature and voltage dependence of the conductance and differential conductance. Using a Schwinger boson approach, we show how these qualitative expectations are borne out in a detailed many body calculation.

Pause

TT 22.8 Mo 16:00 TU H2053

Nonequilibrium Kondo physics in double quantum dots — •YIFENG YANG and KARSTEN HELD — MPI for solid state research, Stuttgart

We study the multi-orbital Kondo effect at a finite bias, generalizing the nonequilibrium scaling approach suggested recently by Rosch et al. [Phys. Rev. Lett. 90, 076804 (2003)]. The finite current through the quantum dots gives rise to a cutoff of the scaling equations, which is calculated from the spin susceptibility. We study in detail the strong orbital Kondo effect in a parallel double quantum dot. The results are consistent with recent experiments. Moreover, we also report on genuine nonequilibrium effects like a negative differential conductance at finite bias voltage.

TT 22.9 Mo 16:15 TU H2053

Electron transport through strongly correlated nanostructures: Frequency vs. real-time approach within DMRG — •PETER SCHMITTECKERT — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

We provide an overview over various strategies to study the problem of electron transport through onedimensional, strongly correlated quantum systems within the framework of density matrix renormalization group calculations. Specifically we compare the Kubo formalism approach in frequency space, in which we calculate the linear dc conductance, with real time simulations, where we extract the conductance from the real-time evolution of suitably chosen initial states.

TT 22.10 Mo 16:30 TU H2053

Full Counting Statistics in Non-Markovian Interacting Electron Systems — •ALESSANDRO BRAGGIO^{1,2}, JÜRGEN KÖNIG¹, and ROSARIO FAZIO³ — ¹Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²LAMIA-INFN, Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16133 Genova, Italy — ³NEST-INFN & Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy

Full counting statistics for electron transport is generalized to interacting electron systems with non-Markovian dynamics. In deriving a general expression for the cumulant generating function, we develop a method to properly account for the non-Markovian nature of the system. We compare with both the limits of Markovian dynamics and with transport through non-interacting systems, and discuss under which circumstances non-Markovian effects appear in the transport properties. As specific examples, we consider transport through a single-level quantum dot in second order of the tunnel coupling strength.

TT 22.11 Mo 16:45 TU H2053

Adiabatic pumping and Berry's phase in a mesoscopic ring — •ANGELIKA BENDER^{1,2}, FRANK W. J. HEKING², ALEXANDER SHNIRMAN¹, and YUVAL GEFEN³ — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS, BP 166, F-38042 Grenoble, France — ³Department of Condensed Matter Physics, The Weizmann Institut of Science, Rehovot 76100, Israel

We study parametric pumping of charge in a mesoscopic system, induced by adiabatic and periodic changes of system parameters. Adiabatic changes of a Hamiltonian lead to phases in the wavefunction. We study the physical meaning of these phases for a loop with an impurity. The loop is threaded by a magnetic flux that induces persistent currents. We compute the total charge that passes the system upon a periodic change of flux and impurity strength and show that it is directly related to the phases of the wavefunction. We find in particular the link between pumped charge and Berry's phase. Further calculations include noise and decoherence due to the coupling of the system to its environment.

TT 22.12 Mo 17:00 TU H2053

Spin and Charge Channels in Zero Dimensional Systems — •MIKHAIL KISELEV¹ and YUVAL GEFEN² — ¹Institut für Theoretische Physik, Universität Würzburg, D-97074 Würzburg, Germany — ²Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

We consider the effects of the charge and spin zero-mode interactions in quantum dots. The non-perturbative effects of zero-mode interaction are described in terms of the propagation of gauge bosons associated with U(1) charge and SU(2) spin fluctuations in the dot. The Coulomb and longitudinal spin components are accounted for "exactly", while transverse spin fluctuations are analyzed perturbatively (with the easy-axis anisotropy). These fluctuations become important as one approaches the Stoner instability. We study the influence of spin on the differential conductance as well as the dynamic spin susceptibility.

TT 22.13 Mo 17:15 TU H2053

On the visibility of electron-electron interaction effects in field emission spectra of single-wall carbon nanotubes — •THOMAS SCHMIDT and ANDREI KOMNIK — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

The electron-electron interaction effects turn out to alter considerably the energy-resolved current measured in field emission experiments. The most prominent feature is the so-called secondary current, which is related to the energy spectrum of the emitted electrons above the Fermi edge and which is brought about by processes of second order in tunnelling. The latter can be calculated exactly for a wide variety of emitters and turns out to be divergent towards E_F . We perform an analysis of tunnelling processes of higher orders and show that they are divergent as well and overcome the leading order contributions sufficiently close to E_F . Another effect which complicates the measurement of the secondary current is the thermal broadening of the Fermi edge. We discuss this aspect as well and make estimations for the energy and temperature windows for the secondary current to be reliably observable during field emission experiments from single-walled carbon nanotubes.

TT 23 Posters Superconductivity, Solids at Low Temperature

Zeit: Montag 14:00–18:00

Raum: Poster TU D

TT 23.1 Mo 14:00 Poster TU D

Superconducting properties of HoNi₂B₂C single crystals — •DMITRI SOUPEL, GÜNTER BEHR, WOLFGANG LÖSER, KONSTANTIN NENKOV, and GÜNTER FUCHS — IFW Dresden, Helmholtzstr. 20, 01171 Dresden

High-quality single crystals of HoNi₂B₂C intermetallic compounds have

been grown by a floating zone technique with optical heating. Depending on small composition variation and the temperature of heat treatment single crystalline HoNi₂B₂C samples 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 2 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.

TT 23.2 Mo 14:00 Poster TU D

In-situ synthesis of MgB₂ thin films for tunnel junctions — ●R. SCHNEIDER, J. GEERK, F. RATZEL, A.G. ZAITSEV, R. HEID, and K.-P. BOHNEN — Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe

A novel approach to the in-situ preparation of as-grown MgB₂ thin films is presented. It comprises a conventional B sputter gun and a special Mg evaporator that provides a high Mg vapor pressure at the position of the substrate. Thin films deposited on r-plane sapphire substrates at a temperature of 440°C had a zero resistance T_c of 33 K and a residual resistivity of approximately 100 $\mu\Omega\text{cm}$. Sandwichtype tunnel junctions with a natural MgB₂ oxide as the potential barrier were prepared for superconducting tunneling spectroscopy. Conductance measurements up to 500 mV revealed estimates of the barrier thickness of 1.5 nm and height of 1.6 eV. The slowly varying conductance between ± 100 mV allowed us to determine the tunneling density of states. The inversion of the tunnel data using the standard single-band Eliashberg equations yielded an effective electron-phonon spectral function accounting for the smaller energy gap. The features of the tunneling spectrum were analyzed by ab-initio LDA calculations and the two-band Eliashberg equations.

TT 23.3 Mo 14:00 Poster TU D

Laserablatierte Magnesium / Bor Multilagen in Kombination mit in-situ Temperschritten: eine Methode zur Herstellung von MgB₂-Schichten — ●ANDREAS KLIMMER¹, ROLAND STEINER¹, ALFRED PLETTL¹, PAUL ZIEMANN¹, JUN CAI² und JÜRGEN BEHM² — ¹Abt. Festkörperphysik, Universität Ulm — ²Abt. Oberflächenchemie und Katalyse, Universität Ulm

Es wurden unter UHV-Bedingungen dünne Multilagen aus Magnesium und Bor bei Raumtemperatur mit Hilfe eines 193 nm - Excimer-Lasers bei hohen Energiedichten auf c-Saphir abgeschieden. Dabei wurden die Schichtdicken so eingestellt, dass sowohl nominell stöchiometrisches als auch Mg-reiches MgB₂ resultieren sollte. Als abschließende Deckschichten wurden dicke Mg-B- bzw. reine B-Schichten verwendet. Ein anschließender in-situ Temperschritt mittels eines CO₂-Lasers ermöglicht in den bereits bei der Ablation durchmischten Schichten eine Reaktion zu MgB₂. Temperatur und Dauer des Temperschritts wurden systematisch variiert und die resultierende Probenzusammensetzung und Struktur mittels Röntgen-, RBS- und XPS-Tiefenprofilmessungen bestimmt. Die Charakterisierung der supraleitenden Eigenschaften erfolgte durch Magnetisierungs- bzw. Transportmessungen.

Erste Ergebnisse liefern Schichten mit einer maximalen Sprungtemperatur von 23,8 K. Dieser, im Vergleich zum Maximalwert von 39 K reduzierte Wert wird auf Mg-Verluste während des Temperns und relativ hohe C-Verunreinigungen aus dem benutzten B-Target zurückgeführt.

TT 23.4 Mo 14:00 Poster TU D

Preparation and Characterization of thin Superconducting MgB₂ Films — ●A. SIDORENKO^{1,2}, V.I. ZDRAVKOV², E. NOLD³, TH. KOCH⁴, and TH. SCHIMMEL^{1,4} — ¹Institute of Applied Physics, Universität Karlsruhe, D-76128 Karlsruhe — ²Institute of Applied Physics, MD-2028 Kishinev, Moldova — ³Institute of Materials Research I, Forschungszentrum Karlsruhe, D-76021 Karlsruhe — ⁴Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe

Superconducting MgB₂ films with a critical temperature, T_c , up to 39.3 K were prepared in a new way by DC-magnetron sputtering from a composite target containing MgB₂ and metallic Mg in approximately equal amounts and ex-situ annealing in Mg vapour using an especially designed Nb reactor. The AFM imaging show a very smooth and homogeneous morphology of the film surfaces which were deposited with this method on (100) - sapphire substrates. Depth profile scanning auger analysis of the thin MgB₂ layers detected the presence of oxygen in only small regions of 10 nm thickness near the surface of the film and near the interface between the substrate and the MgB₂ layer. The parameters of the MgB₂ films which influence T_c , are discussed.

TT 23.5 Mo 14:00 Poster TU D

Mn substitution in MgB₂ single crystals: influence on structural properties — ●G. SCHUCK, N.D. ZHIGADLO, S.M. KAZAKOV, K. ROGACKI, and J. KARPINSKI — Solid State Physics Laboratory ETH-Hönggerberg, CH-8093 Zürich, Switzerland.

Superconducting single crystals of Mn-doped MgB₂ phase have been grown at a pressure of 30 kbar using cubic anvil technique. Critical temperature versus Mn content dependence of single crystals shows different behavior from that of polycrystalline samples [1], because even small substitution of 1.5% of Mn decreases T_c by about 15K. The lattice constant remains almost unchanged while the c parameter slightly decreases with Mn content. Single crystal X-ray and EDX investigations show the existence of single phase crystals up to 2% Mn substitution. For crystals with higher Mn content we present single crystal determination in order to get information on what crystallographic position Mn is substituted in the MgB₂ crystal structure.

[1] S. Xu, Y. Moritomo, K. Kato and A. Nakamura, J. Phys. Soc. Japan, 70 (2001) 1889-1891

TT 23.6 Mo 14:00 Poster TU D

Influence of the stoichiometry variations on the properties of MgB₂ prepared by mechanical alloying — ●MARKO HERRMANN, OLAF PERNER, WOLFGANG HÄSSLER, CHRISTIAN RODIG, and BERNHARD HOLZAPFEL — Institut für Festkörper- und Werkstofforschung (IFW) Dresden

MgB₂ powder was prepared by mechanical alloying of Mg and amorphous boron powder which gives a partially reacted nanosized precursor powder with a high reactivity. For studying the influence of the stoichiometry the Mg/B-ratio was varied in the range of 0.8 to 1.2. Furthermore different boron qualities were used. These precursor powders were hot pressed to bulk samples and were used for the preparation of tapes with an iron sheath. The structural and superconducting properties of bulk samples and tapes are described in detail. The samples with a Mg/B-ratio > 1 show the highest critical temperature (36K) and the best current density (40 kA/cm² at 4.2K and 7.5T).

TT 23.7 Mo 14:00 Poster TU D

Magnetron sputtering of TiN thin films for superconducting single-photon detector — ●KONSTANTIN ILIN¹, MICHAEL SIEGEL¹, ALEXEI SEMENOV², HEINZ-WILHELM HÜBERS², EUGEN HOLLMANN³, and ANDREAS ENGEL⁴ — ¹Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe — ²DLR Institut für Planetenforschung, Berlin — ³Forschungszentrum Jülich GmbH, Jülich — ⁴Physik-Institut der Universität Zürich

Thin and especially ultra-thin superconducting films are widely used for the development of modern radiation sensors, e.g. direct detectors and mixers, providing ultimate performance in a wide range of the electromagnetic spectrum. Recently proposed single-photon detector also utilize ultra-thin films. In order to shift the cut-off wavelength of these devices to infrared and far-infrared spectral range, a superconducting material with a small value of the energy gap and an ability to form superconducting thin films is required. In this report we present our results on the development of the growing technology of thin titanium nitride films. The TiN thin films were deposited on sapphire substrate by dc magnetron sputtering of Ti target in Ar+N₂ atmosphere. The substrates were heated up to 850°C. The superconducting transition temperature of about 5 K has been obtained for 30-nm thick films. We will discuss the dependencies of the film composition, transition temperature, and residual resistivity on the deposition regime.

TT 23.8 Mo 14:00 Poster TU D

Synthesis and Characterization of new Re_xW_{1-x}O₃ Phases — ●CH. HELBIG¹, B. ROHRMOSER¹, K. TRÖSTER¹, D. SHOROKHOV¹, G. HEYMANN², G. EICKERLING¹, R. HERRMANN¹, E.-W. SCHEIDT¹, and W. SCHERER¹ — ¹CPM, Universität Augsburg, 86135 Augsburg, Germany — ²Department Chemie, LMU, 81377 München, Germany

In this presentation we outline new synthetic routes to the small class of vacancy perovskites M_{1-x}M'_xO₃ (M, M' = transition metal) which allows to control their physical properties by variation of the ratio of the metal cations. Employing highly topotactical *Chimie Douce* methods [1] or alternatively high pressure/high temperature routes [2] we were able to synthesize mixed WO₃ and ReO₃ phases and characterize them with respect to their crystal chemistry and physical properties. The chosen parent compounds strongly differ in their electronic and structural behavior. The d¹-system ReO₃ has metallic character and cubic symmetry (*Pm $\bar{3}$ m*), whereas the d⁰-system WO₃ is an insulator and displays various structural phase transitions between 1170 K and 230 K. However, the structures of all these WO₃ phases can be derived by group-subgroup relationships from the ReO₃ structure [3]. For Re_xW_{1-x}O₃ ($x = 0.25$) a metal to semiconductor transition was predicted in the literature [2].

In this contribution, however, we provide for the first time a systematic study of the electronic and magnetic properties of mixed WO_3 and ReO_3 phases. [1] See for example: M. Figlarz, *Chemica Scripta* 28, 3, (1988) [2] A. W. Sleight, J. L. Gillson, *Sol. St. Comm.* 4, 601, (1966) [3] O. Bock, U. Müller, *Z. Anorg. Allg. Chem.* 628, 987, (2000)

TT 23.9 Mo 14:00 Poster TU D

$\text{La}_2\text{Zr}_2\text{O}_7$ buffer layers on Ni RABiTS for YBCO coated conductors using chemical solution deposition — ●KERSTIN KNOTH, SEBASTIAN ENGEL, RUBEN HÜHNE, HEIKE SCHLÖRB, LUDWIG SCHULTZ, and BERNHARD HOLZAPFEL — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden

Chemical Solution Deposition (CSD), as a low-cost method for producing YBCO coated conductors, has been used to prepare $\text{La}_2\text{Zr}_2\text{O}_7$ (LZO) buffer layers on Ni RABiTS. The LZO precursor solution was prepared by dissolving La-, and Zr-2.4-pentanedionates in propionic acid. Solutions with different concentrations as well as variable dip coating speeds were examined to obtain thick and crack free LZO layers on Ni substrates (10 mm x 10mm). During the heat treatment at temperatures around 900°C in a reducing atmosphere, highly textured LZO buffer layers were grown. The texture quality was determined using X-Ray Diffraction (XRD) and Reflection High Energy Electron Diffraction (RHEED). The LZO buffer layers show a strong c-axis orientation in $\theta - 2\theta$ scans and a very good in-plane alignment on Ni, with FWHM values of 6.9° (Ni: 6.0°) and 7.2° (Ni:6.0°) for the in-plane and out-of-plane orientations. Further analyses by SEM and Atomic Force Microscopy (AFM) show dense and crack free layers. The LZO solution was also applied to long lengths using a reel-to-reel dip coating and drying unit. XRD analyses of first longer samples show good c-axis orientation. AFM and SEM investigations are in progress.

TT 23.10 Mo 14:00 Poster TU D

Preparation of buffer layer architectures based on surface oxidized Ni tapes for coated conductor applications — ●R. HÜHNE, D. SELBMANN, J. EICKEMEYER, L. SCHULTZ, and B. HOLZAPFEL — IFW Dresden, Germany

The preparation of cube textured NiO buffer layers on biaxially textured Ni tapes (RABiTS) using surface oxidation epitaxy (SOE) offers a cheap and scalable route for the production of long-length YBCO coated conductors. Therefore, thin highly textured NiO layers have been grown on different microalloyed Ni-tapes. A second buffer layer is necessary to ensure epitaxial growth of the YBCO as well as to prevent Ni contamination of the superconducting layer. Different perovskite buffer were successfully grown on SOE-NiO using pulsed laser deposition (PLD). Among them, BaZrO_3 and SrZrO_3 buffers show a high quality epitaxial growth on NiO with an in-plane orientation similar to the underlying NiO. The subsequent deposition of YBCO on top of these buffers requires a thin intermediate SrTiO_3 layer resulted in epitaxial layers with a T_c above 87 K and J_c up to 1.6 MA/cm². Microstructural investigations showed that the surface topography of the buffer layers and the YBCO is mainly determined by the quality of the NiO layer.

TT 23.11 Mo 14:00 Poster TU D

Optimization of thick $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ coated conductors produced by the TFA process — ●THOMAS THERSLEFF, MARTINA FALTER, HEIKE SCHLÖRB, LUDWIG SCHULTZ, and BERNHARD HOLZAPFEL — IFW Dresden, Helmholtzstr. 20, 01069 Dresden

In this study, the effect of layer thickness, furnace ramp rate, and peak reaction temperature on YBCO layers chemically deposited onto single-crystal STO using the TFA process is assessed. First, layer thickness was increased by coating substrates multiple times. After each coating, the substrates were pyrolyzed up to 400°C in a humid flowing gas O_2 furnace. A single coating with our standard TFA precursor produces a layer ~ 200 nm thick. Second, single layers were subjected to a slow heating ramp rate of 150 K/h in the 400-750°C region. Third, other single layer samples were reacted at a depressed peak temperature of 760°C to avoid reaction at the film boundary. Results show that substrates coated up to three times retain superconductivity with a ΔT_c of 3.9 K. XRD indicates the presence of BaF_2 , suggesting further temperature refinement is necessary. The slower ramp rate for single layers results in superior current transport properties, with J_c as high as 5 MA/cm². Samples reacted at 760°C maintain superconductivity with a ΔT_c as low as 1.4 K.

TT 23.12 Mo 14:00 Poster TU D

$\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ -Schichten und Schichtsysteme für supraleitende Bauelemente — ●ULRIKE BALDEWEG, PIERRE LORENZ, SUSAN BIERING, VEIT GROSSE, CHRISTOPH BECKER, RALF BECHSTEIN, TOBIAS FÖRSTER, HAGEN WALD, FRANK SCHMIDL und PAUL SEIDEL — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

Es werden Ergebnisse zur LASER-gestützten, großflächigen Abscheidung von supraleitenden $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO)-Schichten vorgestellt. Verschiedene Technologien zur Mikrostrukturierung und Passivierung werden hinsichtlich der elektrischen Eigenschaften der Proben und ihrer Stabilität verglichen. Mögliche Einsatzgebiete dieser Schichten sind Antennenstrukturen für Magnetometer und Gradiometer.

TT 23.13 Mo 14:00 Poster TU D

Optimierung von HTSC FlipChip-Gradiometern mit SiO_2 als Isolationsmaterial — ●SUSAN BIERING, ULRIKE BALDEWEG, RALF BECHSTEIN, CHRISTOPH BECKER, VEIT GROSSE, FRANK SCHMIDL und PAUL SEIDEL — Institut für Festkörperphysik, Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

Es wurden Untersuchungen zur Optimierung gradiometrischer Sensoren mit einer auf einem separaten Substrat befindlichen Antenne, welche in einer FlipChip-Konfiguration mit dem Gradiometer verbunden ist, durchgeführt. Dabei wurden zur Realisierung der Josephson-Kontakte $\text{YBa}_2\text{Cu}_3\text{O}_7$ -Schichten auf SrTiO_3 -Bikristallen eingesetzt. Um langzeitstabile, gegenüber äußeren Einwirkungen unempfindliche Sensoren herstellen zu können, ist ein Isolationsmaterial erforderlich, das zudem eine sehr niederohmige Ankontaktierung ermöglicht. In den Mittelpunkt des Interesses ist dabei das Material SiO_2 gerückt. Erste Erfahrungen mit diesem Material werden vorgestellt.

TT 23.14 Mo 14:00 Poster TU D

Elektrische Eigenschaften von SrTiO_3 als Isolationschicht für Tieftemperaturanwendungen — ●VEIT GROSSE, HAGEN WALD, MICHAEL MANS, FRANK SCHMIDL und PAUL SEIDEL — Institut für Festkörperphysik, Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

Mittels Laserdeposition auf dünnen YBCO-Schichten abgeschiedenes SrTiO_3 wurde hinsichtlich seiner elektrischen Eigenschaften und Eignung als Isolationschicht für supraleitende Bauelemente untersucht. Neben dem erwarteten Verhalten als Schottky-Kontakt, zeigten sich auch Widerstandsänderungen, die zu einem hysteretischen Verlauf der I-U-Kennlinien führten. Es werden Erklärungsversuche für diesen Effekt präsentiert. Des weiteren wird näher auf die dielektrischen Eigenschaften des SrTiO_3 bei tiefen Temperaturen, sowie die supraleitenden Eigenschaften der YBCO-Schichten in einem YBCO-STO-YBCO-System eingegangen.

TT 23.15 Mo 14:00 Poster TU D

Reversible and irreversible magnetostrictive effects in untwinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ crystals — ●P. POPOVICH¹, R. LORTZ^{1,2,3}, C. MEINGAST¹, S. TAJIMA⁴, and T. MASUI⁴ — ¹Forschungszentrum Karlsruhe, IFP, Germany — ²Fakultät für Physik, Universität Karlsruhe, Germany — ³present address: DCMP, University of Geneva, Switzerland — ⁴ISTEC, Tokyo, Japan

The magnetostriction coefficients, $\lambda_i = 1/L_i \cdot dL_i/dH$ (i=a,b,c), of high-pressure oxygenated untwinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ single crystals are determined between 40 K and 150 K and in fields up to 10 T. Above 55K, λ is nearly reversible and is, thus, proportional to the uniaxial pressure dependence of the magnetization, which in turn provides important information about the pressure dependencies of $T_c(H)$, the vortex melting transition $T_m(H)$, the thermodynamical critical field $H_c(T=0)$, κ , and the normal state susceptibility. Clear signatures in $\lambda(H)$ are seen at $T_m(H)$ and at the broadened H_{c2} . Both transitions exhibit good 3D-XY scaling, which clearly demonstrate the importance of thermal phase fluctuations. The driving force for most of the reversible magnetostriction is due to dT_c/dp_i . Below 55K and above 6-8T, $\lambda(H)$ becomes irreversible due to increased flux pinning at the order-disorder Bose-glass to vortex-glass transition. In contrast to the magnetization, which shows the typical monotonic peak effect, the irreversible magnetostriction exhibits reproducible fine structure within the transition region. This may be due to nucleation of distinct vortex domains in the crystal, which would provide clear evidence for a first-order transition.

TT 23.16 Mo 14:00 Poster TU D

Raman scattering from charge ordering fluctuations in cuprates — ●LEONARDO TASSINI¹, FRANCESCA VENTURINI¹, RUDI HACKL¹, QING-MING ZHANG², ANDREAS ERB¹, NAOKI KIKUGAWA³, and TOSHIZO FUJITA³ — ¹Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, D-85748 Garching — ²Department of Physics, Nanjing University, Nanjing 210093, P.R. China — ³ADSM, Hiroshima University, Higashi-Hiroshima 739-8526

The electronic Raman effect has been studied in differently doped single crystals of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) and of $\text{Y}_{0.97}\text{Ca}_{0.03}\text{Ba}_2\text{Cu}_3\text{O}_6$ (YBCO). The experimental data provide direct evidence of the formation of one-dimensional charged structures in the two-dimensional CuO_2 planes. The stripes manifest themselves in a Drude-like peak at low energies and temperatures. The selection rules allow to determine the orientation to be along the principle axes at $x = p = 0.10$ in LSCO and along the diagonals at $p = 0.02$ in LSCO and YBCO. The stripes fluctuate, and the correlation length is of the order of the electronic mean free path. In LSCO the temperature is the only scale of the response at different doping levels demonstrating the importance of quantum critical behavior. We provide an estimate of the quantum critical point in LSCO at $x_c = 0.18$.

TT 23.17 Mo 14:00 Poster TU D

Change of quasiparticle dispersion in crossing T_c in the underdoped cuprates — ●THOMAS ECKL¹, WERNER HANKE¹, SERGEY V. BORISENKO², and JÖRG FINK² — ¹Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — ²Institute for Solid State Research, IFW-Dresden, P.O. Box 27 00 16, D-01171 Dresden, Germany

One of the most remarkable properties of the high-temperature superconductors is a pseudogap regime appearing in the underdoped cuprates above the superconducting transition temperature T_c . The pseudogap continuously develops out of the superconducting gap. In this contribution, we demonstrate by means of a detailed comparison between theory and experiment that the characteristic change of quasiparticle dispersion in crossing T_c in the underdoped cuprates can be understood as being due to phase fluctuations of the superconducting order parameter. In particular, we show that within a phase fluctuation model the characteristic back-turning BCS bands disappear above T_c whereas the gap remains open. Furthermore, the pseudogap rather has a U-shape instead of the characteristic V-shape of a $d_{x^2-y^2}$ -wave pairing symmetry and starts closing from the nodal $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ directions, whereas it rather fills in at the anti-nodal $\vec{k} = (\pi, 0)$ regions, yielding further support to the phase fluctuation scenario.

TT 23.18 Mo 14:00 Poster TU D

Dynamical spin susceptibility in the d -density wave state: a comparison of theory and experiment — ●JAN-PETER ISMER and ILYA EREMIN — Institut für Theoretische Physik, Freie Universität Berlin, D-14195 Berlin, Germany

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. Furthermore, we investigate the structure of the particle-hole continuum, the formation of so-called 'silent' bands, and most interestingly, the behavior of the upward part of the resonance peak dispersion. The new features arising due to DDW ordering are discussed.

TT 23.19 Mo 14:00 Poster TU D

Surface critical currents below and above $H_{c2}(T)$ of Niobium — ●LARS VON SAWILSKI and JÜRGEN KÖTZLER — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

By using a conventional and a novel gradient [1] inductive method, the critical current at the surface of Nb-cylinders is measured below and above the upper critical field, respectively. Upon smoothing the surface of as-grown cylinders by chemical and electrical polishing from some 100 nm to 1 nm, not only the critical current below H_{c2} is decreased by a factor of three but also the flux-jumps disappears, possibly due to a reduction of pinning at the surface. On the other hand, $j_c(H > H_{c2})$ increased towards the value predicted for a multiply connected superconducting surface [2].

However, chemical impurities induced by polishing, may cause a strong degradation of j_c , though the critical fields are enhanced.

[1] J. Kötzler et al., PRL **92**, 067005 (2004)[2] H. J. Fink and L. J. Barnes, PRL **15**, 792 (1965)

TT 23.20 Mo 14:00 Poster TU D

Feldabhängigkeit grenzflächeninduzierter Supraleitung — ●V. KOERTING^{1,2}, QINGSHAN YUAN³, P.J. HIRSCHFELD⁴, T. KOPP¹, J. MANNHART¹ und C.W. SCHNEIDER¹ — ¹Center for Electronic Correlations and Magnetism, EP6, Univ. Augsburg, Germany — ²Institut fuer Theorie der Kondensierten Materie, Univ. Karlsruhe, Germany — ³Texas Center for Superconductivity and Advanced Materials, Univ. Houston, USA — ⁴Department of Physics, Univ. of Florida, Gainesville, USA

In einem zwei-dimensionalen (2D) Elektronengas betrachten wir die Cooper-Paarbildung, die durch einen benachbarten Film, bestehend aus polarisierbaren lokalen Anregungen, feldabhängig induziert wird. Im Rahmen eines Modells, das die Wechselwirkung zwischen 2D Elektronen und lokalisierten Zwei-Niveau Systemen beschreibt, berechnen wir die kritische Temperatur T_c in Abhängigkeit der angelegten Spannung. Ausgehend von der Annahme, dass eine ausreichende Ladungsträgerdichte in diesem Feldeffekt-Bauelement induziert werden kann, zeigen wir, dass es möglich sein sollte, Supraleitung in solchen Systemen zu beobachten. Für die Sprungtemperatur T_c finden wir eine nicht-monotone Abhängigkeit sowohl von dem elektrischen Feld als auch von der Anregungsenergie der Zwei-Niveau Systeme.

TT 23.21 Mo 14:00 Poster TU D

Effects of disorder with finite range on the properties of d -wave superconductors — ●SIMON SCHEFFLER, KURT SCHARNBERG, CARSTEN T. RIECK, and ATIF ISMAIL — I. Institut für Theoretische Physik, Universität Hamburg

It has long been established that disorder has profound effects on unconventional superconductors and it has been suggested repeatedly that observation and analysis of these disorder effects can help to identify the order parameter symmetry. In much of the relevant literature, including very sophisticated calculations of interference and weak localization effects, the disorder is represented by delta-function scatterers of arbitrary strength. One obvious shortcoming of this approximation is that resonant scattering resulting from the wavelength of the scattered quasiparticle matching the spatial extent of the defect is not included. We find that the mitigation of the T_c -reduction, expected when d -wave scattering is included, is very sensitive to the average strength of the scattering potential and is most effective for weak scatterers. Disorder with finite range not only has drastic effects on the predicted density of states at low energies, relevant for transport properties, but affects the spectral function at all energies up to the order parameter amplitude. The gap structure, which does not appear to be of the simplest d -wave form, should show a defect-dependent variation with temperature, which could be detected in ARPES experiments.

TT 23.22 Mo 14:00 Poster TU D

Exchange integrals in 1D versus 2D cuprates - an electronic structure study — ●ULRIKE NITZSCHE¹, STEFAN-LUDWIG DRECHSLER¹, and HELGE ROSNER² — ¹Leibniz Institute for Solid State and Materials Research Dresden — ²MPI for Chemical Physics of Solids

We present a systematic study of the electronic structure and the exchange integrals for different types of 1D and 2D cuprate networks: edge and corner shared single-chain (Li_2CuO_2 , Sr_2CuO_3), double-chain (SrCuO_2), ladder-type ($\text{Sr}_2\text{Cu}_2\text{O}_3$) and planar (CaCuO_2 , $\text{Sr}_2\text{CuO}_2\text{Cl}_2$) 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 models from one-band and multi-band approaches. We investigate the effect of the network configuration (edge shared vs. corner shared CuO_2 plaquettes) and of the dimensionality on the coupling strength. The influence of external parameters like pressure and doping is briefly discussed.

TT 23.23 Mo 14:00 Poster TU D

Strong spin triplet contribution of the first removal state in the insulating regime of Bi-cuprates — ●R.-S. UNGER¹, C. JANOWITZ¹, U. SEIDEL¹, A. KRAPP¹, R. MANZKE¹, V. A. GAVRICHKOV², and S. G. OVCHINNIKOV² — ¹Humboldt Universität zu Berlin, Institut für Physik, 12489 Berlin — ²L.V.Kirensky Institute of Physics of the Siberian Branch of the Russian Academy of Science, Krasnoyarsk, 660036, Russia

The experimental dispersion of the first removal state in the insulating regime of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$ is found to differ significantly from that of other parent materials: oxycloides and La_2CuO_4 . For Y-contents of $0.92 \geq x \geq 0.55$ the crystal lattice parameters a,b,c change very strongly. This (a,b) parameter increase and c parameter decrease results in an unconventional three peak structure at $(0,0)$; $(\frac{\pi}{2}, \frac{\pi}{2})$; (π, π) for $x = 0.92$. We can describe the experimental data only beyond the framework of the 3-band pd-model involving the representations of a new triplet counterpart for the Zhang-Rice singlet state [1]. The former results, obtained on a cuprate with two CuO_2 -layers per unit cell, is found to be universal. Measurements on single layered $Bi_2Sr_{2-x}La_xCu_2O_{6+\delta}$ give similar results.

[1] JETP Lett, 80(11) in print. (2004)

TT 23.24 Mo 14:00 Poster TU D

Angular resolved photoemission on Pb-Bi2201: Doping-dependent evolution of the pseudogap in the underdoped case — ●L. DUDY¹, B. MÜLLER¹, L. LASOGGA¹, A. KRAPP¹, H. DWELK¹, C. JANOWITZ¹, R. MANZKE¹ und H. HÖCHST² — ¹Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — ²Synchrotron Radiation Center (SRC), Madison/Wisconsin (USA)

In search for the pairing mechanism of the hole doped HTSCs there is still a debate about the pseudogap [1]. Some groups report a vanishing pseudogap around optimum doping [2]. Other measurements show in the overdoped region a smooth convergence of the pseudogap temperature with T_c , which gives the idea to treat the pseudogap state as a normal state precursor of the superconducting gap due to local, dynamic pairing correlations in a state without long range phase coherence[3]. An important point has been observed in the layered cuprates, which show that the pseudogap temperature T^* is almost not dependent of the number of CuO layers[4]. We focus our work on measurements of the Pb and La doped one-layer Bi2201 single crystals. Here we present temperature dependent ARPES data from the optimum doped Pb-Bi2201 ($T_c = 32K$) down to the strongly underdoped ($T_c \sim 0K$) case. The data shows the evolution of the pseudogap temperature T^* and the magnitude Δ^* with respect to doping. [1] T. Timusk et al., Rep. Prog. Phys. **62** (1999), 61-122 [2] J.L. Tallon et. al., Physica C **282-287** (1997) 236-239 [3] V.J. Emery et al., Nature **374** (1995), 434 [4] T. Honma et al., cond-mat/0309597 (2003), accepted for Phys. Rev. B

TT 23.25 Mo 14:00 Poster TU D

Four-Unit-Cell Superstructure in the Optimally Doped $YBa_2Cu_3O_{6.92}$ Superconductor — ●Z. ISLAM¹, X. LIU², S.K. SINHA², J.C. LANG¹, S.C. MOSS³, D. HASKEL¹, G. SRAJER¹, P. WOCHNER⁴, D.R. LEE¹, D.R. HAEFFNER¹, and U. WELP⁵ — ¹Advanced Photon Source, ANL, Argonne, USA — ²University of California, San Diego, USA — ³University of Houston, USA — ⁴MPI f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ⁵Materials Science Division, ANL, Argonne, USA

Diffuse x-ray scattering measurements reveal that the optimally doped $YBa_2Cu_3O_{6.92}$ superconductor is intrinsically modulated due to the formation of a kinetically limited 4-unit-cell superlattice, $q_0 = (1/4, 0, 0)$, along the shorter Cu-Cu bonds. Long-range strains emanating from these modulated regions generate an inhomogeneous lattice which may play a fundamentally important role in the electronic properties of yttrium-barium-copper-oxides.

TT 23.26 Mo 14:00 Poster TU D

Competing magnetic instabilities in 214-ruthenates — ●P. STEPFENS¹, O. SCHUMANN¹, O. FRIEDT¹, M. BRADEN¹, Y. SIDIS², J. KULDA³, S. NAKATSUJI⁴, N. KIKUGAWA⁴, and Y. MAENO⁴ — ¹II. Physikal. Institut, Uni Köln — ²LLB, France — ³ILL, France — ⁴Kyoto University, Japan

We present the results of inelastic neutron scattering on pure and doped Sr_2RuO_4 .

The role of magnetic excitations in the pairing mechanism of the spin-triplet superconductor Sr_2RuO_4 is still unclear. The excitation spectrum is dominated by incommensurate fluctuations (caused by Fermi-surface-

nesting) at $q=(0.3,0.3,q_l)$. We determined their anisotropy of in-plane and out-of-plane component. In addition, we found a broad ferromagnetic signal (presumably the γ -band contribution) around $q=0$.

On minor substitution of Ru^{4+} by Ti^{4+} , the incommensurate fluctuations get enhanced and finally condense into static order. We present first results on the excitation spectra of samples with and without order.

Doping with La increases the number of electrons, and the shift of the nesting signal indicates that the filling occurs predominantly in the one-dimensional bands.

Especially interesting is the phase diagram created by substitution of Sr by Ca. The compounds near $Ca_{1.5}Sr_{0.5}RuO_4$ show almost ferromagnetic behaviour. In contrast to Sr_2RuO_4 , the excitation spectrum is dominated by fluctuations at $(0.22,0,0)$. At low energy and temperature the spectrum becomes ferromagnetic.

TT 23.27 Mo 14:00 Poster TU D

Renormalization group studies of pairing mechanism and order parameter symmetry in Sr_2RuO_4 — ●ANDREY KATANIN^{1,2}, ARNO KAMPF³, and IVAN LEONOV³ — ¹Max-Planck-Institut fuer Festkoerperforschung, 70569 Stuttgart, Germany — ²Institute of Metal Physics, 620219 Ekaterinburg, Russia — ³Institut fuer Physik, Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universitaet Augsburg, 86135 Augsburg, Germany

We study superconducting pairing in Sr_2RuO_4 by application of the functional renormalization group method combined with the Bethe-Salpeter analysis to realistic 3-band Hubbard model, which describes this compound. The competition of singlet and triplet pairings with different symmetries is investigated within this model. The results are compared to earlier proposals on the mechanism of triplet pairing in Sr_2RuO_4 .

TT 23.28 Mo 14:00 Poster TU D

Magnetic quantum oscillations in the normal and superconducting state of YNi_2B_2C — ●O. IGNATCHIK¹, J. WOSNITZA¹, M. JÄCKEL¹, D. SOUPTTEL², G. BEHR², and P. CANFIELD³ — ¹Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — ²Leibniz-Institut für Festkörper- und Werkstofforschung (IFW), D-01069 Dresden, Germany — ³Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

The de Haas-van Alphen (dHvA) effect, or quantum oscillations of the magnetization, is the most direct method to study Fermi-surface properties in metals. It is remarkable, that these magnetic quantum oscillations persist deep into the vortex state of many type-II superconductors. The damping of the oscillation amplitude below the upper critical field can be related to the magnitude of the superconducting gap. For YNi_2B_2C , however, quite controversial results for the dHvA signal in the superconducting state have been reported. We will present dHvA measurements of YNi_2B_2C single crystals prepared by different methods. The flux-grown crystals exhibit dHvA oscillation in the superconducting state down to 3 T as reported in literature. However, we observed an unexpectedly sudden vanishing of the dHvA signal in the mixed state for crystals grown by a zone-melting method. The very quick disappearance of the oscillating signal below B_{c2} suggests an unexpected fast opening of a large superconducting gap. At high magnetic fields six different dHvA frequencies could be detected.

TT 23.29 Mo 14:00 Poster TU D

Lattice dynamics and electron-phonon coupling in $YBa_2Cu_4O_8$ — ●V. PANKOKE¹, R. HEID² und K.-P. BOHNEN² — ¹Forschungszentrum Karlsruhe, Institut für Wissenschaftliches Rechnen, P.O.B. 3640, D-76021 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe

The superconducting properties of $YBaCuO$ depend strongly on the oxygen content thus it is of crucial importance to understand the lattice dynamics and the electron-phonon coupling as function of doping. While it has been possible to investigate these quantities recently with modern ab-initio methods [1] studying doping effects is a much more difficult task due to the loss of translational invariance. Fortunately, some ordered structures exist which can be treated rigorously with modern density functional methods. Among these $YBa_2Cu_4O_8$ plays a special role due to the fact that this compound contains double Cu-O chains a structural building block which is very rare in the high- T_c compounds. Using the density functional perturbation approach we have studied the lattice dynamics and electron-phonon coupling of $YBa_2Cu_4O_8$. Results will be compared with available experimental data. Good agreement between

calculated and measured vibration frequencies was obtained however eigenvectors inferred from experiments differ in some cases substantially from the calculated ones. These differences will also be discussed.

[1] K.-P. Bohnen, R. Heid, M. Krauss, *Europhys. Lett.* **64**, 104 (2003)

TT 23.30 Mo 14:00 Poster TU D

Electronic structure and weak electron-phonon coupling in TiB₂ — ●EUGENIO FORZANI¹ and HELGE ROSNER² — ¹I. Physikalisches Institut, Universität Göttingen — ²MPI for Chemical Physics of Solids, Dresden

The Fermi surface of TiB₂ was studied with the de Haas-van Alphen (dHvA) effect in order to clarify the electronic analogies with the previously investigated ZrB₂ [1]. This effort intends to revise a past work [2], which accused sample limitations, and to extend the investigation of the transition metal diborides of the fourth group. For a definite assignment of all the dHvA frequencies the angular dependencies of the extremal cross-section areas are estimated from full-potential band structure calculations [3]. In order to explain the absence of conventional superconductivity also in this diboride compound, the electron-phonon coupling constants are deduced from the experimental and theoretical datas. Developments of the measurement technique and new goals are discussed.

[1] S.L. Drechsler et al., *J. of Low Temp. Phys.* **131**, 5/6 (2003)

[2] T. Tanaka and Y. Ishizawa, *J. Phys. C: Solid St. Phys.* **13**, 6671-6 (1980)

[3] H. Rosner et al., *Phys. Rev. B* **66**, 024521 (2002)

*With grant of the Göttingen Graduate School of Physics

TT 23.31 Mo 14:00 Poster TU D

Electronic structure and electron phonon coupling in Sc doped MgB₂ — ●VIVIEN PETZOLD and HELGE ROSNER — MPI for Chemical Physics of Solids

Recently, Agrestini et al. reported a detailed study of the effects of Sc substitution in Mg_{1-x}Sc_xB₂ [1]. For the achievable Sc doping levels ($x=0.12\dots0.27$), the compound shows only a very small lattice expansion, allowing this way the separation of lattice and doping effects on the critical temperature $T_c(x)$ and on the frequency $\omega_{E_{2g}}$ of the E_{2g} phonon. To investigate the influence of the Sc concentration x 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 lead to consistent results with respect to lattice expansion and electronic properties (density of states, Fermi surfaces). We demonstrate that the doping dependent changes in the electronic structure are strongly influenced by the $sp^2(\text{B})-d(\text{Sc})$ hybridization. The dependence of the electronic topological transition proposed by Agrestini et al.[1] from the Sc concentration is discussed.

[1] Agrestini et al. *Phys. Rev. B* **70** 134514 (2004).

TT 23.32 Mo 14:00 Poster TU D

Observation of a second energy gap in Nb₃Sn — ●M. MARZ¹, R. LORTZ², A. JUNOD², W. GOLDACKER³, and G. GOLL¹ — ¹Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²Department of Condensed Matter Physics, University of Geneva, CH-1211 Geneva 4, Switzerland — ³Forschungszentrum Karlsruhe, Institut für Technische Physik, D-76021 Karlsruhe, Germany

Nb₃Sn is a well-known technically applied superconductor with critical temperature $T_c \approx 18$ K. Recently, a low-temperature anomaly in the specific-heat data on a particularly dense and homogeneous polycrystalline sample has been interpreted in terms of the presence of a second superconducting gap [1]. We performed point-contact spectroscopy on samples of the same batch using the break-junction technique. A small bar of Nb₃Sn has been broken at liquid-helium temperature in order to obtain a freshly cleaved surface. We measured the differential resistance as a function of applied voltage in the temperature range between 1.5 and 20 K. Several characteristic minima in the dV/dI vs V curves can be interpreted only under the assumption of two superconducting energy gaps in Nb₃Sn. From a comparison with calculated curves for superconductor-superconductor contacts we deduced a large gap $\Delta_L = 3.5 \pm 0.2$ meV and a small gap of $\Delta_S = 0.8 \pm 0.2$ meV. This is the first spectroscopic confirmation of two-gap superconductivity in Nb₃Sn. We note that Δ_L is in line with previous tunnelling measurements and the result confirms the interpretation of the specific-heat data.

[1] V. Guritanu *et al.*, *Phys. Rev. B* (2004) in print.

TT 23.33 Mo 14:00 Poster TU D

Investigation of CeCoIn₅/Pt point contacts in the normal and superconducting states — ●STEFAN KONTERMANN¹, GERNOT GOLL¹, TODD SAYLES², and M. BRIAN MAPLE² — ¹Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — ²Institute for Pure and Applied Physical Sciences, University of California, San Diego, La Jolla, CA 92093, USA

The ternary rare-earth compound CeCoIn₅ becomes superconducting for temperatures $T \leq 2.3$ K, the highest transition temperature among the heavy-fermion superconductors. Power-law behavior of the specific heat and the thermal conductivity in the superconducting state give evidence that the superconductivity in this material is unconventional. We report on investigations of CeCoIn₅ by point-contact spectroscopy with Pt as the normal-metal counterelectrode. In the normal state a pronounced asymmetry of the differential resistance dV/dI as a function of applied bias V is observed which becomes more pronounced as the temperature is reduced. For a contact in the ballistic regime the asymmetry can be attributed to the emergence of the coherent heavy-fermion liquid. In the superconducting state Andreev reflection of quasiparticles at a normal metal/superconductor interface leads to characteristic minima in the dV/dI vs V spectra. We measured spectra which show either a reduced resistance for bias $|V| < \Delta/e$ or a single minimum of dI/dV for $V = 0$, i. e. a zero-bias anomaly. The observation of a zero-bias anomaly is expected only if the order parameter exhibits a sign change as a function of k which leads to an Andreev bound state at the surface.

TT 23.34 Mo 14:00 Poster TU D

Unusual electronic and magnetic properties of intermetallic antiperovskites — ●CLAIRE LOISON, ANDREAS LEITHE-JASPER, and HELGE ROSNER — Max Planck Institut für Chemische Physik fester Stoffe, Nöthnitzerstrasse 40, 01187 Dresden, Germany

In the last years, cubic perovskites XYT_3 ($X=\text{Mg,Cu,La}\dots$, $Y=\text{B,C,N}\dots$ and T a transition metal) have received considerable attention because of many unusual physical properties caused by different competing interactions. Examples are the recently discovered superconductor MgCNi₃ or the non-collinear magnet CuNMn₃. Here, we present a systematic study of a series of antiperovskites ($RB_x\text{Pd}_3$ where R is a rare-earth metal, and x varies between 0 and 1) using density functional theory (DFT) electronic structure calculations within the local spin density approximation (LSDA). To investigate the role of possible strong Coulomb repulsion we applied as well LSDA+ U . We investigate the effects of pressure and doping on the electronic properties and magnetism. In order to interpret the discrepancies between the results on the lattice constants of LaB_xPd₃ as published by Dhar et al.[1] and our theoretical calculations, we examined this compound experimentally too. The insertion of boron in LaPd₃ ($a=4.1862(1)\text{\AA}$) could not be detected, but the exposure to oxygen resulted in an increased lattice constant of $a=4.2368(2)\text{\AA}$ close to the value published in [1]. They report a lattice constant independent of x ; according to our calculations, it should increase almost linearly and substantially with x . Thus, our results are inconsistent with the formation of LaB_xPd₃.

[1] Dhar et al. *Mat. Res. Bull.* **16** 1557 (1981).

TT 23.35 Mo 14:00 Poster TU D

Mirage phenomena in quantum corrals of s-wave superconductors — ●MARKUS SCHMID and ARNO P. KAMPF — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg

We investigate the local density of states (LDOS) for an s-wave superconductor in an elliptic quantum corral. Using a T-matrix analysis we explore the spatial structure of the LDOS in the presence of one or two magnetic/non-magnetic impurities and observe a variety of quantum mirage phenomena. In particular, we discuss mirage effects for localized impurity bound states and analyze the interference patterns for the scattering processes from two magnetic impurities in the quantum corral.

TT 23.36 Mo 14:00 Poster TU D

Josephson current through a Pb/Cu/Pb nanobridge — ●JONAS HANISCH¹, ALEXANDER COSCEEV¹, CHRISTOPH SÜRGER¹, HILBERT V. LÖHNESEN^{1,2}, and GERNOT GOLL¹ — ¹Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

The superconducting state is a macroscopic quantum state characterized by a macroscopic wave function with amplitude and phase. The

Josephson effect which occurs through a weak link between two superconductors is a direct consequence of the macroscopic phase carried by each superconductor. There exist several possibilities to manufacture a weak link. Here we report on a simple fabrication method and the characterization of planar Josephson contacts between two Pb electrodes weakly coupled through a Cu nanobridge on a sapphire substrate. In these superconductor (S)/normal metal (N)/superconductor junctions the Josephson coupling is mediated via the proximity effect at the S/N interfaces. For a long dirty junction ($l \ll \xi_N$, where l is the mean-free-path and ξ_N is the coherence length in N) the Josephson current I_c is proportional to $L/\xi_N \cdot \exp(-L/\xi_N)$ which gives an upper limit for the length L of the normal-metal bridge in order to observe Josephson coupling. A Josephson current of up to $750 \mu\text{A}$ at 1.5K was observed in junctions with L well below $1 \mu\text{m}$ which is only $1/8$ of the theoretically expected value. The reduction might originate from oxide layers at the normal metal/superconductor interfaces. The temperature and magnetic-field dependence of the Josephson current was investigated as well.

TT 23.37 Mo 14:00 Poster TU D

Alternative mechanism of the sign-reversal effect in Superconductor-Ferromagnet-Superconductor Junctions — ●ALEXANDRA ANISHCHANKA¹ and ANATOLI VOLKOV^{1,2} — ¹Theoretische Physik III, Ruhr-Universität Bochum, D-44801, Germany — ²Institute of Radioengineering and Electronics of the Russian Academy of Sciences, 103907 Moscow, Russia

We consider a simple model of a multidomain superconductor-ferromagnet-superconductor (SFS) Josephson junction. Sign-alternating magnetization M in domains leads to a spatial modulation of the phase difference $\phi(x)$. Due to this modulation the Josephson critical current I_c may have a different sign depending on the ratio of the magnetic flux in a domain, $4\pi Ma(2d_F)$, and the magnetic flux quantum. Just this, but not a nonmonotonic dependence of the local critical current density j_c , may be the reason for oscillations of the current I_c as a function of the F layer thickness $2d_F$ or temperature, observed in experiments.

TT 23.38 Mo 14:00 Poster TU D

Superconducting/ferromagnetic proximity effect mediated by Cr-spacer layers in the Fe/Cr/V/Cr/Fe thin film system — ●M. FATTAKHOV¹, I. GARIFULLIN², L. R. TAGIROV³, K. WESTERHOLT¹, and H. ZABEL¹ — ¹Institut für Experimentalphysik/Festkörperphysik Ruhr-Uni 44780 Bochum — ²Zavoisky Physical-Technical Institute, 420029 Kazan, Russia — ³Kazan State University, 420008 Kazan, Russia

We have studied the superconducting proximity effect in the thin film system Fe/Cr/V/Cr/Fe where the Cr layers play the role of screening layers between the superconducting V-layer and the strongly pair breaking Fe-layers. When keeping the thickness of the Fe-layers d_{Fe} fixed and varying the thickness of the Cr-layers d_{Cr} , the superconducting transition temperature T_c first rises reaching a maximum at $d_{Cr}=40 \text{ \AA}$ and then sharply drops for larger Cr-thickness. Keeping d_{Cr} constant and varying d_{Fe} the superconducting transition temperature becomes independent on d_{Fe} for $d_{Cr} > 40 \text{ \AA}$. The results demonstrate that the Cooper pairs penetrate into the Cr-layer to a depth of about 40 \AA . From our experimental results we suggest that the Cr-layer is nonmagnetic for $d_{Cr} < 40 \text{ \AA}$ and undergoes a transition to an incommensurate spin density wave state for $d_{Cr} > 40 \text{ \AA}$.

TT 23.39 Mo 14:00 Poster TU D

Non-ideal artificial phase discontinuity and fractional vortex dynamics in long Josephson 0- κ -junctions. — ●EDWARD GOLDOBIN¹, TOBIAS GABER¹, DIETER KOELLE¹, REINHOLD KLEINER¹, MICHAEL SIEGEL², and MANFRED NEUHAUS² — ¹Physikalisches Institut — Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen — ²Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe, Hertzstr. 16, 76187 Karlsruhe

We investigate the creation of an arbitrary κ -discontinuity of the Josephson phase in a long Nb-AlO_x-Nb Josephson junction (LJJ) using a pair of tiny current injectors, and study the formation of fractional vortices formed at this discontinuity. The current I_{inj} , flowing from one injector to the other, creates a phase discontinuity $\kappa \propto I_{inj}$. The calibration of injectors is discussed in detail. The small but finite size of injectors leads to some deviations of the properties of such a 0- κ -LJJ from the properties of a LJJ with an ideal κ -discontinuity. These experimentally observed deviations in the dependence of the critical current on I_{inj} and magnetic field can be well reproduced by numerical simulation assuming a finite injector size. The physical origin of these deviations is discussed.

Furthermore, we present new experimental results on the dynamics of arbitrary fractional vortices and report the observation of semi-integer zero field steps corresponding to $n = \frac{3}{2}$ and $n = \frac{5}{2}$.

TT 23.40 Mo 14:00 Poster TU D

Polarised SANS measurements of the FLL in niobium — ●SEBASTIAN MÜHLBAUER¹, ROBERT GEORGI² und PETER BÖNI¹ — ¹TU-München Physikdepartment E21 — ²ZWE FRM II TU-München

We report on polarised small angle neutron scattering (SANS) on the flux line lattice (FLL) of a well known classic superconductor, niobium on the reflectometer MIRA at the FRM-II in Garching. The six-fold symmetry of the scattering pattern of the FLL was recorded with a two-dimensional position sensitive SANS detector using a horizontal and vertical field geometry and an incident wavelength of 10 \AA . Even the second order peaks could be observed. We examined the chirality of the FLL, especially close to the on-set of the so-called flux line melting. The results of these measurements will be discussed with special emphasis on future measurements on high T_c superconductors.

TT 23.41 Mo 14:00 Poster TU D

Surface potential in superconductors — P. LIPAVSKÝ¹, ●K. MORAWETZ^{2,3}, JAN KOLÁČEK¹, J.J. MAREŠ¹, E.H. BRANDT⁴, and M. SCHREIBER² — ¹Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16258 Praha 6, Czech Republic — ²Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ³Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — ⁴Max-Planck-Institute for Metal Research, D-70506 Stuttgart, Germany

The electrostatic potential close to the surface of superconductors in the Meissner state is discussed. We show that beside the Bernoulli potential, the quasiparticle screening, and the thermodynamic contribution due to Rickayzen, there is a non-local contribution which is large for both type-I and weak type-II superconductors [1]. A generalization of the Budd-Vannimenus theorem is found which allows one to evaluate the observed potential without the explicit solution of the charge profile at the surface [2]. The electrostatic potential above the Abrikosov vortex lattice is evaluated numerically. We propose an experimental measurement by NMR [3] to access this field which can yield informations about material parameters.

[1] P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, M. Schreiber, Phys. Rev. B 69 (2004) 024524-1-7

[2] P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, M. Schreiber, Phys. Rev. B 70 (2004) 104518-1-7

[3] P. Lipavský, J. Kolacek, K. Morawetz, E. H. Brandt, Phys. Rev. B 66 (2002) 134525

TT 23.42 Mo 14:00 Poster TU D

Vortex dynamics in Nb films on faceted substrate surfaces — ●OLEKSIY K. SOROKA¹, MICHAEL HUTH², VALERIY A. SHKLOVSKIY³, JENS OSTER¹, and HERMANN ADRIAN¹ — ¹Institute of Physics, Johannes Gutenberg-University, Staudinger Weg 7, D-55099 Mainz, Germany — ²Institute of Physics, Johann Wolfgang Goethe-University, Robert-Mayer-Str. 2-4, D-60054 Frankfurt, Germany — ³Kharkiv National University, Physical Department, 4 Svobody Sq., 61077 Kharkiv, Ukraine

Anisotropy of the viscous damping force in superconductor can lead to the existence of the preferred directions for the vortices to move. Such a guided vortex motion leads to the appearance of new components in the galvanomagnetic response of the sample: an additional odd longitudinal and even transversal magnetoresistive components with respect to magnetic field reversal.

Perfect vortex guiding along the facet ridges was proved in Nb-films on faceted $\alpha\text{-Al}_2\text{O}_3$ by magnetoresistivity measurements. The thin film sample consisted of five microbridges oriented at the angles 0° , 30° , 45° , 60° and 90° with respect to the facet ridges. Field inversion was used to separate the even and odd components of the magnetoresistivities to obtain the contributions caused by the guided vortex motion.

The temperature dependences of the even longitudinal magnetoresistivity of the samples could be well fitted within the theoretical approach proposed by V. A. Shklovskij, using for the isotropic and anisotropic pinning potential a simple potential with a symmetric triangular wells whose depths were estimated from the experimental data.

TT 23.43 Mo 14:00 Poster TU D

Einfluss akustischer Oberflächenwellen auf die gemischte Phase in MgB_2 — ●ANDREAS HEINRICH¹, CHRISTIAN LEIRER¹, RUDOLF SCHNEIDER², BERND STRITZKER¹ und ACHIM WIXFORTH³ — ¹Universität Augsburg, EP IV, 86135 Augsburg — ²Forschungszentrum Karlsruhe, IFP, Karlsruhe — ³Universität Augsburg, EPI, 86135 Augsburg

Durch Einkoppeln elektromagnetischer Wellen in piezoelektrische Substrate können in diesen akustische Oberflächenwellen erzeugt werden. Dabei begleitet die Gitterdeformation einer solchen Welle immer auch ein elektrisches Feld. Beide Größen können dazu genutzt werden, um dünne Filme, welche auf das Substrat abgeschieden wurden, zu untersuchen bzw. zu beeinflussen. In dieser Arbeit wollen wir die Untersuchung von MgB_2 in der gemischten Phase mit Hilfe von akustischen Oberflächenwellen vorstellen. Einerseits wird auf die strukturellen und supraleitenden Untersuchungen der auf $LiNbO_3$ abgeschiedenen Schichten eingegangen. Trotz der stark unterschiedlichen Gitterparameter zwischen MgB_2 und $LiNbO_3$ konnten Schichten mit hoher kritischer Temperatur abgeschieden werden. Andererseits werden die Ergebnisse der Dämpfungsmessungen vorgestellt. Dabei zeigt sich, dass der Verlauf der Dämpfung durch ein BCS-artiges Verhalten beschrieben werden kann. Letztlich werden noch Anzeichen eines Akusto-elektrischen Effektes skizziert.

TT 23.44 Mo 14:00 Poster TU D

Shadow on the wall cast by an Abrikosov vortex — ●SIEGFRIED GRASER, CHRISTIAN INIOTAKIS, THOMAS DAHM, and NILS SCHOPHIL — Lehrstuhl für Theoretische Festkörperphysik, Auf der Morgenstelle 14, 72076 Tübingen

At the surface of a d -wave superconductor, a zero-energy peak in the quasiparticle spectrum can be observed. This peak appears due to Andreev bound states and is maximal if the nodal direction of the d -wave pairing potential is perpendicular to the boundary. We examine the effect of a single Abrikosov vortex in front of a reflecting boundary on the zero-energy density of states. We can clearly see a splitting of the low-energy peak and therefore a suppression of the zero-energy density of states in a shadow-like region extending from the vortex to the boundary. This effect is stable for different models of the single Abrikosov vortex, for different mean free paths and also for different distances between the vortex center and the boundary. This observation promises to have also a substantial influence on the differential conductance and the tunneling characteristics for low excitation energies.

TT 23.45 Mo 14:00 Poster TU D

Vortex core structure of a two-gap superconductor — ●ANDREAS GUMANN, SIEGFRIED GRASER, THOMAS DAHM und NILS SCHOPHIL — Universität Tübingen, Lehrstuhl für Theoretische Festkörperphysik, Auf der Morgenstelle 14, 72076 Tübingen, Germany

The recently discovered superconductor MgB_2 is believed to be a superconductor with two gaps. A single vortex line in such a system thus consists of two components, which are coupled to each other. Here, we present theoretical calculations of the core structure of such a vortex. Recently, it has been argued that Ginzburg-Landau theory cannot give a sufficient description of this situation. Therefore, we use quasiclassical Eilenberger theory employing the Riccati method. We present results for the self-consistently determined gap function and the local density of states in the vicinity of the vortex in the clean limit.

TT 23.46 Mo 14:00 Poster TU D

Local density of states at faceted boundaries of d -wave superconductors — ●CHRISTIAN INIOTAKIS, SIEGFRIED GRASER, THOMAS DAHM, and NILS SCHOPHIL — Universität Tübingen, Lehrstuhl für Theoretische Festkörperphysik, Auf der Morgenstelle 14, 72076 Tübingen, Germany

The local density of states at the boundary of a superconductor is a crucial factor in many experiments, for example tunneling measurements. For conventional s -wave superconductors, the local density of states at the boundary is practically the same as in the bulk. In particular, the specific boundary geometry is irrelevant. In the case of d -wave symmetry, however, the situation is completely different. Apart from the well-known formation of Andreev bound states at the surface, it is important to realize that for d -wave symmetry also the boundary geometry itself can have strong influence on the local density of states. In this work, we examine the local density of states at the surface of a d -wave superconductor for some basic examples of polygonal and faceted boundary geometries. We

also consider the additional influence of a single Abrikosov vortex pinned near the boundary geometry.

TT 23.47 Mo 14:00 Poster TU D

Elektrische Untersuchung serieller intrinsischer Josephsonkontaktarrays an dünnen $Tl_2Ba_2CaCu_2O_{8+x}$ Schichten auf r -cut Saphir und 20° vicinalem $LaAlO_3$ — ●MATTHIAS BÜENFELD¹, RALF BECHSTEIN¹, MICHAEL MANS¹, FRANK SCHMIDL¹, ALEXANDR GRIB², HENRIK SCHNEIDEWIND³ und PAUL SEIDEL¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743-Jena, Deutschland — ²Physics Department, Kharkov National University, 61077 Kharkov, Ukraine — ³IPHT Jena, Albert - Einstein - Str. 9, 07745-Jena, Deutschland

Zur Messung intrinsischer Josephsoneffekte wurden TBCCO Schichten zum einen auf Saphir hergestellt und zu Mesas strukturiert, zum anderen auf 20° vicinalem $LaAlO_3$ hergestellt und zu brückenartigen Strukturen strukturiert. Für eine Anwendung dieser Kontaktarrays ist es wichtig eine Synchronisation der Kontakte zu erreichen. Aus diesem Grund haben wir die Arrays in Resonatoren platziert. Zur Optimierung der Resonatoreigenschaften für Mesa-artige Arrays ist es nötig die Eigenschaften der dielektrischen Zwischenschicht zu kennen. Zu diesem Zweck wurden verschiedene Isolatormaterialien von uns untersucht. Für die brückenartigen Kontaktarrays wird gezeigt, wie sich ein zusätzlicher normalleitender Shunt auf die Möglichkeit der Synchronisation auswirkt. Sie wurden hierzu mit Goldschichten versehen und in einem Resonator platziert. Erste Ergebnisse werden vorgestellt. Diese Arbeit wurde gefördert durch die DFG (Nr. Se 664/10-3)

TT 23.48 Mo 14:00 Poster TU D

Intrinsic Josephson effects in the ferromagnetic superconductor $RuSr_2GdCu_2O_8$ — ●T. NACHTRAB¹, D. KOELLE¹, R. KLEINER¹, C. T. LIN², C. BERNHARD², R. KOCH³, and P. MÜLLER³ — ¹Physikalisches Institut - Experimentalphysik II, Universität Tübingen, 72076 Tübingen — ²Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — ³Physikalisches Institut III, Universität Erlangen-Nürnberg, 91058 Erlangen

The crystal lattice of the ruthenocuprate $RuSr_2GdCu_2O_8$ ($Ru1212$) can be described as an alternating stack of weakly ferromagnetic ($T_{mag} \approx 130$ K) RuO_2 and superconducting ($T_c \approx 55$ K) CuO_2 layers, separated by an insulating barrier of SrO . Besides the existence of an intrinsic Josephson effect as, e.g., in $Bi_2Sr_2CaCu_2O_{8+\delta}$ ($Bi2212$), more exotic phenomena, like the formation of intrinsic π -junctions, have been predicted due to the coexistence of ferromagnetism and superconductivity.

We present magnetization and electrical interlayer transport measurements on micron-sized single crystals of $Ru1212$. The magnetization data differ from former results on polycrystalline samples, confirming the anisotropic structure of the system. The transport measurements show clear evidence for an intrinsic Josephson effect below T_c [1]. Data obtained in magnetic fields reveal that fluxon motion takes place in a very similar fashion as in $Bi2212$. Although the RuO_2 subsystem gives a clear fingerprint in the transport data near T_{mag} , we did not observe any unconventional behavior due to the interplay of magnetism and superconductivity at low temperatures.

[1] T. Nachtrab *et al.*, Phys. Rev. Lett. **92**, 117001 (2004)

TT 23.49 Mo 14:00 Poster TU D

A LT-STM for spectroscopy on finite superconducting proximity structures — ●CHRISTIAN DEBUSCHEWITZ, FRANK MÜNSTERMANN, VOJKO KUNEJ, and ELKE SCHEER — Department of Physics, University of Konstanz, 78457 Konstanz

We present a low temperature STM for spectroscopy on finite superconducting proximity structures. The nonmagnetic STM head is based on a slip-stick coarse approach and works in a conventional ³He cryostat at $T = 240$ mK and a magnetic field up to 1 T. All electrical lines are radio-frequency filtered at low temperature in order to achieve the required energy resolution. For the determination of the energy resolution we measure the superconducting gap of aluminium at 240 mK. The proximity structure is fabricated by e-beam lithography and consists of normal metal islands (Au) on top of a superconducting plane (Al).

TT 23.50 Mo 14:00 Poster TU D

Fractional thermal magnetoconductance of one-dimensional proximity systems — ●GRIGORY TKACHOV — Institute for Theoretical Physics, Regensburg University, 93040 Regensburg, Germany

While phase-coherent charge transport in mesoscopic normal metal/superconductor systems has been receiving considerable attention, heat conduction properties of such proximity structures have been explored to a much lesser extent (see, e.g. Refs. [1,2]). The purpose of this talk is to present a theoretical study of anomalous magnetic field behaviour of heat transport in quasi-one-dimensional ballistic wires coupled in parallel to superconductors [3,4]. The proximity effect is described in terms of Andreev bound states whose spectrum acquires a minigap due to the mixing of particle and hole states in the wire. In the presence of a magnetic field B , a specific interplay between the Zeeman spin splitting and the effect of a proximity-induced screening supercurrent is found to preserve time-reversal symmetry for certain groups of Andreev states with the minigap independent (or weakly dependent) of B . In this regime the low-temperature thermal magnetoconductance of the wire is predicted to increase in portions equal to half of the thermal conductance quantum.

[1] J. Eom, C.-J. Chien, and V. Chandrasekhar, Phys. Rev. Lett. **81** 437 (1998); A. Parsons, I. A. Sosnin, and V. T. Petrushov, Phys. Rev. B **67** 140502 (2003).

[2] E. V. Bezuglyi and V. Vinokur, Phys. Rev. Lett. **91** 137002 (2003).

[3] G. Tkachov, to appear in Physica C (2005);cond-mat/0402158.

[4] G. Tkachov and V. I. Fal'ko, Phys. Rev. B **69** 092503 (2004).

TT 23.51 Mo 14:00 Poster TU D

Oscillations of Superconducting T_c in Nb/Cu_xNi_{1-x} Bilayers With Subnanometer Thick Ferromagnetic Layer — ●V. I. ZDRAVKOV^{1,2}, A. S. SIDORENKO^{1,3}, V. RYAZANOV⁴, V. OBOZNOV⁴, M. SCHRECK², S. GSELL², S. HORN², C. MUELLER², and A. WIXFORTH² — ¹Institute of Applied Physics, MD-2028 Kishinev, Moldova — ²Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — ³Institute of Applied Physics, Universität Karlsruhe, D-76128 Karlsruhe — ⁴Institute of Solid State Physics, RU-Chernogolovka, Russia

Present work reports the results of proximity effect investigation for superconducting Nb/CuNi-bilayers with the thickness of the ferromagnetic layer (Cu_xNi_{1-x}) being in sub-nanometer scale. It was found a non-monotonic behavior of the critical temperature, T_c , i.e. its growth with the ferromagnetic layer thickness increasing, dF , for series of samples with constant thicknesses of Nb layer, $dNb = \text{const}$. The samples were prepared on Si substrates using magnetron sputtering for Nb layer and RF-cathode sputtering for CuNi layer. Each set of the samples (with constant thickness of Nb layer and variable ferromagnetic layer thickness) was prepared within a one-deposition run using the special method of wedge-shaped films deposition technique. The thickness dF and the Cu/Ni-ratio were precisely measured by RBS spectroscopy. The possible reasons of the T_c non-monotonic behavior at the sub-nanometer range of dF variation are discussed.

TT 23.52 Mo 14:00 Poster TU D

Superconductivity in Pd films on Eu_xSr_{1-x}S — ●A. COSCEEV^{1,2}, A. FAISS¹, C. PFLEIDERER¹, C. SÜRGER^{1,2}, and H. v. LÖHNESEN^{1,2,3} — ¹Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — ³Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

Superconductivity in Pd was reported earlier for He⁺-irradiated films [1] and for Ag/Pd/Ag sandwiches [2]. Here we investigate the effect of ferromagnetic order on the superconductivity of Pd films (thickness $d_{Pd} = 5 - 20$ nm) deposited on insulating Eu_xSr_{1-x}S. Samples have been prepared at different substrate temperatures T_S on 50-nm thick Eu_xSr_{1-x}S films on Si(111). For films with $d_{Pd} \leq 7$ nm prepared at $T_S = 300$ K a maximum $T_c = 0.9$ K is observed for $x = 0$, i.e. on nonmagnetic SrS. T_c decreases to 0.7 K for $x = 0.6$ possibly due to the contact with the magnetic insulator. For larger d_{Pd} , superconductivity is suppressed towards lower T which suggests that the superconducting phase is only stabilized in a narrow region near the Pd/Eu_xSr_{1-x}S interface. Application of a magnetic field clearly shows the gradual transition towards insulating behavior as seen by a logarithmic increase of the resistance R with decreasing temperature T . The magnetoresistance is positive up to a maximum field of 18 T supporting the presence of strong electron-electron interaction effects.

[1] B. Stritzker, Phys. Rev. Lett. **42**, 1769 (1979)[2] M. B. Brodsky, Phys. Rev. B **25**, 6060 (1982)

TT 23.53 Mo 14:00 Poster TU D

Andreev reflection in nanostructured Al/Ni point contacts — ●D. WEISSENBARGER^{1,2}, F. PÉREZ-WILLARD^{2,3}, C. SÜRGER^{1,2}, and H. v. LÖHNESEN^{1,2,4} — ¹Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — ²DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ³Laboratorium für Elektronenmikroskopie, Universität Karlsruhe, D-76128 Karlsruhe — ⁴Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The electronic transport through nanostructured Al/Ni contacts is studied by point-contact spectroscopy at low temperatures. Samples were fabricated by means of electron-beam lithography, reactive ion etching, and deposition of Al and Ni onto both sides of a Si₃N₄ membrane as previously reported [1]. Andreev spectra, i.e. conductance vs. voltage, were measured in dependence of temperature and applied magnetic field. The degree of current spin polarization P is obtained by fitting the whole set of experimental data with a theoretical model [1] which takes into account the spin-dependent transmission coefficients due to the majority and minority spin bands of the ferromagnet. For Ni the value of P determined from the spectra is smaller than for Co reported earlier [1].

[1] F. Pérez-Willard et al., Phys. Rev. B **69**, 140502(R) (2004)

TT 23.54 Mo 14:00 Poster TU D

Superconducting noise bolometer as a direct detector — ●ALEXEI SEMENOV¹, HEINZ-WILHELM HÜBERS¹, KONSTANTIN ILIN², MICHAEL SIEGEL², and ANDREAS ENGEL³ — ¹DLR Institute of Planetary Research, Berlin — ²Institute of Micro- and Nanosystems, University of Karlsruhe — ³Institute of Physics, University of Zürich

An advantage of superconducting detectors is a much lower noise in comparison to their semiconductor counterparts. We have studied the magnitude and spectrum of electric noise in thin superconducting NbN nanostrips carrying a subcritical current. Analysis of the experimental data suggests that the noise appears due to fluctuations in the two-dimensional vortex gas below the Kosterlitz-Thouless phase transition. Basing on our understanding of the noise source, we proposed a novel detector concept. The novelty is the use of the noise, which generally hampers the performance of conventional detectors, as the physical quantity that itself senses radiation. Our detector is a meander line patterned from a superconducting thin film and connected to the terminals of a planar log-periodic antenna. The detector operates in the current-carrying superconducting state and exhibits the noise that changes under irradiation. At 4.2 K measured noise-equivalent power amounted at 10^{-14} W Hz^{-1/2} and is likely to improve at lower temperatures.

TT 23.55 Mo 14:00 Poster TU D

Design und Entwicklung von Arrays kalorimetrischer Tieftemperatur Detektoren für die Energiemessung von Schwerionen — ●J.P. MEIER^{1,2}, A. BLEILE^{1,2}, P. EGELHOF^{1,2}, A. KISELEVA¹, O. KISELEV¹ and S. KRAFT-BERMUTH^{1,2} — ¹Gesellschaft für Schwerionenforschung, Darmstadt — ²Institut für Physik, Johannes Gutenberg Universität, Mainz

Kalorimetrische Tieftemperatur Detektoren mit Al-Phasenübergangsthermometer haben sehr gute Auflösungen für den Energienachweis von Schwerionen in einem breiten Energie- und Massenbereich. Für Schwerionen mit Energien von $E = 0.1-100$ MeV/amu wurde $\Delta E/E = 1-5 \times 10^{-3}$ erzielt. Damit eignen sich die Detektoren für den Energienachweis in verschiedenen Anwendungen der Schwerionen-Physik. Das aktuelle Detektor-konzept hat eine aktive Detektorfläche von ca. 2×3 mm². In Anwendungen wie der Identifikation superschwerer Elemente, der Beschleuniger-Massenspektrometrie oder für Reaktionen mit radioaktiven Schwerionenstrahlen werden größere aktive Detektorflächen gefordert. Hierfür ist der Aufbau eines Detektor-Arrays notwendig. In einem ⁴He-Badkryostaten sollen die einzelnen Pixel eines Arrays mit deren spezifischen Arbeitstemperaturen im Bereich von $T_{WP} = 1.4-1.5$ K betrieben werden. Im Design eines Prototypen-Arrays sind 5×2 Pixel vorgesehen. Resultate erster Testmessungen mit einem 2-Pixel-Detektor werden diskutiert.

TT 23.56 Mo 14:00 Poster TU D

Metallic magnetic calorimeters: design considerations for large area detectors and arrays — ●M. LINCK, A. BURCK, T. DANILYAROV, H. ROTZINGER, T. SCARBROUGH, A. FLEISCHMANN, and C. ENNS — Kirchhoff-Institut für Physik, Heidelberg, Germany

Metallic magnetic calorimetry is well suited for energy dispersive quantum detection. A metallic paramagnetic sensor, which is in tight thermal contact with a metallic absorber, is placed in a weak magnetic field. The sensor's magnetization is used to monitor the temperature. Changes in magnetization upon the absorption of a quantum are measured by a low-noise, high-bandwidth DC SQUID system.

Design considerations have been made to find different geometries of metallic magnetic calorimeters. Different shapes and sizes of a possible detector have been simulated, the energy resolution of such detectors has been calculated. It can be shown, that it is possible to increase the signal size and therefore the energy resolution by optimizing the geometry. We present the first results with a meander shaped geometry, which was also developed for large area detection. We discuss the energy resolution and show applications, such as the detection of molecule fragments, which require large detection areas.

TT 23.57 Mo 14:00 Poster TU D

Neues Verfahren zur räumlichen Abbildung der Leistungsverteilung von Mikrowellen — ●ANDRÉ KAESTNER, FELIX STEWING und MEINHARD SCHILLING — Institut für elektrische Messtechnik und Grundlagen der Elektrotechnik, TU Braunschweig, Hans-Sommer-Straße 66, D-38106 Braunschweig

Die Leistungsverteilung von Mikrowellen-Signalen auf dem Chip ist in sehr vielen Anwendungen eine wichtige Messgröße, insbesondere wenn es um die Analyse und Reduktion von parasitären Effekten geht. Bei den Frequenzen oberhalb von 100 GHz, die inzwischen in der Kommunikationstechnik erreicht werden, ist die Minimierung des Übersprechens zwischen den Mikrowellenleitungen und die Charakterisierung neuer dielektrischer Dünnschichtmaterialien interessant.

Unser messtechnischer Ansatz zur räumlichen Abbildung der Leistungsverteilung von Mikrowellen erlaubt durch den Einsatz von Josephson-Kontakten aus Hochtemperatur-Supraleitern eine Analyse der Signale von wenigen GHz bis weit in den THz-Bereich hinein. Die räumliche Auflösung hängt von den eingesetzten Antennenstrukturen und damit von der angestrebten Messbandbreite ab und kann vom Millimeterbereich bis unter 1 μm variiert werden. Die minimale Schrittweite unseres Scanners liegt in allen drei Raumrichtungen bei 100 nm.

TT 23.58 Mo 14:00 Poster TU D

Josephson effects in cold atomic fermionic gases near a Feshbach resonance — ●FLAVIO NOGUEIRA — Institut für Theoretische Physik, Freie Universität Berlin

The Josephson effects that emerge out of a system featuring two fermionic atomic gases in contact through a weak link is considered. The subsystems are assumed to be near a Feshbach resonance. The results will be derived both microscopically and phenomenologically. In the Josephson current appears three types of phase differences: (i) a phase difference $\Delta\theta = \theta_1 - \theta_2$ corresponding to the phases θ_1 and θ_2 of the molecular bosons of subsystems 1 and 2, respectively; (ii) a phase difference $\Delta\varphi = \varphi_1 - \varphi_2$, corresponding to the phases φ_1 and φ_2 of the Cooper pairs of subsystems 1 and 2, respectively; (iii) and a phase difference between molecular bosons and Cooper pairs across the link. The time dependence of the phase difference between molecules can be controlled by the detuning parameter. While for $\Delta\varphi$ the familiar Josephson time evolution holds, i.e., $d\Delta\varphi/dt = 2\Delta\mu$, where $\Delta\mu = \mu_1 - \mu_2$ is the difference between the chemical potentials, we obtain $d\Delta\theta/dt = 2\Delta\mu + \Delta\delta$, where $\delta_1 - \delta_2$ is the detuning difference. This type of effect may be used experimentally to probe the presence of Cooper pairs in the system by controlling the BCS-BEC crossover.

TT 23.59 Mo 14:00 Poster TU D

Density fluctuations of a hard-core Bose gas in a one-dimensional lattice — ●CHRISTOPHER MOSELEY, CENAP ATES, and KLAUS ZIEGLER — Institut für Physik, Universität Augsburg, 86135 Augsburg

We consider a hard-core Bose gas on a one-dimensional optical lattice with and without confining potential. For this purpose a model of the statistics of directed polymers in two dimensions is applied to the world lines of the hard-core bosons, such that a crossing of different world lines is prohibited. We find characteristic oscillations in the density-density

correlation function. Their wavelength diverges as the system undergoes a continuous transition from an incommensurate to a Mott insulating phase. The associated static structure factor vanishes as the Mott insulating phase is approached.

TT 23.60 Mo 14:00 Poster TU D

Magnetic field dependence of polarisation echos generated in mixtures of amorphous glycerin and heavy water — ●C. FISCHER, M. BARTKOWIAK, S. HUNKLINGER, and C. ENSS — Kichhoffinstitut für Physik, Universität Heidelberg, Germany

The properties of glasses at temperatures below a few kelvin are dominated by atomic tunneling systems. Measuring dielectric polarization echos are one way to gain a better understanding of these energetically low-lying excitations.

In this work we present measurements on glassy mixtures of glycerin and heavy water as well as on deuterated glycerin. We observed oscillations superimposed on the decay of spontaneous echos, the so-called quantum beating, as well as the alteration of the integrated echo amplitude by the application of an external magnetic field.

Both effects originate from the introduction of nuclear quadrupole moments to the amorphous system, they are a direct consequence of the deuteration. The beating frequencies measured were in good agreement with quadrupole frequencies determined in NMR experiments.

Having a technique sensitive to tunneling systems with nuclear quadrupoles only, we can use selective isotopic substitution as a marker method. This opens a new way to microscopic studies of the tunneling systems.

TT 23.61 Mo 14:00 Poster TU D

1/f-noise in quench condensed Ag films — ●MICHAEL BURST¹, SWASTIK KAR², ARUP K. RAYCHAUDHURI³, and GEORG WEISS¹ — ¹Physikalisches Institut, Universität Karlsruhe, Karlsruhe, Germany — ²Rensselaer Polytechnic Institute, Troy, USA — ³Indian Institute of Science, Bangalore, India

We present data of quench condensed silver films with a thickness of 10-20 nm. The samples are as small as $300 \times 100 \text{ nm}^2$. Experiments focus on the temperature region between 350 mK and 4.2 K. We show measurements on virgin films immediately after the deposition at low temperatures as well as measurements after annealing of the films. Our results of annealed films are in good agreement with former experiments under similar conditions. New and surprising results are obtained of the virgin samples: non-linear I-V characteristics and normalized noise power which is up to 5 orders of magnitude higher than those of annealed samples.

TT 23.62 Mo 14:00 Poster TU D

Low-temperature investigation on thermal properties of glasses — ●ASTRID NETSCH, HSIN-YI HAO, SABINE WOLF, ANDREAS ROST, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

The thermal conductivity of glasses at temperatures below 1 K is generally described by phonon thermal transport. The mean free path of the phonons is limited by scattering processes between the heat-carrying phonons and the tunneling systems in the glasses. At further low temperature, it is possible that the interactions between the tunneling systems also contribute to the thermal conductivity. To investigate such an additional heat transport mechanism one has to reduce the phonon mean-free-path to cut down the phonon contribution. That means one has to make some restrictions to the geometry of the glass sample.

We present measurements of the thermal conductivity of a glass capillary array which is used to introduce extra scattering of the thermal phonons. For measuring thermal conductivity of such diminutive magnitude, our contact-free technique is proved to be ideal owing to its surpassingly small parasitic heating to the system. Our results show a thermal conductivity, which varies proportional to T^3 down to about 50 mK as expected for boundary scattering. Below this temperature the heat transport deviates from this dependence, being larger than expected. This might be an indication for non-phonon thermal transport of heat in glasses.

TT 24 Symposium Nanomechanics

Zeit: Dienstag 10:15–12:50

Raum: TU H104

Hauptvortrag

TT 24.1 Di 10:15 TU H104

Single-Electron Transport in Nano-Electromechanical Devices — ●YAROSLAV M. BLANTER — Kavli Institute of NanoScience, Delft University of Technology, 2628 CJ Delft, The Netherlands

We first review existing experimental and theoretical developments in nanoelectromechanical systems (NEMS) in the single-tunneling regime. Next, we discuss effect of electric degrees of freedom on the mechanical properties and show that eigenfrequencies of suspended beams can be tuned by the gate voltage (as confirmed recently by the Cornell group). Then, we consider the situation of a strong mechanical feedback and discuss the modification of transport properties by mechanical motion.

Hauptvortrag

TT 24.2 Di 10:50 TU H104

Nano-Electromechanical Systems with Carbon Nanotubes — ●YUVAL YAISH, VERA SAZONOVA, ETHAN D. MINOT, HANDE ÜSTÜNEL, DAVID ROUNDY, TOMAS A. ARIAS, and PAUL L. MCEUEN — Laboratory of Atomic and Solid-State Physics, Cornell University, Ithaca, NY 14853, USA

Carbon nanotubes (NTs) offer a unique opportunity to scale down Nano Electro Mechanical Systems (NEMS) to the nanometer scale. Here we present our recent results in which guitar-string-like oscillation modes of doubly clamped nanotube oscillators were found. These resonance frequencies can be widely tuned electrostatically and their quality factor increases as temperature decreases. The static behavior of suspended NTs is intriguing as well. We will discuss their electrical response to mechanical perturbations and magnetic fields.

Fachvortrag

TT 24.3 Di 11:25 TU H104

Some Quantum Phenomena in Nanoelectromechanical Systems — ●JÖRG P. KOTTHAUS — Department für Physik and Center for NanoScience, LMU München

In an effort to create a single electron shuttle we study a nanoelectromechanical system (NEMS) etched out of Si and containing a metallic island which driven by Coulomb forces mechanically oscillates and transfers charge between two contacts. With increasing ac bias we find in the dc current a transition from charge transport via normal tunneling to transport via field emission from the isolated nanoscale island. It deviates in a characteristic fashion from the usual Fowler Nordheim description of field emission [1]. GaAs-based NEMS containing a low-dimensional electron gas are fabricated suitably to enable the definition of an individual quantum dot within a suspended beam. The low temperature electron transport through such a suspended quantum dot is found to exhibit a new characteristic gap in the diamond-like conductance spectra caused by Coulomb blockade. It is interpreted as a phonon blockade [2] caused by coherent transfer of electronic energy to a quantized thickness vibration of the thin suspended cavity, in analogy to the Franck-Condon principle in molecular systems [3].

[1] A. D. V. Scheible, C. Weiss, J. P. Kotthaus, and R. H. Blick, Phys. Rev. Lett. 93, 186801 (2004)

[2] E. M. Weig, R. H. Blick, T. Brandes, J. Kirschbaum, W. Wegscheider, M. Bichler, and J. P. Kotthaus, Phys. Rev. Lett. 92, 046804 (2004)

[3] J. Koch and F. von Oppen, cond-mat/0409667

Fachvortrag

TT 24.4 Di 12:00 TU H104

Cooling and squeezing nanomechanical resonators with Josephson qubits — ●ALEXANDER SHNIRMAN¹, PETER RABL², IVAR MARTIN³, LIN TIAN^{1,2}, and PETER ZOLLER² — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — ²Institute for Theoretical Physics, University of Innsbruck, A-6020 Austria — ³Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

We propose an application of a single Cooper pair box (Josephson qubit) for active cooling of nanomechanical resonators. Latest experiments with Josephson qubits demonstrated that long coherence time of the order of microsecond can be achieved in special symmetry points. Here we show that this level of coherence is sufficient to perform an analog of the well known in quantum optics “laser” cooling of a nanomechanical resonator capacitively coupled to the qubit. By applying an AC driving to the qubit or the resonator, resonators with frequency of order 100 MHz and quality factors higher than 10^3 can be efficiently cooled down to their ground state, while lower frequency resonators can be cooled down to micro-Kelvin temperatures.

In addition we show how the resonator can be driven into a squeezed state by choosing the appropriate coupling to a Josephson charge qubit. The stationary squeezed state of the resonator exhibits a reduced noise in one of the quadrature components by a factor of 0.5 - 0.2. These values are obtained for a 100 MHz resonator with a Q-value of 10^4 to 10^5 and for $T \approx 25$ mK. We show that the coupling to the charge qubit can be used to detect the squeezed state via measurements of the excited state population. Furthermore, by extending this measurement procedure a complete quantum state tomography of the resonator state can be performed. This provides a universal tool to detect a large variety of different states and to prove the quantum nature of a nanomechanical oscillator.

TT 24.5 Di 12:35 TU H104

Charge transport through a SET with a mechanically oscillating island — ●WOLFGANG BELZIG¹, NIKOLAI M. CHTCHELKATCHEV², and CHRISTOPH BRUDER¹ — ¹Department of Physics and Astronomy, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — ²L.D. Landau Institute for Theoretical Physics, Russian Academy of Sciences, 117940 Moscow, Russia

We consider a single-electron transistor (SET) whose central island is a nanomechanical oscillator. The gate capacitance of the SET depends on the mechanical displacement, thus, the vibrations of the island may influence the transport properties. Harmonic oscillations of the island and thermal vibrations change the transport characteristics in different ways. The changes in the Coulomb blockade oscillations and in the current noise spectral density help to determine in what way the island oscillates, and allow to estimate the amplitude and the frequency of the oscillations.

TT 25 Correlated Electrons - Low-dimensional Systems: Models

Zeit: Dienstag 09:45–13:00

Raum: TU H2053

TT 25.1 Di 09:45 TU H2053

Finite-frequency transport properties of dimerized and frustrated spin-1/2 chains — ●FABIAN HEIDRICH-MEISNER, ANDREAS HONECKER, and WOLFRAM BREINIG — Technische Universität Braunschweig, Institut für Theoretische Physik, Mendelssohnstraße 3, 38106 Braunschweig

We present a numerical study of both spin and thermal transport in dimerized and frustrated spin-1/2 chains at finite temperatures. Since both models are nonintegrable, the Drude weights scale to zero in the thermodynamic limit [1]. We therefore focus on the behavior of the conductivities at finite frequencies, studying the scaling with system size as well as the extrapolation to the zero-frequency limit. Results for three examples are presented. First, the dimerized chain is studied in the limit of weakly coupled dimers. In this case, interactions of the elementary triplet excitations are weak, which allows us to compute the life-times

of the energy and the spin current analytically in a perturbative scheme within a bond-boson operator representation. Second, we compare the conductivities of the frustrated chain in the massless and the massive regime of this model. Finally, we extract the zero-frequency thermal conductivity of the isotropic two-leg spin ladder from the numerical data and suggest a comparison with experimental results for $\text{La}_5\text{Cu}_9\text{Cu}_{24}\text{O}_{41}$ [2].

[1] F. Heidrich-Meisner et al., Phys. Rev. B 68, 134436 (2003).

[2] C. Hess et al., Phys. Rev. B 64, 184305 (2001).

TT 25.2 Di 10:00 TU H2053

Adaptive time-dependent DMRG: simulating the dynamics of strongly correlated systems — ●ULRICH SCHOLLWÖCK — Institut für Theoretische Physik C, RWTH Aachen, 52056 Aachen

The integration of concepts from quantum information theory has recently allowed the extension of DMRG to the high-precision calculation of the time-evolution of one-dimensional strongly correlated quantum systems at low algorithmic cost (Daley, Kollath, Schollwoeck, Vidal and White, Feiguin). The key idea is that the reduced Hilbert space generated by DMRG does not remain static in time or is enlarged at substantial computational cost, but adapts itself optimally to the time-evolving quantum state. I want to present the potential of this method for the calculation of far-from-equilibrium time-evolutions of quantum spin chains as well as the time-evolution of electronic models.

TT 25.3 Di 10:15 TU H2053

Adaptive time-evolution with DMRG for low dimensional correlated systems — ●SALVATORE MANMANA^{1,2}, ALEJANDRO MURAMATSU¹, and REINHARD NOACK² — ¹Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57/V, 70550 Stuttgart — ²AG Vielteilchennumerik, Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg

Only little is known about the physics of time-dependent problems in the field of strongly correlated quantum systems due to the lack of effective controlled approaches. Recently there has been progress in this direction for one dimensional systems. We present further developments in the construction of numerical schemes, in particular using exact diagonalization techniques and the density matrix renormalization group method (DMRG), which can be applied to correlated low-dimensional systems. Results for the collapse and revival of the metallic state in systems of spinless fermions with nearest-neighbour-interaction are discussed and the accuracy of these methods is compared with exact results.

TT 25.4 Di 10:30 TU H2053

Charge inhomogeneities in the one-dimensional t - J model — ●D. PERTOT, J. HUB, C. LAVALLE, and A. MURAMATSU — Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart

We study phase separation and related phenomena in the one-dimensional t - J model using a recently performance-improved version of our hybrid-loop QMC algorithm [1], which combines the loop and determinantal algorithms. The boundary of the phase-separated regime is determined and compared with previous results obtained by different techniques. In the phase-separated regime we find low energy spatially charge-ordered excited states ($\Delta E \ll J$). These excited states can be thought of as the electron-rich region of the phase-separated ground state being split up into multiple electron-rich regions with hole-rich regions in between. We discuss the behavior of the excitations far away from and close to the phase separation boundary when approaching the thermodynamic limit. Possible implications for experimental observations of charge-ordering in cuprates are pointed out.

[1] C. Lavalle *et al.*, Phys. Rev. Lett. **90**, 216401 (2003)

TT 25.5 Di 10:45 TU H2053

Anomalous self-energy and Fermi surface quasi-splitting in the vicinity of a ferromagnetic instability — ●ANDREY KATANIN^{1,2} and ARNO KAMPP³ — ¹Max-Planck-Institut fuer Festkoerperforschung, 70569 Stuttgart, Germany — ²Institute of Metal Physics, 620219 Ekaterinburg, Russia — ³Institut fuer Physik, Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universitaet Augsburg, 86135 Augsburg, Germany

We discuss the low-temperature behavior of the electronic self-energy in the vicinity of a ferromagnetic instability in quasi-dimensional systems. We show, that in the paramagnetic phase, where the long-range magnetic order is absent, the self-energy has a non-Fermi liquid form at low energies $|\omega| < \Delta_0$ near the Fermi level, where Δ_0 is the ground-state spin splitting. The spectral function at temperatures $T < \Delta_0$ has a two-peak structure with finite spectral weight at the Fermi level. The simultaneous inclusion of self-energy and vertex corrections shows that the above results remain qualitatively unchanged down to very low temperatures $T_C < T \ll \Delta_0$. It is argued, that this form of the spectral functions implies the quasi-splitting of the Fermi surface in the paramagnetic phase in the presence of strong ferromagnetic fluctuations.

TT 25.6 Di 11:00 TU H2053

Effects of Frustration in The Auxiliary-Fermion Approach to The 2D Quantum Heisenberg Model — ●JAN BRINCKMANN and PETER WÖLFLE — Institut für Theorie der Kondensierten Materie, Uni Karlsruhe, D-76128 Karlsruhe

Recently we studied the nearest-neighbor quantum-antiferromagnetic Heisenberg model for spin 1/2 on a two-dimensional square lattice [1]. A self-consistent approach based on the auxiliary-fermion representation of spin operators yields a correlation length $\xi(T) \propto \exp(2\pi\rho_S/T)$ as well as signatures of short-range order in the dynamical structure factor, in good agreement with the literature.

In the present work we study the effect of quantum fluctuations caused by an additional next-nearest-neighbor coupling J_2 (J_1 - J_2 -model). In mean-field theory the order parameter is finite at the border $\eta = J_2/J_1 = 1/2$ between the Néel and collinear ground states, corresponding to a finite stiffness ρ_S at $T > 0$. Within the self-consistent approach, however, we find that strong fluctuations drive $\rho_S \rightarrow 0$ at $\eta = 1/2$. We also study the influence of the local Hilbert-space constraint on the auxiliary particles by comparing two variations of the approach: First the constraint is approximately replaced by a global one (as has been utilised in [1]), second the constraint is imposed exactly using a method proposed in [2].

[1] J. Brinckmann, P. Wölffe, Phys. Rev. **B70**, in press (cond-mat/0405438)

[2] V. N. Popov, S. A. Fedotov, JETP **67**, 535 (1988)

TT 25.7 Di 11:15 TU H2053

Heat Transport in Almost Integrable Spin-Chains — ●PETER JUNG, ROLF HELMES, and ACHIM ROSCH — Institute of Theoretical Physik, Cologne University, Zùlpicher Str. 77, 50937 Köln, Germany

Integrable quantum spin chains are characterized by an infinite heat conductivity. We study the effect of small perturbations which destroy integrability. We evaluate a perturbation theory for $1/\kappa(T, \omega)$ using both exact diagonalization and a high temperature expansion which reconstructs the relevant correlation functions from its moments.

TT 25.8 Di 11:30 TU H2053

Excitation content of spectral functions in the 1D t-J model — ●C. LAVALLE¹, M. ARIKAWA², and A. MURAMATSU¹ — ¹Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany — ²Bergische Universität Wuppertal, Fachbereich Physik, D-42097 Wuppertal, Germany

The excitation content of spectral functions of the 1D t-J model with nearest neighbor interactions is obtained from the Bethe Ansatz solution at the supersymmetric point and compared with quantum Monte Carlo (QMC) simulations based on the hybrid-loop algorithm [1]. We consider the one-particle spectrum as well as the dynamical spin and charge structure factors. The connection to the 1D supersymmetric t-J model with $1/r^2$ interaction will be explained and the extension to experimentally relevant values of J/t will be discussed on the basis of QMC results.

[1] C. Lavalle *et al.*, Phys. Rev. Lett. **90**, 216401 (2003).

TT 25.9 Di 11:45 TU H2053

Spin Gap in a Spiral Staircase Model — ●MIKHAIL KISELEV¹, DIMITRY ARISTOV², and KONSTANTIN KIKOIN³ — ¹Institut für Theoretical Physics and Astrophysics, Würzburg University, 97074 Würzburg, Germany — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — ³Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

We investigate the formation of spin gap in one-dimensional models characterized by the groups with hidden symmetries. We introduce a new class of Hamiltonians for description of Spin Staircases - the spin systems intermediate between 2-leg ladders and S=1 spin chains. The spin exchange anisotropy along legs is described by the angle of spiral twist. The properties of a special case of Spin Rotator Chain (SRC) corresponding to a flat 1-leg ladder is considered by means of fermionization approach based on Jordan-Wigner transformation. The influence of dynamical hidden symmetries on the scaling properties of the spin gap is discussed.

TT 25.10 Di 12:00 TU H2053

Thermodynamics of a t - J chain with boundary impurities — ●GUILLAUME PALACIOS and HOLGER FRAHM — Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany

We consider a supersymmetric t - J chain with integrable boundary impurities. Within the framework of the Quantum Inverse Scattering Method (QISM), these impurities are constructed by the combination of boundary fields with an integrable impurity [1]. The impurity site differs from the bulk chain by allowing double occupancy of the local orbitals. In addition to the boundary fields, that can be either a chemical potential or a magnetic field imposed at the ends of the chain, the model possesses

two free parameters which allow to control the coupling between the Anderson-like impurity and the rest of the chain and the on-site interaction on the impurity site. It is of interest to mention that the latter can be tuned continuously without breaking the integrability of the model [2].

Starting from the Bethe Ansatz equations for the chain spectrum, our goal is to evaluate such impurities' contribution to thermodynamics quantities like magnetic susceptibilities or electronic densities.

[1] G. Bedürftig and H. Frahm, *J. Phys A* **32** (1999) 4585

[2] G. Bedürftig, F. H. L. Essler and H. Frahm, *Nucl. Phys. B* **489** (1997) 697

TT 25.11 Di 12:15 TU H2053

Quantum Creep and Variable Range Hopping of One-dimensional Interacting Electrons — •THOMAS NATTERMANN, SERGUEI MALININ, and BERND ROSENOW — Institut für Theoretische Physik der Universität zu Köln, Zùlpicher Str. 77, 50937 Köln

The variable range hopping results for non-interacting electrons of Mott and Shklovskii are generalized to 1D disordered charge density waves and Luttinger liquids using an instanton approach. Following a recent paper by Nattermann, Giamarchi and Le Doussal [*Phys. Rev. Lett.* **91**, 56603 (2003)] we calculate the quantum creep of charges at zero temperature and the linear conductivity at finite temperatures for these systems. The hopping conductivity for the short range interacting electrons acquires the same form as for non-interacting particles if the one-particle density of states is replaced by the compressibility. In the present paper we extend the calculation to dissipative systems and give a discussion of the physics after the particles materialize behind the tunneling barrier. It turns out that dissipation is crucial for tunneling to happen. Contrary to pure systems the new meta-stable state does not propagate through the system but is restricted to a region of the size of the tunneling region. This corresponds to the hopping of an integer number of charges over a finite distance. A global current results only if tunneling events fill the whole sample. We argue that rare events of extra low tunneling probability are not relevant for realistic systems of finite length. Finally we show that an additional Coulomb interaction only leads to small logarithmic corrections.

TT 25.12 Di 12:30 TU H2053

Nonlinear ac conductivity of disordered interacting 1d electrons — •BERND ROSENOW and THOMAS NATTERMANN — Institut für Theoretische Physik, Universität zu Köln, D-50932 Germany

We consider low energy charge transport in one-dimensional (1d) electron systems with short range interactions under the influence of a random potential. For not too attractive interactions, such systems are insulators and the ac conductivity $\sigma_{ac} \sim \omega^2 \ln(1/\omega)^2$ is described by a modified Mott-Halperin law [1]. At zero frequency, charge transport is only possible by the tunneling of charge carriers and the nonlinear dc conductivity is characterized by $I \sim \exp(-\sqrt{E_0/E})$ [2]. Combining RG and instanton methods, we calculate the nonlinear ac conductivity and discuss the crossover between the nonanalytic field dependence of the electric current at zero frequency and the linear ac conductivity at small electric fields and finite frequency [3].

[1] M. Fogler, *Phys. Rev. Lett.* **88**, 186402 (2002).

[2] T. Nattermann, T. Giamarchi, and P. Le Doussal, *Phys. Rev. Lett.* **91**, 056603 (2003).

[3] B. Rosenow and T. Nattermann, cond-mat/0408042.

TT 25.13 Di 12:45 TU H2053

Fermi Edge Singularities in the Mesoscopic Regime: From Rounded to Peaked Edge — •MARTINA HENTSCHEL^{1,2}, DENIS ULLMO¹, and HAROLD U. BARANGER¹ — ¹Duke University, Durham NC 27708-0305 (USA) — ²Universität Regensburg, D-93040 Regensburg

We study many-body effects associated with a sudden perturbation in a mesoscopic system, finding substantial differences from the bulk case. One example is the sudden, localized perturbation caused by an x-ray exciting a core electron into the conduction band. Here, Anderson orthogonality catastrophe (AOC) competes with a many-body effect caused by the interaction of the conduction electrons with the core hole. In the bulk, this produces deviations from the naively expected photoabsorption cross section in the form of a peaked or rounded edge. For a coherent system with chaotic dynamics, such as a nanoparticle or quantum dot, we use a random matrix model and find substantial changes: (1) the finite number of particles leads to an incomplete AOC, (2) the sample-to-sample fluctuations of the discrete energy levels produce a distribution of AOC overlaps, and (3) most importantly, the dipole matrix elements connecting the core and conduction electrons are substantially modified. One of our key results is that a photoabsorption cross section showing a rounded edge in the bulk will change to a slightly peaked edge on average as the system size is reduced to a mesoscopic (coherent) scale.

Supported in part by the NSF (DMR-0103003) and the Humboldt Foundation.

TT 26 Superconductivity - Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

Zeit: Dienstag 10:15–11:45

Raum: TU H3027

TT 26.1 Di 10:15 TU H3027

Heterstructures of YBCO and spin-polarized manganites - Playing around with superconducting properties — •JOACHIM ALBRECHT^{1,2}, SOLTAN SOLTAN² und HANNS-ULRICH HABERMEIER² — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

We have grown epitaxial bilayers of $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (LCMO) and optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) on single-crystalline substrates. Owing to the vicinity of the ferromagnetic, highly spin-polarized LCMO layer the properties of the YBCO film can change substantially. We investigated in detail the transition temperature [1], the critical current density [2] and the resistivity in the normal conducting state [3] of YBCO films in bilayers and heterostructures with different geometry. It is shown in this contribution that both the magnetic stray field and the spin polarization of the manganite strongly influences the properties of the YBCO thin film.

[1] S. Soltan, J. Albrecht and H.-U. Habermeier, *Phys. Rev. B* **70**, 144517 (2004).

[2] J. Albrecht, S. Soltan and H.-U. Habermeier, *Physica C* **408-410**, 482 (2004).

[3] S. Soltan, J. Albrecht and H.-U. Habermeier, *Solid State Comm.*, submitted

TT 26.2 Di 10:30 TU H3027

Experimental evidence for crossed Andreev reflections — •DETLEF BECKMANN¹, HEIKO B. WEBER¹, and HILBERT V. LÖHNEISEN^{2,3} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie — ²Forschungszentrum Karlsruhe, Institut für Festkörperforschung — ³Physikalisches Institut, Universität Karlsruhe

In our recent work [1], we have shown experimentally that electronic subgap transport in a superconducting non-local spin-valve can be described by the superposition of crossed Andreev reflection, i.e. the splitting of a Cooper pair into two different leads, and electron cotunneling, i.e. the transmission of an electron through the superconducting gap. Here, we report on experiments which allow us to discriminate both processes. We have extended our investigation from metallic point contacts to planar tunnel junctions, and replaced the non-local voltage detection (i.e. outside the current path) by a local detection scheme (along the current path). We observe a negative resistance which allows us to give a lower bound to the contribution due to crossed Andreev reflections alone. [1] D. Beckmann *et al.*, *PRL* **93** (2004) 197003

TT 26.3 Di 10:45 TU H3027

Andreev reflection in hybrid InGaAs/InP structures with superconducting NbN contacts — •I. E. BATOV¹, TH. SCHÄPERS², A. A. GOLUBOV³, and A. V. USTINOV¹ — ¹Physikalisches Institut III, Universität Erlangen-Nürnberg — ²ISG-1, Forschungszentrum Jülich — ³Faculty of Applied Physics, University of Twente, The Netherlands

We have studied magnetotransport and differential current voltage

characteristics of highly transparent superconductor/normal metal/two-dimensional electron gas junctions formed by a superconducting NbN electrode, a thin (10nm) Au interlayer, and a two-dimensional electron gas in an InGaAs/InP heterostructure. A decrease in the differential resistance with pronounced double dip structure has been observed within the superconducting energy gap. It is argued that the double-dip structure in the differential resistance is related to the transport in SN-2DEG contacts in the ballistic regime. It has been found that the reduced subgap resistance is preserved in high quantizing magnetic fields. We observed resistance oscillations as a function of magnetic field at zero dc bias current in our junctions. The effect of temperature and dc bias current on the amplitude of the magnetoresistance oscillations was studied. The experimental results are qualitatively explained by taking Andreev reflection in high magnetic fields into account.

TT 26.4 Di 11:00 TU H3027

Diamagnetic screening in Nb/Ag double layers in contact with a ferromagnet — ●H. STALZER¹, A. COSCEEV¹, C. SÜRGER¹, and H. V. LÖHNEYSEN^{1,2} — ¹Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The magnetization $M(T, B)$ of planar superconducting Nb/Ag and Nb/Ag/Fe heterostructures (thicknesses $d_{\text{Nb}} = 200$ nm, $d_{\text{Ag}} = 35 - 800$ nm, and $d_{\text{Fe}} = 40$ nm) epitaxially grown on sapphire (11 $\bar{2}$ 0) is studied in parallel magnetic fields B between temperatures of $T = 0.06 - 10$ K. Below the superconducting phase transition of Nb a further diamagnetic signal occurs at a temperature T^* due to screening currents in Ag induced by the proximity effect. In contact with an additional Fe layer the proximity effect vanishes for thick Ag layers ($d_{\text{Ag}} \geq 200$ nm). Surprisingly the diamagnetic transition at T^* reappears in Nb/Ag/Fe triple layers with a thickness of 20-35 nm. Furthermore, we investigate the effect of an additional SiO₂ spacer layer of thickness $d_{\text{SiO}_2} = 1 - 5$ nm, separating the Ag

and Fe film, on the diamagnetic phase diagram. We propose the realization of a tunable π -contact using weak ferromagnets.

TT 26.5 Di 11:15 TU H3027

Switching superconductivity in S/F bilayers by multiple-domain structures — ●THIERRY CHAMPEL and MATTHIAS ESCHRIG — Institut TFP, Universitaet Karlsruhe, 76128 Karlsruhe, GERMANY

We consider the effect of a multiple magnetic domain structure in a superconductor/ferromagnet bilayer, modeled by a ferromagnetic layer with a rotating magnetic moment. The domain walls in this model are of equal size as the domains, and are of Néel type. We study the superconducting critical temperature as a function of the rotation wavelength of the magnetic moment. The critical temperature of the bilayer is found to be always enhanced by the domain structure, and exhibits an interesting reentrant behavior. We suggest that this effect can be used for a new device where superconductivity may be controlled by the domain structure of the magnetic layer.

TT 26.6 Di 11:30 TU H3027

Charge Transport in Andreev Billiards with a Superconducting Antidot — ●A. LASSL¹, K. RICHTER¹, P. SCHMELCHER², F. DI-AKONOS³, M. SCHEID¹, and N. FITAS³ — ¹University of Regensburg — ²University of Heidelberg — ³University of Athens

We study the transport properties of a normal conducting electron billiard in contact with a superconductor. In particular we are interested in the magnetic field dependence of the particle and hole transmission and reflection coefficients. For our numerical simulations we chose a Sinai billiard with a superconducting antidot in the center of the quadratic scattering region. The presence of the superconductor changes the dynamics of the system due to Andreevreflection. The results of a purely classical and a quantum mechanical approach are presented and they show to be in very good agreement.

TT 27 Solids at Low Temperature - New Materials

Zeit: Dienstag 12:00–12:30

Raum: TU H3027

TT 27.1 Di 12:00 TU H3027

Wigner crystallization in Na₃Cu₂O₄ and Na₈Cu₅O₁₀ chain compounds — ●P. HORSCH, M. SOFIN, M. MAYR, and M. JANSEN — Max-Planck-Institut fuer Festkoerperforschung, D-70569 Stuttgart, Germany

We report the synthesis of novel edge-sharing chain systems Na₃Cu₂O₄ and Na₈Cu₅O₁₀, which form insulating states with commensurate charge order. We identify these systems as one-dimensional Wigner lattices, where the charge order is determined by long-range Coulomb interaction and the number of holes in the d-shell of Cu. Our interpretation is supported by X-ray structure data as well as by an analysis of magnetic susceptibility and specific heat data. Remarkably, due to large second neighbor Cu-Cu hopping, these systems allow for a distinction between the (classical) Wigner lattice and the $4k_F$ charge-density wave of quantum mechanical origin.

TT 27.2 Di 12:15 TU H3027

Influence of structural distortions on electronic properties of Ba₆Ge₂₅ clathrate — ●IVICA ZEREC¹, WILDER CARRILLO-CABRERA¹, VLADIMIR VOEVODIN¹, JÖRG SICHELSCHEIDT¹, ALEXANDER YARESKO², PETER THALMEIER¹, and YURI GRIN¹ — ¹Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

Clathrates are cage compounds, recently investigated as interesting candidates for thermoelectric applications. The complex structure poses a major challenge in understanding the variety of their interesting physical properties. We present the electronic band structure calculations for Ba₆Ge₂₅ clathrate. It undergoes an involved structural phase transition, accompanied with stepwise changes of many physical quantities. We construct the ordered structural models for different temperatures, in accordance with the experimental data and calculate the corresponding electronic band structures. We show how the changes of electronic properties across the phase transition may be understood from the modifications of the band structure induced by the structural distortions. In particular we show how the shift of the optical spectral weights towards higher frequencies, observed in the optical conductivity below the phase transition, is well reproduced by the theoretical calculations based on the electronic band structure.

TT 28 Superconductivity - Applications I : Cryodetectors

Zeit: Dienstag 14:00–16:00

Raum: TU H104

TT 28.1 Di 14:00 TU H104

Hauptvortrag

Cryogenic Detectors for X-ray Astronomy — ●PIET DE KORTE — Sorbonnelaan 2, 3584CA Utrecht, The Netherlands

The future of X-ray astronomy will be directed towards the study of very high redshift sources, that are therefore extremely weak. Some observational cases will be presented.

In addition to extremely large area collection optics this requires detectors with a high detection efficiency in combination with very good spectral resolution and imaging. Such a mission is conceptualized by the European Space Agency under the name XEUS.

The only type of sensors fulfilling those requirements are cryogenic sensors with single photon detection capability and an intrinsic en-

ergy resolution of a few eV at photon energies of a few keV. Microcalorimeters making use of the phase-transition between the normal-to-superconducting state for thermometry are at presently the most promising devices.

This paper will describe the characteristics of these so-called transition-edge-sensors (TES), their present performance and the means to make large imaging pixel arrays. Also the characteristics of SQUID-based read-out electronics will be presented.

TT 28.2 Di 14:30 TU H104

EDS- material analysis with Microcalorimeters — ●CHRISTIAN HOLLERITH¹, MATTHIAS BÜHLER², FRANZ V. FEILITZSCH¹, JENS HÖHNE², CHRISTIAN ISAILA^{1,3}, MICHAEL HUBER¹, JOSEF JOCHUM¹, KEVIN PHELAN², BIRGIT SIMMNACHER³, RAINER WEILAND³, and DOREEN WERNICKE^{2,1} — ¹Physik-Department E15, TU München, James-Franck-Straße, 85747 Garching — ²VeriCold Technologies GmbH, Bahnhofstr. 21, 85757 Ismaning — ³Infineon Technologies AG, Otto-Hahn-Ring 6, 81739 München

Energy dispersive X-ray spectroscopy (EDS) of samples mounted in scanning electron microscopes (SEM) is a standard technique for elemental material analysis. Today Si(Li)-detectors are used in this field with a maximum energy resolution of about 130eV at a X-ray energy of 6keV. This energy resolution is unsatisfactory for the separation of the low energetic lines like M-lines of heavy elements, L-lines of medium heavy elements and K-lines of light elements. But for excitation of small volumes like particles in samples with the electron beam in the SEM only low acceleration voltages may be used and therefore only low energetic lines are excited. A high resolution spectrometer with a microcalorimeter detector cooled by a pulse tube refrigerator with an ADR unit has been installed on a SEM for this purpose. It shows an average energy resolution of better than 10eV @ 1.5keV. The low countrate in comparison to Si(Li) detectors due to the small area of the microcalorimeter has been increased by the application of a polycapillary X-ray optics. This way the microcalorimeter is a promising tool for material analysis of thin layers and small samples.

TT 28.3 Di 14:45 TU H104

Development of metallic magnetic calorimeters for high-resolution X-ray spectroscopy — ●M. LINCK, A. BURCK, T. DANIYAROV, H. ROTZINGER, T. SCARBROUGH, A. FLEISCHMANN, and C. ENSS — Kirchhoff-Institut für Physik, Heidelberg, Germany

X-ray detectors based on the concept of magnetic calorimetry are well suited for high-resolution spectroscopy. Metallic magnetic calorimeters (MMC) make use of a metallic paramagnetic temperature sensor, which is in tight thermal contact with a metallic X-ray absorber. The paramagnetic sensor is placed in a weak magnetic field; its magnetization is used to monitor the temperature. High-energy resolution can be obtained by using a low-noise, high-bandwidth DC SQUID system to measure the small change in magnetization upon the absorption of a X-ray.

We present the state of development of the current prototype detectors. We discuss noise contributions and the energy resolution observed in MMCs. Applications in material analysis and in metrology, such as absolute activity measurements of low-energy emitting radionuclides, will also be shown.

TT 28.4 Di 15:00 TU H104

Development of Detectors for High Count Rate Calibration Measurements in CRESST — ●WOLFGANG WESTPHAL, FRANZ VON FEILITZSCH, CHIARA COPPI, THOMAS JAGEMANN, JAN KÖNIG, WALTER POTZEL, WOLFGANG RAU, MICHAEL STARK, and HESTI WULANDARI — Technische Universität München, Physik Department E15, James-Franck-Straße, 85748 Garching

CRESST is an experiment for the direct search of dark matter particles (WIMPs) using cryogenic detectors. The detectors are designed as "double detectors" for the simultaneous measurements of the phonon signal and the scintillation light from a recoil event in a CaWO₄ crystal. The phonon signal is read out via a tungsten transition edge sensor (TES) evaporated directly onto the crystal. For the measurement of the light signal there is a silicon light detector, also read out by a TES, mounted together with the CaWO₄ inside a reflective housing. This design allows

for discriminating the relevant nuclear recoils from the background electron recoils due a different light output.

At TU München we are performing calibration measurements for the better understanding of the detector response on various event types (e.g. neutrons scattering on different nuclei). For this purpose we are developing a special version of the CRESST detector optimized for higher count rates. In our design we are using a TES based on Ir/Au multilayers instead of tungsten.

TT 28.5 Di 15:15 TU H104

Untergrundarmer 4π-Kryodetektor zur Messung des ⁷¹Ge-Zerfalls bei GNO — ●WALTER POTZEL, TOBIAS LACHENMAIER, JEAN-CÔME LANFRANCHI und FRANZ VON FEILITZSCH — Physik-Department E15, James-Franck-Str, 85748 Garching

Tieftemperaturdetektoren könnten aufgrund ihrer hohen Energieauflösung, niedrigen Energieschwelle und hohen Nachweeffizienz den bisher bei GNO (Gallium Neutrino Observatory) eingesetzten miniaturisierten, radioaktivitätsarmen Proportionalzählrohren deutlich überlegen sein. Nach der erfolgreichen Entwicklung eines hocheffizienten 4π-Detektors und der Optimierung der thermischen Ge-Deposition auf das Detektorsubstrat, konzentriert sich unsere derzeitige Aktivität auf die Unterdrückung des Untergrundes. Neben dem Aufbau eines Myon-Vetos und einer externen Bleiabschirmung wurde auch, nach eingehender Materialanalyse, eine interne, den besonderen Ansprüchen von GNO genügende Abschirmung und Detektorhalterung entworfen. Desweiteren soll über erste langzeit-stabile Messungen im Untergrundlabor (15m.w.e.) in Garching berichtet werden.

TT 28.6 Di 15:30 TU H104

Low Temperature Calorimeters for Precise Lamb shift Measurements on Hydrogen-Like Heavy Ions — ●ALEXANDER BLEILE¹, V. ANDRIANOV¹, P. EGELHOF¹, S. KRAFT¹, D. MCCAMMON², H.J. MEIER¹, J.P. MEIER¹ und C. STAHL³ — ¹GSI, Darmstadt / Univ. Mainz — ²Univ. of Wisconsin, Madison, USA — ³Goddard Space Flight Center, Greenbelt, 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 ²³⁸U⁹¹⁺ ions at the ESR storage ring at GSI, a calorimetric low temperature detector for hard X-rays was developed. The experimental requirements for the detector are the high absorption efficiency and the relative energy resolution of the order of 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 8 pixels was recently set up and tested, the achieved energy resolution ΔE=75-140 eV @ 60 keV is close to fulfill the demands of the experiment. The status of the experiment will be presented and results of first test measurements at the ESR will be discussed.

TT 28.7 Di 15:45 TU H104

Untersuchung und Optimierung extrem dünner NbN-Filme für die Herstellung phonon-gekühlter Hot-Electron-Bolometer (HEB) — ●T. A. SCHERER, M. SCHICKE und K. SCHUSTER — IRAM, Domaine Universitaire, St-Martin-d'Hères, France

Supraleitende HEBs für radioastronomische Anwendungen im THz-Bereich bestehen aus extrem dünnen Mikrobrücken. Diese Bauelemente arbeiten im Gegensatz zu konventionellen SIS-Mischern auch oberhalb der Bandlückenfrequenz. Zum Verständnis des Phonon-Kühlmechanismus in HEBs auf der Basis von NbN-Mikrobrücken werden zunächst ultradünne NbN-Filme auf Quartz-Substrat reaktiv aufgesputtert. Die Deposition erfolgt mittels eines Nb-bestückten RF-Magnetrons in einer Mischgasatmosphäre bestehend aus Argon, Stickstoff und Methan. Mit Hilfe ellipsometrischer und profilometrischer Messungen wird die Schichtdicke der NbN-Filme kalibriert. Vorgestellt werden das Verhalten der kritischen Temperatur in Abhängigkeit von der Schichtdicke sowie korrespondierende Raman-Messungen und daraus resultierende Interpretationen der Phononenableitgeschwindigkeit zur Kühlung der Mikrobrücke. Der Einfluss von Film-Stress und Wachstum auf die Eigenschaften des Bolometers werden diskutiert.

TT 29 Measuring Devices, Cryotechnique

Zeit: Dienstag 16:15–16:45

Raum: TU H104

TT 29.1 Di 16:15 TU H104

³He/⁴He-Mischkryostat mit mechanischer Pulsrohrvorkühlung — ●DOREEN WERNICKE¹, MATTHIAS BÜHLER¹, JENS HÖHNE¹ und KURT UHLIG² — ¹VeriCold Technologies GmbH, Bahnhofstraße 21, D-85737 Ismaning — ²Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner Str. 8, D-85748 Garching

Eines der Hauptgeschäftsfelder der VeriCold Technologies GmbH liegt im Bereich der Entwicklung und Fertigung von Geräten zur Erzeugung tiefer Temperaturen.

Die zunehmende Verwendung von Tieftemperaturbauelementen in der industriellen Anwendung hat insbesondere die Entwicklung von mechanischen Kühlsystemen für 4K voran getrieben. Aber auch Laboranwendungen stellen immer höhere Anforderungen an Bedienbarkeit und Funktionalität. Am Walther-Meissner-Institut (WMI) in München wurde ein Mischkryostat mit 4K-Pulsrohrkühlung für kontinuierliche Kühlung unterhalb von 10mK entwickelt. Basierend auf diesem Design hat VeriCold gemeinsam mit dem WMI einen Mischkryostaten für die Atom-spektroskopie im Temperaturbereich um 100mK gefertigt. Dieser Kryostat verfügt über Öffnungen in den Schilden und im Dewar, so dass ein Atom- oder Molekülstrahl ungehindert in einen kalten, supraleitenden Resonator eingestrahlt werden kann.

In dem Vortrag werden der Aufbau und die Funktionsweise dieses mechanisch gekühlten Mischkryostaten vorgestellt und die Vorteile gegenüber der Kühlung mit Kryoflüssigkeiten diskutiert.

TT 29.2 Di 16:30 TU H104

Kryogene Gütemessung an optischen Komponenten für Gravitationswellendetektoren — ●RONNY NAWRODT, ANJA ZIMMER, SANDOR NIETZSCHE, RALF NEUBERT, MATTHIAS THÜRK, WOLFGANG VODEL und PAUL SEIDEL — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena

Die Existenz von Gravitationswellen wurde von Einstein im Rahmen seiner Allgemeinen Relativitätstheorie postuliert. Für den experimentellen Nachweis dieser Wellen mittels interferometrischer Gravitationswellendetektoren ist es von besonderer Bedeutung, das thermische Rauschen durch die Anwendung von Kryotechniken zu minimieren. Es wird ein spezieller Messaufbau vorgestellt, mit dem es möglich ist, Untersuchungen des thermischen Rauschens von optischen Komponenten wie Interferometer-Endspiegel oder -Strahlteiler in einem Temperaturbereich von 300 K bis zu 5 K durchzuführen. Besonderes Interesse liegt dabei auf den festkörperphysikalischen Prozessen, die das thermische Rauschen hervorrufen. Die vorerst zu untersuchenden Substratmaterialien sind synthetisches Quarzglas (fused silica), Quarzeinkristall, Silizium und Saphir. Es werden sowohl der Einfluss des Materials und dessen Verarbeitungsprozesse als auch die Einflüsse etwaiger Beschichtungen bzw. Strukturierungen untersucht. Die Arbeiten finden im Rahmen des DFG-geförderten Sonderforschungsbereiches TR7 "Gravitationswellenastronomie" statt.

TT 30 Superconductivity - Applications II : Levitation, SQUID-based Sensors, Devices

Zeit: Dienstag 16:45–18:15

Raum: TU H104

TT 30.1 Di 16:45 TU H104

Levitation and guidance system for a superconductively levitated transport system — ●CHRISTOPH BEYER, O. DE HAAS, P. VERGES, G. FUCHS, and L. SCHULTZ — IFW Dresden, Helmholtztrasse 20, 01069 Dresden

The insight into technology and physics of the levitation and guidance system for the SupraTrans project, a prototype of a superconductively levitated transport system, will be delivered. The technology used herein bases on the flux pinning in melt-textured bulk YBCO that stabilizes the lateral and the vertical position of the vehicle above the magnetic track. A track made out of permanent magnets and soft magnetic steel-yokes acting as flux collectors has been constructed and its capability will be presented.

To establish a highly branched transportation network with short switching times a non-mechanic turnout switch operated by electromagnets has been constructed for a toy sized model and will complete the SupraTrans demonstrator.

TT 30.2 Di 17:00 TU H104

Hochempfindliche und robuste SQUID-Stromsensoren für Tieftemperaturanwendungen — ●FRANK RUEDE, DIETMAR DRUNG, JÖRN BEYER, MARGRET PETERS, CORNELIA ASSMANN und THOMAS SCHURIG — Physikalisch Technische Bundesanstalt Institut Berlin

SQUID-basierte Stromsensoren sind praktisch konkurrenzlos für die Auslesung von niederohmigen Tieftemperaturdetektoren, z.B. supraleitende und magnetische Mikrokalorimeter. Kombiniert mit Feldaufnahmespulen sind SQUID-Stromsensoren wesentliche Komponenten in magnetischen Messsystemen für neue medizinisch-diagnostische Verfahren. In diesem Beitrag werden Stromsensoren präsentiert, die in der PTB für derartige Anwendungen entwickelt wurden. Diese Sensoren basieren auf einer Serienschaltung von gradiometrischen Nb-dc-SQUIDS. Die Eingangsspule der Stromsensoren ist über eine Transformatorschaltung an die SQUID-Serienschaltung angekoppelt. Dieses Sensorkonzept ermöglicht anpassbare Eingangsinduktivitäten zwischen 70 nH und 1.4 μ H sowie eine minierte Rückwirkung der SQUID-Ausleseelektronik auf die Eingangsbeschaltung der Sensoren. Eine hohe Stromempfindlichkeit bei gleichzeitiger Unempfindlichkeit gegenüber magnetischen Umgebungsstörungen wurde in den neuen Sensordesigns erzielt. Es werden Stromrauschwerte unter 1 pA/ \sqrt Hz für Frequenzen oberhalb 10 Hz bei einer Sensor-Temperatur von 4.2 K erreicht. Mit einer neuen Hochgeschwindigkeits-Ausleseelektronik ist es möglich, die Stromsensoren mit einer Bandbreite von bis zu 20 MHz

in einer Flussregelschleife zu betreiben. Es werden Entwurf, Eigenschaften und Einsatzbeispiele der Stromsensoren vorgestellt.

TT 30.3 Di 17:15 TU H104

Entwicklung eines SQUID-basierten Systems mit integrierter Abschirmung zur Messung des Herzmagnetfeldes von Mäusen — ●R. ACKERMANN¹, M. BADER², D. DRUNG¹, S. KNAPPE-GRÜNEBERG¹, H. KOCH¹, A. SCHNABEL¹, TH. SCHURIG¹, U. STEINHOFF¹ und F. WIEKHORST¹ — ¹Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — ²Max-Delbrück-Centrum, Robert-Rössle-Str. 10, 13125 Berlin, Germany

Bei der Entwicklung neuer Therapieverfahren für Herz-Kreislauf-Krankheiten werden gentechnisch veränderte Tiere phänotypisiert. Üblicherweise wird an anästhesierten Tieren das EKG gemessen oder es werden telemetrische Geräte implantiert. Ein alternatives Verfahren ist die berührungsfreie SQUID-Magnetokardiografie, bei der das Magnetfeld der zeitlich veränderlichen elektrischen Ströme im Herzen gemessen wird.

Mit einem vorhandenen SQUID-System gelang uns die Messung des Herzmagnetfeldes von Mäusen mit Feldamplituden zwischen 1 pT und 10 pT sowie die Bestimmung der Herzrate und detaillierterer elektrophysiologischer Parameter. Auf dieser Grundlage entstand die Konstruktion eines für Messungen an Mäusen optimierten Systems: Das Helium-Dewar-Gefäß besitzt eine horizontale 25 mm Warmbohrung, sechs Low- T_c -SQUIDS sind im Umkreis der Maus optimal angeordnet. Eine zylindrische supraleitende 50 mm Nb-Schirmung umschließt die Warmbohrung und die SQUIDS zur Unterdrückung äußerer Störungen. Simulationen ergeben einen Abschirmfaktor $> 10^6$. Wir stellen bisherige experimentelle Resultate, die Details der Konstruktion und die optimale Sensoranordnung vor.

TT 30.4 Di 17:30 TU H104

Novel, non-contact noise thermometer for milli-Kelvin temperatures — ●ASTRID NETSCH, ELENA HASSINGER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

The temperature dependence of thermal voltage noise of an electrical resistance is described by the dissipation-fluctuation theorem, which directly reflects our basic understanding of statistical physics and thermodynamics. This made the measurement of noise an attractive option for primary thermometry in a wide range of temperatures. A lot of in-

vestigations have been made on that topic but parasitic heat input and the suitable fabrication of the resistor still causes frequently problems.

We present a novel technique for Johnson-noise thermometry which 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 high purity gold, which cause fluctuations of magnetic flux in a pickup coil being connected to the input coil the SQUID-magnetometer. The thermometer is easy to fabricate, shows a linear dependence of spectral power density upon temperature below 4 K and is rather insensitive to typical sources of parasitic heating. We discuss general design considerations of such thermometers as well as the dependence of temperature uncertainty upon measurement time and show a comparison of our prototype to the present international temperature scale PLTS-2000 provided by a superconducting reference device (SRD1000) which contains ten fixed-points between 15.4 mK and 1175.8 mK.

TT 30.5 Di 17:45 TU H104

Superconductivity Controlled by Interface Polarization: Novel Perspectives for Superconducting Field-Effect Devices — ●NATALIA PAVLENKO — Institute of Physics, University of Augsburg, Universitaetstr.1, D-86135 Augsburg, Germany

Recent experiments performed on the high- T_c superconducting films clearly demonstrate that an external electric field applied across a dielectric/ferroelectric gate can effectively control a reversible superconductor-insulator switching behavior which plays a key role in the superconducting oxide electronics. On the basis of our recently developed microscopic approach [1,2], we show that the electric polarization at the interface

with ultrathin superconducting films sandwiched between ferroelectric layers allows the achievement of a substantially stronger modulation of the inner carrier density and superconducting transition temperature as compared to ferroelectric-superconducting bilayers typically used in superconducting field-effect devices. We propose a novel design concept for superconducting electric field-effect transistors and provide theoretical calculations that indicate how the field effect in these devices could be amplified.

[1] N. Pavlenko and F. Schwabl, Phys.Rev.B 67, 094516 (2003). [2] N.Pavlenko, Phys.Rev.B 70, 094519 (2004); N.Pavlenko et al., cond-mat/0407696.

TT 30.6 Di 18:00 TU H104

New Concepts for Superconducting Memory Elements — ●RAINER HELD¹, JUN XU¹, CHRISTOF SCHNEIDER¹, JOCHEN MANNHART¹, and MALCOLM BEASLEY² — ¹Lehrstuhl für Experimentalphysik VI, Institut für Physik, Universität Augsburg, D-86135 Augsburg — ²Theodore H. Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California 94305-4045, USA

Superconducting memory is an essential requirement for integrated high-density superconducting digital electronics. Josephson junctions based memory cells have a high clock-speed and a very small power dissipation. Limited by the size of a flux quanta and thereof required inductancies, such elements are difficult to scale to small dimensions. In this presentations, we introduce a new superconducting memory concept, which potentially allows a large integration density.

TT 31 Correlated Electrons - Low-dimensional Materials I

Zeit: Dienstag 14:00–16:00

Raum: TU H2053

TT 31.1 Di 14:00 TU H2053

Scaling Behavior of the Longitudinal and Transverse Transport in Quasi One-Dimensional Organic Conductors — ●MARTIN DRESSEL¹, KONSTANTIN PETUKHOV¹, BELAL SALAMEH¹, PEDRO ZORNOZA¹, and THIERRY GIAMARCHI² — ¹Physikalisches Institut, Universität Stuttgart, Germany — ²DPMC, University of Geneva, Switzerland

The organic conductors (TMTSF)₂PF₆ and (TMTSF)₂ClO₄ are model systems to study the Luttinger-liquid behavior in one dimension. We have investigated the dc and microwave transport properties along the a , b' , and c^* directions. In the normal state of (TMTSF)₂PF₆ below $T = 70$ K, the dc resistivity follows a power-law with ρ_a and $\rho_{b'}$ proportional to T^2 while $\rho_{c^*} \propto T$. Above $T = 100$ K the exponents extracted from the data for the a and c^* axes are consistent with what is to be expected for a system of coupled one-dimensional chains (Luttinger liquid) and a dimensional crossover at a temperature of about 100 K. The b' axis shows anomalous exponents that could be attributed to a large crossover between these two regimes. The organic superconductor (TMTSF)₂ClO₄ is more a two-dimensional metal with an anisotropy $\rho_a/\rho_{b'}$ of approximately 2 at all temperatures. Such a low anisotropy is unexpected in view of the transfer integrals. Slight indications to one-dimensionality are found in the temperature dependent transport only above 200 K. Even along the least conducting c^* direction no region with semiconducting behavior is revealed up to room temperature

TT 31.2 Di 14:15 TU H2053

Numerical study of the two-chain Hubbard model: possible relevance with triplet superconductivity in Bechgaard salts — ●SATOSHI NISHIMOTO¹, YUKINORI OHTA², TOMONORI SHIRAKAWA², and YUJII YAMAGUCHI² — ¹Institut für Theoretische Physik, Universität Göttingen, Germany — ²Department of Physics, Chiba University, Japan

The properties of quasi-one-dimensional Bechgaard salts (TMTSF)₂X have been extensively studied in recent years. This system exhibits a rich phase diagram and the superconducting phase is in proximity to the insulating phase. This is similar to the quasi-two-dimensional organic conductor (BEDT-TTF)₂X and the high- T_c superconductor, in which the d -wave singlet pairing is realized. However, most of recent experiments show strong evidences of triplet pairing in (TMTSF)₂X, and the mechanism of pairing and symmetry of superconducting order parameter are still an open issue. Motivated by such a situation, we study the ground-state properties of a two-chain Hubbard model with zigzag

bonds where we include the intra- and inter-site Coulomb repulsions as well as anisotropic hopping parameters. We use the density-matrix renormalization group and exact diagonalization methods to calculate the spin, charge, and pairing correlations of the model. We thereby find enhancement of triplet pairing correlations for some sets of parameter values, which may have some relevance with triplet superconductivity in (TMTSF)₂X.

TT 31.3 Di 14:30 TU H2053

Comparative resistivity studies under hydrostatic pressure on different variants of the organic superconductor κ -(ET)₂Cu[N(CN)₂]Br — ●CHRISTIAN STRACK¹, CEMIL AKINCI¹, BERND WOLF¹, MICHAEL LANG¹, JOHN SCHLUETER², JOCHEN WOSNITZA³, and DIETER SCHWEITZER⁴ — ¹Physikalisches Institut, J.W. Goethe-Universität Frankfurt, FOR 412 — ²Materials Science Division, Argonne NL, Illinois, USA — ³Institut für Festkörperphysik, TU Dresden — ⁴Physikalisches Institut, Universität Stuttgart

Resistivity measurements on four samples of κ -(ET)₂Cu[N(CN)₂]Br, synthesized by following two different preparation routes, yield strongly sample-dependent $\rho(T)$ profiles. By comparing the interlayer resistivities and their response to hydrostatic pressure we infer: (i) a significant part of the inelastic-scattering contribution, causing the anomalous $\rho(T)$ maximum around 90K, is extrinsic in nature, (ii) the abrupt change in the slope of $\rho(T)$ around $T^* \approx 40$ K is sample independent and most likely marks a second-order phase transition, (iii) the origin of the $\rho(T) \propto AT^2$ dependence at low temperatures, with a strongly sample dependent coefficient A and range of validity, is different from coherent Fermi-liquid excitations.

TT 31.4 Di 14:45 TU H2053

Spin-Charge Separation in TTF-TCNQ — ●HOLGER BENTHIE¹, FLORIAN GEBHARD¹ und ERIC JECKELMANN² — ¹Fachbereich Physik, Philipps-Universität Marburg — ²Fachbereich Physik, Johannes Gutenberg-Universität

Correlated electrons in one spatial dimension have very unusual properties such as the dynamical separation of spin and charge degrees of freedom. Typically, dynamical correlation functions of these systems are investigated with field theoretical methods that are valid in the limit of vanishingly low energies. However, there are few reliable results at *finite* energies which can be directly compared with spectra of scattering experiments. It has therefore been difficult to find direct spectroscopic evidence of spin-charge separation in experimental realizations of quasi

one-dimensional electron systems.

The Dynamical Density-Matrix Renormalization Group [1] can accurately determine spectral properties of correlated one-dimensional lattice models for all energy scales and interaction strengths. We use this method to calculate the one-particle spectral function of Hubbard chains both above and below half-filling [2]. We argue that the ARPES spectrum of the quasi one-dimensional organic conductor TTF-TCNQ [3] can be consistently explained by essentially uncoupled TTF and TCNQ chains with short-ranged Coulomb interactions at electron densities $n = 1.4$ and $n = 0.6$, respectively.

[1] E. Jeckelmann, Phys. Rev. B **66**, 045114 (2002);

[2] H. Benthien *et al.*, Phys. Rev. Lett. **92**, 256401 (2004);

[3] R. Claessen *et al.*, Phys. Rev. Lett. **88**, 096402 (2002).

TT 31.5 Di 15:00 TU H2053

Strong evidence for Luttinger Liquid behaviour in quasi-one-dimensional Lithium purple bronze — ●J. HAGER and R. MATZDORF — FB 18, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

We have measured the density of states at energies near the Fermi energy ϵ_F using scanning tunneling spectroscopy on cleaved $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ samples. In literature the discussion about the electronic structure, especially a phase transition at $T = 24\text{K}$ remains controversial. Localization effects, charge density wave and spin density wave transitions, as well as a Luttinger Liquid scenario are used to explain experiments. Our dI/dV measurements at 5K show strong depression of the dI/dV signal at ϵ_F . Our experimental spectra near the Fermi energy can be explained excellently by Luttinger Liquid theory at low and ambient temperatures. Our data excludes current zero bias anomaly theories for explanation, which would predict a similar behaviour.

TT 31.6 Di 15:15 TU H2053

Thermodynamische Messungen an der Hochdruckphase von $(\text{VO})_2\text{P}_2\text{O}_7$ — ●ANDREAS BRÜHL, MICHAEL LANG, BERND WOLF, VOLODYMYR PASHCHENKO, CHRISTOPH GROSS, WOLF ASSMUS und ANDREI PROKOFIEV — Physikalisches Institut, J. W. Goethe-Universität Frankfurt, 60054 Frankfurt am Main, DFG-SP 1073

Vanadylpyrophosphat ($(\text{VO})_2\text{P}_2\text{O}_7$) kann je nach Züchtungsbedingungen in einer Umgebungsdruck- und einer Hochdruckphase hergestellt werden, abgekürzt mit AP-VOPO bzw. HP-VOPO. Nach dem zur Zeit geläufigsten Modell bilden die V^{4+} -Ionen in beiden Phasen $S=1/2$ -Spinketten mit einer alternierenden Wechselwirkung zwischen nächsten Nachbarn. Während zur Beschreibung von AP-VOPO zwei verschiedene Arten dieser Ketten benötigt werden, kommt man bei HP-VOPO mit einer aus, wie es auch durch die einfachere Kristallstruktur nahegelegt wird. In beiden Fällen wird von einer nur schwachen Kopplung der Ketten untereinander ausgegangen.

Messungen der thermischen Ausdehnung, spezifischen Wärme, elastischen Konstanten und der Magnetisierung zeigen jedoch, dass für HP-VOPO dieses einfache Bild nicht ausreichend ist. Insbesondere das Auftreten einer sehr deutlichen Anomalie magnetischen Ursprungs bei

$T \approx 15\text{ K}$ in der thermischen Ausdehnung und die Feld- und Temperaturabhängigkeit der elastischen Konstanten lassen sich nicht durch das genannte Modell erklären.

TT 31.7 Di 15:30 TU H2053

Infrared properties of the quasi-one-dimensional superconductor $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$ under pressure — ●C. A. KUNTSCHER¹, S. FRANK¹, I. LOA², K. SYASSEN², T. YAMAUCHI³, and Y. UEDA³ — ¹Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — ³Institute for Solid State Physics, University of Tokyo, Tokyo, Japan

At ambient pressure $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$ shows a quasi-one-dimensional metallic character at room temperature, which can be explained by its highly anisotropic crystal structure consisting of chains and ladders of VO_6 octahedra and chains of VO_5 square pyramids. Upon cooling it undergoes a metal-insulator transition at 135 K due to charge ordering on the V sites. The pressure-temperature phase diagram of $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$ is remarkable, since it shows a superconducting phase for pressures higher than 7 GPa in direct vicinity to the charge-ordered phase [1]. The mechanism of the observed superconductivity and its relation to the charge ordering is not clear. Besides, electron-phonon interaction seems to play a role as well, influencing the conduction mechanism.

We carried out polarization-dependent reflectivity measurements on $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$ at room temperature as a function of pressure (<20 GPa). The results are discussed in terms of the conduction mechanism, pressure-induced structural changes, and charge ordering/redistribution. *Supported by the DFG, Emmy Noether-program.*

[1] T. Yamauchi, Y. Ueda, and N. Mori, Phys. Rev. Lett. **89**, 057002 (2002).

TT 31.8 Di 15:45 TU H2053

Field induced magnetic phase transition in Cs_2CuCl_4 as a magnon Bose-Einstein condensation — ●TEODORA RADU¹, HERIBERT WILHELM¹, VIKTOR YUSHANKHAI¹, DMITRY KOVRIZHIN², RADU COLDEA³, THOMAS LÜHMANN¹, and FRANK STEGLICH¹ — ¹MPI für Chemische Physik fester Stoffe D-01187 Dresden, Germany — ²MPI für Physik komplexer Systeme D-01187 Dresden, Germany — ³Oxford Physics, Clarendon Laboratory Oxford, OX1 3PU, UK

We report on results of specific heat $C(T)$ measurements on single crystals of the frustrated quasi-2d spin $-1/2$ antiferromagnet Cs_2CuCl_4 in the external magnetic field $0 \leq B \leq 12\text{ T}$ and in the temperature range $0.3\text{ K} < T < 6\text{ K}$. For different orientation of the applied magnetic field, B with respect to the crystallographic axes, the magnetic phase diagrams are obtained and compared with the previous neutron scattering results. For $\vec{B} \parallel \vec{a}$, the magnetic phase transition near the critical field $B_c \simeq 8.44\text{ T}$ is treated as a magnon Bose Einstein condensation (BEC). In this context, the phase boundary $T_N \sim (B_c - B)^{1/\phi}$ is described with the critical exponent $\phi \simeq 1.5$. This result is discussed in terms of a simple mean-field theoretical study of the magnon BEC.

TT 32 Correlated Electrons - Low-dimensional Materials II

Zeit: Dienstag 16:15–18:30

Raum: TU H2053

TT 32.1 Di 16:15 TU H2053

Magnetic ground state of the quantum spin magnet CaCu_2O_3 probed by high field ESR — ●V. KATAEV¹, M. GOIRAN², M. COSTES², J. M. BROTO², F. C. CHOU³, E. ARUSHANOV^{1,2}, S. DRECHSLER¹, and B. BÜCHNER¹ — ¹Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — ²Laboratoire National des Champs Magnétiques Pulsés, 31432 Toulouse Cedex 04, France — ³Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

We report an electron spin resonance (ESR) study of the $S = 1/2$ -Heisenberg pseudo-ladder magnet CaCu_2O_3 in pulsed magnetic fields up to 40 T. At sub-Terahertz frequencies we observe an ESR signal originating from a small amount of uncompensated spins residing presumably at the imperfections of the strongly antiferromagnetically correlated host spin lattice. The data give evidence that these few percent of extra spin states are coupled strongly to the bulk spins and are involved in the antiferromagnetic ordering at $T_N = 25\text{ K}$. By mapping the frequency/resonance field diagram we have determined the spin gap for magnetic excitations below T_N amounting to $\sim 0.3\text{ meV}$. The small value

of the gap explains the occurrence of the spin-flop transition in CaCu_2O_3 at the critical magnetic field $H_{sp} \sim 3\text{ T}$. Qualitative changes of the ESR response with increasing the field strength give indications that strong magnetic fields reduce antiferromagnetic fluctuations and may even suppress the long-range magnetic order in CaCu_2O_3 . ESR data support theoretical predictions of a significant role of the extra spin states for the properties of the low-dimensional quantum magnets.

TT 32.2 Di 16:30 TU H2053

Evidence for "ferromagnetic" helimagnetism in compounds with frustrated edge-shared CuO_2 chains — ●S.-L. DRECHSLER¹, J. RICHTER², J. MÁLEK¹, A. MOSKVIN³, H. ROSNER⁴, A. GIPPIUS⁵, R.E. KREMER⁶, and M. ENDERLE⁷ — ¹IFW-Dresden — ²Universität Magdeburg — ³Ural State University Ekaterinburg, Russia — ⁴MPI f. CPfS, Dresden — ⁵State University, Moscow, Russia — ⁶MPI f. Festkörperforsch., Stuttgart — ⁷Inst. Laue-Langevin, Grenoble, France

We present a combined theoretical and experimental study of the electronic structure and helimagnetism in compounds with frustrated edge-shared CuO_2 chains: LiVCuO_4 and LiCu_2O_2 vs. the ferromagnetic

(fm) inchain ordering in Li_2CuO_2 . Based on full potential L(S)DA and LSDA+ U band structure calculations, exact diagonalization studies of multi-band Hubbard and Heisenberg models, we estimate sign and magnitude of the most relevant exchange integrals J . Strongly competing fm nearest neighbor (nn) and anti-fm next nn J 's are found for the inchain direction. This frustration scenario well describes magnetic susceptibility, specific heat, spin entropy, inelastic neutron scattering, and NMR data. The influence of interchain couplings is briefly discussed.

TT 32.3 Di 16:45 TU H2053

One-dimensional magnetic thermal conductivity of Ca-doped SrCuO_2 — ●PATRICK RIBEIRO¹, CHRISTIAN HESS², and BERND BÜCHNER¹ — ¹IFW-Dresden, Germany — ²DPMC-Geneva, Switzerland

We present results on the heat conduction of the Ca-doped SrCuO_2 -system, which is a prototype system for spin 1/2 Heisenberg-chains. 1D-magnetic heat transport is present in this compound, giving rise to a strong anisotropy of the heat conduction tensor. The separation of the magnetic contributions from the phonon background is ambiguous in the pure material SrCuO_2 . By doping it with Ca, the phononic contribution to the heat conduction is partially suppressed by enhanced phonon-defect scattering. Concomitantly, the electronic configuration of Cu is only weakly affected, since Ca is isovalent to Sr. Hence, no strong changes in the magnetic conductivity are to be expected. This leads to a better separation of both contributions. First results of the thereby obtained magnetic heat conduction will be presented and discussed.

TT 32.4 Di 17:00 TU H2053

Thermal conductivity of single-layered cuprates $R_2\text{CuO}_4$ — ●K. BERGGOLD¹, T. LORENZ¹, M. HOFMANN¹, J. BAIER¹, M. KRIENER¹, H. ROTH¹, A. FREIMUTH¹, and S. BARILO² — ¹II. Physikalisches Institut 50937 Köln — ²Inst. of Sol. State & Semicond. Phys., Minsk

Thermal conductivity of low-dimensional spin systems is investigated because of the possibility of a large magnetic contribution to the heat transport. There is a lot of evidence for such a contribution in various 1D systems, but it is less investigated in 2D systems. We present measurements of the thermal conductivity κ of $\text{SrCuO}_2\text{Cl}_2$ [1] and $R_2\text{CuO}_4$ with $R = \text{Pr, Nd, Sm, Eu}$ and Gd . For all samples, κ is anisotropic with a conventional low-temperature maximum for a heat current perpendicular to the Cu-O-planes, whereas for a heat current within the Cu-O-planes a second high-temperature maximum or shoulder occurs. In principle, two mechanisms could explain a double-peak structure of κ . One is an unusual phonon-damping, which is e.g. relevant in the 2D-System $\text{SrCu}(\text{BO}_3)_2$ [2]. Such a damping could arise from soft phonon modes caused by structural instabilities. The other is an additional contribution by magnetic excitations of the spin system. However, a structural instability is only present for $R=\text{Eu}$ and Gd . Thus, the observation of a double-peak structure in all samples gives clear evidence for a sizeable heat transport by magnetic excitations. We also show, that weak charge-carrier doping strongly suppresses the magnetic contribution.

[1] M. Hofmann et al. PRB 67, 184502 (2003)

[2] M. Hofmann et al. PRL 87, 047202 (2001)

Supported by the DFG through SFB 608

TT 32.5 Di 17:15 TU H2053

$\text{Sr}_2\text{Cu}(\text{PO}_4)_2$ - an unexpected one dimensional spin 1/2 Heisenberg system with isolated CuO_4 units — ●HELGE ROSNER¹, MICHELLE JOHANNES², JOHANNES RICHTER³, and STEFAN-LUDWIG DRECHSLER⁴ — ¹MPI for Chemical Physics of Solids, Dresden — ²NRL Washington, USA — ³Otto-von-Guericke-University Magdeburg — ⁴Leibniz Institute for Solid State and Materials Research Dresden

Recently, Belik *et. al.* [1] reported synthesis and physical properties of the compound $\text{Sr}_2\text{Cu}(\text{PO}_4)_2$. The measured magnetic susceptibility [1] exhibits a broad maximum at 92 K characteristic for quasi-1D systems, but shows no long range magnetic ordering down to 0.45 K. Here, we present full potential electronic structure calculations within the local spin density approximation, followed by a subsequent mapping to a one-band tight-binding model and an extended Heisenberg model. Although the crystal structure of $\text{Sr}_2\text{Cu}(\text{PO}_4)_2$ is formed by unlinked CuO_4 units, we find a surprisingly pronounced one dimensional behaviour with substantial coupling between nearest neighbors (NN) only. The calculated NN exchange coupling $J_1 \sim 180$ K is in good agreement with the experimental estimate. It exceeds all other couplings by at least two orders of magnitude, placing the system in the forefront of 1D spin 1/2 model compounds. Model calculations using the derived exchange constants suggest that no long range magnetic ordering should be expected down to very

low temperatures.

[1] Belik *et. al.*, J. of Sol. Stat. Chem. 177, 883 (2004).

TT 32.6 Di 17:30 TU H2053

Evidence for bound holes in the doped spin ladders of $(\text{Sr,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$ — ●C. HILGERS¹, M. GRÜNINGER¹, A. FREIMUTH¹, U. AMMERLAHL^{2,3}, P. RIBEIRO⁴, B. BÜCHNER⁴, and A. REVCOLEVSCHI³ — ¹II. Physikalisches Institut, Universität zu Köln — ²II. Physikalisches Institut, RWTH-Aachen — ³Laboratoire de Physico-Chimie de L'Etat Solides, Université Paris-Sud, France — ⁴IFW Dresden

In the telephone-number compounds $(\text{Sr,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$ the interplay of spin and charge degrees of freedom gives rise to a competition between charge-density wave (CDW) and superconducting (SC) ground states. Superconductivity was found in $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ under external pressure for $x \geq 11.5$, whereas for $x \leq 8$ a charge ordering in the chains and a CDW ground state in the ladders were observed. However, the nature of the CDW ground state is still unresolved. We present a detailed study of the doping dependence of the optical conductivity in the far-infrared range as a function of temperature and polarization ($E||a,c$). Between $x = 6$ and $x = 8$, we observe a qualitative change of $\sigma_a(\omega)$ and $\sigma_c(\omega)$ with new collective modes for $x = 8$. We interpret these modes as evidence for bound holes in the ladders. For $x \leq 8$, we observe a new optical phonon mode at low temperatures which can be attributed to a Raman-active ladder mode activated by the CDW. We report an interesting correlation between transition temperatures of the CDW ground state in the ladders and charge ordering in the chains.

TT 32.7 Di 17:45 TU H2053

Spin chains in $(\text{Ca,L a,Sr})_{14}\text{Cu}_{24}\text{O}_{41}$ — ●COSIMA SCHUSTER and UDO SCHWINGENSCHLÖGL — Institut für Physik, Universität Augsburg

The $(\text{Ca,L a,Sr})_{14}\text{Cu}_{24}\text{O}_{41}$ compounds contain two different structural components, CuO_2 ladders and CuO chains. The compounds are intrinsically doped, whereby the main part of the holes can be assigned to the chains. The spin and charge order on the chains are strongly doping dependent and range from spin dimers over 3D antiferromagnetic order to ferromagnetic order in the La rich compounds. On the basis of the crystal structure we try to form a model for the chains on the basis of the Hubbard model. We choose the Hubbard model, because it is particle-hole-symmetric, and the doping is numerically easy to implement. In addition we study periodic potentials with different period. We examine, which potential is energetically favored and which charge and spin order is linked with this potential. In our investigations we concentrate on the quarter filled band. We find that a $2k_F$ periodic magnetic field leads – with interaction – to the highest energy gain but it is related with a large spin gap. On the other hand a $4k_F$ periodic potential is favored for strong interaction. In this case, we find no spin gap but a $2k_F$ oscillation of the magnetization. The difference to a Heisenberg chain is pointed out.

TT 32.8 Di 18:00 TU H2053

DIMER FORMATION IN THE Cu ($S=1/2$) SPIN CHAINS OF $\text{Sr}_{13}\text{LaCu}_{24}\text{O}_{41}$ — ●H.-H. KLAUSS¹, H. GERDES¹, A. BOSSE¹, H.-J. GRAFE^{1,2}, D. MIENERT¹, J. LITTERST¹, R. KLINGELER², and B. BÜCHNER² — ¹Institut für Metallphysik und Nukleare Festkörperphysik, TU Braunschweig, 38106 Braunschweig — ²Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Helmholtzstr. 20, 01069 Dresden

We present a comparative ^{63}Cu -NMR study on the Cu chain site in $\text{Sr}_{13}\text{LaCu}_{24}\text{O}_{41}$ and $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$. The experiments on the $\approx 60\%$ hole doped antiferromagnetic (AFM) spin chains in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ confirm the existence of local dimers with a spin excitation gap of $\Delta \approx 130$ K in good agreement with [1]. The formation of weakly interacting dimers is explained by a specific charge order model. In $\text{Sr}_{13}\text{LaCu}_{24}\text{O}_{41}$ the hole doping is reduced to $\approx 50\%$. In a static alternating spin/hole charge order model an AFM $S=1/2$ spin chain with a gapless Bonner-Fisher behavior is expected. Susceptibility measurements indeed verify the absence of a spin gap. We present NMR experiments which reveal a strongly temperature dependent Knight shift and T_1 relaxation rate below 150 K which can be described by a thermal activation over a finite spin excitation gap. Possible reasons for this discrepancy will be discussed. [1] M. Takigawa *et al.*, PRB 57 (1998) 1124

TT 32.9 Di 18:15 TU H2053

Strong Coulomb effects in hole-doped Heisenberg chains — ●JÜRGEN SCHNACK — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Substances like the “telephone number compound” $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ are intrinsically hole-doped. The involved interplay of spin and charge dynamics is a challenge for theory. In this Letter we propose to describe hole-doped Heisenberg spin rings by means of complete numerical diagonalization of a Heisenberg Hamiltonian that depends parametrically on

hole positions and includes the screened Coulomb interaction among the holes. It is demonstrated that key observables like magnetic susceptibility, specific heat, and inelastic neutron scattering cross section depend sensitively on the dielectric constant of the screened Coulomb potential which opens the fascinating possibility to determine the in-medium dielectric constant experimentally from such observables [1,2].

[1] J. Schnack, Phys. Rev. Lett., submitted, cond-mat/0409650

[2] J. Schnack, F. Ouchni, J. Magn. Magn. Mater. (2004) accepted, cond-mat/0406592

TT 33 Transport - Nanoelectronics III: Molecular Electronics

Zeit: Dienstag 14:00–18:00

Raum: TU H3027

TT 33.1 Di 14:00 TU H3027

A single-molecule diode — ROLF OCHS¹, MARK ELBING¹, MARCEL MAYOR¹, MAX KÖNTOPP¹, FERDINAND EVERS¹, and ●HEIKO B. WEBER^{1,2} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, D-76021 Karlsruhe — ²Institut für Angewandte Physik, Universität Erlangen, Staudtstr. 7, 91058 Erlangen

We have designed and synthesized an organic molecule such that it can be used as a diode on the single-molecule level. Individual molecules were contacted employing the mechanically controlled break junction technique. The results show indeed diode-like current-voltage characteristics. In contrast to that, control experiments with similar symmetric molecules did not show significant asymmetries in the transport properties. In order to investigate the underlying transport mechanism, phenomenological arguments are combined with calculations based on density functional theory. It turns out that the physics responsible for the asymmetry has several analogies to that in a p-n semiconductor diode.

TT 33.2 Di 14:15 TU H3027

Electrical transport through DNA molecules under stretching — ●NING KANG, ROMAN LEHNER, ARTUR ERBE, and ELKE SCHEER — Department of Physics, University of Konstanz, Germany

Understanding the mechanism of electron motion along DNA is an essential step for the development of DNA-based molecular electronics. However, a number of contradicting findings were reported regarding the electronic properties of DNA. Theoretical calculations have demonstrated that the charge transport through the DNA will be strongly influenced by conformational transitions. To probe this effect, we have measured the resistance of DNA molecules under stretching with the help of the mechanically controllable break junction technique (MCB). Using the break junctions, we are able to fabricate electrodes with nanometer separation and fine-tune the tunneling gap between electrodes down to a resolution in the picometer range. In our experiments, we used 10-nm-long (30 base pairs) DNA with thiol groups at both ends, and stretched continuously the trapped molecules by means of MCB. A discrete two-level resistance switching behavior is observed when changing the distance of the electrodes, which might be related to a conformation transition of the DNA under stretching. To clarify whether the measured signal is from molecules, we also perform the measurements with a specific enzyme that cuts the DNA.

TT 33.3 Di 14:30 TU H3027

Dissipative Effects in the Electronic Transport through DNA molecular wires — ●RAFAEL GUTIERREZ, SUDEEP MANDAL, and GIANAURELIO CUNIBERTI — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg

DNA-based molecular wires have a huge potential for application in molecular electronics. Their electronic transport properties are however not well elucidated. This is mainly due to the extreme sensitivity of charge propagation in DNA to static and dynamic disorder as well as to environmental effects (counterions, water shell, etc). We investigate the influence of a dissipative environment which effectively comprises the effects of counterions and hydration shells, on the transport properties of short DNA wires. For this purpose we use a tight-binding model embedded in a bosonic bath consisting of a collection of harmonic oscillators. In the absence of interactions with the bath, a temperature independent gap opens in the electronic spectrum. Upon allowing for electron-bath coupling the gap becomes temperature dependent. We show that a crossover from semiconducting to metallic behavior in the low-voltage region of the I - V characteristics can be achieved in some parameter regions. The reason is the appearance of bath-induced polaronic states within the elec-

tronic bandgap. We further show that the temperature dependence of the transmission near the Fermi energy displays an Arrhenius-like behavior in agreement with recent transport experiments.

TT 33.4 Di 14:45 TU H3027

Characterization of nanoscale molecular junctions — ●ARTUR ERBE¹, ANAT DE PICCIOTTO², JENNIFER E. KLARE², COLIN NUCKOLLS², KIRK BALDWIN³, and ROBERT WILLET³ — ¹Universität Konstanz, FB Physik — ²Columbia University, NY, USA — ³Lucent Technologies, Bell Labs, NJ, USA

Exploring the electronic possibilities of nanoscale organic materials has become an important challenge as modern lithographical techniques approach ultimate limits. In this regime, the properties of single or a few molecules will dominate the behavior of whole devices. Recent experiments on nanoscale molecular junctions show a large variety of results. Differences in the properties of the molecules themselves cannot fully account for these variations. This fact indicates that contact properties play an important role in the behavior of the whole junction. We present electrical measurements of various types of molecules using an electrical break junction technique. The formation of the junctions relies on electromigration in a narrow gold wire. This technique allows us to test the junctions under varying external conditions. Distinct features are found in the I - V -characteristics at low temperatures indicating that single or a few molecules are contacted. Some of those features can be affected by changes in applied gate voltage. The energy scales associated with these features cannot be explained with molecular properties alone. In order to explain our results we take interactions between the molecules and the contacting metals into account.

TT 33.5 Di 15:00 TU H3027

Electron-phonon interactions in atomic-scale conductors — ●JANNE VILJAS, FABIAN PAULY, and JUAN CARLOS CUEVAS — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

With the recent advances in nanofabrication techniques it has become possible to manipulate and explore the electronic transport through atomic-scale wires and individual molecules. This has posed an exciting theoretical challenge, namely the understanding of the conduction mechanisms at the molecular scale. So far, the effort has been mostly concentrated on analysing the role of the electronic structure of the atomic-scale conductors, but little has been done on the role of their internal degrees of freedom. In this talk I will present our efforts to understand what are the effects of the vibrational modes on conduction at the atomic scale. In particular, making use of a tight-binding approach, we describe the influence of the inelastic electron-phonon processes in metallic atomic wires. This allows us to address many different questions such as (i) what determines that in some experimental situations the vibrational modes enhance the current and in some others they reduce it? (ii) What are the possible signatures of these modes in the current-voltage characteristics? (iii) What are the selection rules that explain why some vibrational modes do not show up in the transport experiments?

TT 33.6 Di 15:15 TU H3027

Electron-phonon coupling mechanisms in molecular electron transport — ●MICHAEL HARTUNG and GIANAURELIO CUNIBERTI — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We study the conductance through a single vibrating molecule contacted to two metallic electrodes. The starting point is a tight-binding Hamiltonian with a linear coupling of the ionic motion to the electronic

degrees of freedom. We distinguish between a coupling to the *onsite* energy of the molecule and a coupling representing a *bond-stretching* vibrational mode.

The full nonequilibrium current, shot noise, and dissipated power is calculated within the Keldysh Green function formalism. As far as transport observables are concerned, onsite and bond-stretching coupling mechanisms differ in several respects: In the latter case satellite peaks in the differential conductance are more pronounced and results closer to the experimental evidence can be obtained.

TT 33.7 Di 15:30 TU H3027

Vibrational effects in transport through a few level molecule. — ●DMITRI RYNDYK — Universität Regensburg

We consider a simple molecule with several electron levels placed between large metallic leads. At finite voltage internal vibrations of the molecule as well as an oscillation of the whole molecule between the leads can be excited. We use the self-consistent nonequilibrium theory to describe electron transport through a molecule and dynamics of vibrations. At small voltage or high temperature current is affected by thermally excited vibrations. At larger voltage and low enough temperature transition into the regime with nonequilibrium vibrations is possible. Phase diagram of the system is controlled by coupling to the leads, electron-vibron coupling, and coupling of vibrations to the thermal bath. The other nonequilibrium effect which should be taken into account is spectrum modification due to nonequilibrium distribution function of electrons at finite voltage.

Pause

TT 33.8 Di 16:00 TU H3027

Theoretical analysis of conductance histograms of Au atomic contacts — ●F. PAULY¹, M. DREHER², J.C. CUEVAS¹, E. SCHEER², and P. NIELABA² — ¹Institut für Theoretische Festkörperphysik, University of Karlsruhe, 76128 Karlsruhe, Germany — ²Physics Department, University of Konstanz, 78457 Konstanz, Germany

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic of the corresponding material. In order to shed some light on the origin of these peaks, we present a theoretical analysis of the conductance histograms of Au atomic contacts, investigating the interplay between mechanical and electrical properties of these nanocontacts. 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. We also compare with experimental results on Au atomic contacts where the individual channel transmissions have been determined.

TT 33.9 Di 16:15 TU H3027

Utilization of Carbon Nanotubes by Surface Acoustic Waves — ●JENS EBEBECKE¹, CHRISTOPH J. STROBL², and ACHIM WIXFORTH¹ — ¹Institut für Physik der Universität Augsburg, Experimentalphysik I, Universitätsstr. 1, 86135 Augsburg — ²Sektion Physik der Ludwig-Maximilian-Universität und Center for Nanoscience (CeNS), Geschwister-Scholl-Platz 1, 80539 München

We report a surface acoustic wave (SAW) mediated carbon nanotube (CNT) alignment parallel to the sample surface. The piezoelectric field of the SAW aligns the CNTs in parallel to the wave vector. Furthermore we have contacted single-walled CNTs after aligning them. The acoustoelectric current has been measured at 4.2 K and a probing of the low-dimensional electronic states by the SAW has been detected. By decreasing the acoustic wavelength resulting in an adjustment to the length of the defined CNT constriction a quantization of the acoustoelectric current has been observed.

TT 33.10 Di 16:30 TU H3027

Magnetoconductance in Disordered Carbon-Nanotubes — ●NORBERT NEMEC and G. CUNIBERTI — Molecular Computing Group, Universität Regensburg, Germany

Single wall carbon-nanotubes in tight-binding approximation are one of the simplest nontrivial theoretical models with physical relevance that can be used for studying quantum mechanical transport mechanisms at the molecular scale. Based on this model, we examine the interplay

of disorder with external magnetic fields, leading to signs of weak localization. As expected, weak localization is enhanced in the energy regions with high density of states. We quantify the resulting energy dependent mean free path in relation to the sample size and the strength of the disorder. “Coating wideband leads” are introduced as a novel approach to model realistic contacts as they are found in experiment, without adding much computational complexity.

TT 33.11 Di 16:45 TU H3027

Non-linear transport properties in commensurate and incommensurate double-walled carbon nanotubes — ●SHIDONG WANG and MILENA GRIFONI — Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

We use a tight-binding model to investigate the effective intershell coupling in double-walled carbon nanotubes. We derive an analytical expression for the effective intershell coupling and find selection rules. The intershell coupling between lowest bands is significantly suppressed if two shells are incommensurate. Including the long-ranged Coulomb interactions, double-walled carbon nanotubes can be described by Luttinger liquid theory at low energies. The tunneling density of states and the non-linear *I-V* characteristics of double-walled carbon nanotubes are also obtained.

TT 33.12 Di 17:00 TU H3027

Franck-Condon blockade and giant Fano factors in transport through single molecules — ●JENS KOCH and FELIX VON OPPEN — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We show that Franck-Condon physics leads to a significant current suppression at low bias voltages (termed Franck-Condon blockade) in transport through single molecules with strong coupling between electronic and vibrational degrees of freedom.

For weak vibrational relaxation, we find that transport in this regime is characterized by remarkably large Fano factors (10^2 – 10^3), which arise due to avalanche-like transport of electrons. Avalanches occur in a self-similar manner over a wide range of time scales, as reflected in power-law dependences of the current noise on frequency and vibrational relaxation rate.

TT 33.13 Di 17:15 TU H3027

Transport calculations for single molecules based on density functional theory: some fundamentals — ●F. EVERS¹, K. BURKE², and R. GAUDOIN² — ¹Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — ²Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, Piscataway NJ 08854

In principle, the use of time dependent density functional theory (TDDFT) allows for exact calculations of the linear and non-linear density and current response of interacting many-body systems. An important application of this method are transport calculations for single molecules. In practice, one is forced to make approximations for the exchange correlation (XC) functional employed which then can put serious limits to the accuracy of TDDFT calculations. We will discuss artifacts that can occur if the non-equilibrium XC-functional is replaced by the equilibrium one. A formalism will be proposed that allows to include the XC-functional in the hydrodynamic approximation (Vignale and Kohn) into the standard DFT-approach to transport.

TT 33.14 Di 17:30 TU H3027

Electron and Exciton Transfer in Donor-Acceptor Systems: Many-Particle Effects and Influence of Electronic Correlations — ●SABINE TORNOW, NING-HUA TONG, and RALF BULLA — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The spin boson model provides a well established description of electron transfer processes from a donor to an acceptor. The redox sites are modelled by two localized quantum states. This picture breaks down in multi electron transfer processes if many particle effects and electron correlations have to be taken into account. We present a theoretical non-perturbative study of the electron and exciton transfer based on an extended spin boson model where the redox sites are modelled more realistically. Using Wilsons Numerical Renormalization Group method we discuss effects of the electron correlations on the transfer rate.

TT 33.15 Di 17:45 TU H3027

Magnetic Field Dependent Band Structure in Multiwall Carbon Nanotubes — ●BERNHARD STOJETZ¹, FRANCOIS TRIOZON², STEPHAN ROCHE², LAZLO FORRÓ³, and CHRISTOPH STRUNK¹ — ¹Institut für Experimentelle und Angewandte Physik, Universität Regensburg — ²Commissariat à l'Énergie Atomique, DRFMC/SPSMS, 38042 Grenoble, France — ³Institute of Physics of Complex Matter, FBS Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

We report conductance measurements for large diameter (30 - 40 nm) individual multiwall carbon nanotubes in magnetic fields both parallel and perpendicular to the tube axis. A prestructured Al backgate allows a substantial shift of the Fermi level. The thin native oxide on the Al

films provides a very efficient electrostatic coupling between the gate and the tube.

The conductance of the nanotube was recorded as a function of the magnetic field B and the gate voltage U . For parallel fields, both h/e - and $h/2e$ -periodic oscillations in the magnetoconductance occur and lead to rhomb-shaped regions of low conductance in the B - U -plane. In the perpendicular case, a region of low conductance forms at small gate voltages, which grows with increasing magnetic field.

The experimental observations are explained well by tight-binding band-structure calculations for the outermost shell of a multiwall nanotube in a magnetic field.

TT 34 Correlated Electrons - Quantum Impurities, Kondo Physics

Zeit: Mittwoch 09:45–11:15

Raum: TU H104

TT 34.1 Mi 09:45 TU H104

Frequency-dependent transport through a quantum dot in the Kondo regime — ●MICHAEL SINDEL¹, WALTER HOFSTETTER², JAN VON DELFT¹, and MARKUS KINDERMANN³ — ¹Physics Department and Center for NanoScience, LMU München, 80333 München — ²Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen — ³Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139, USA

Motivated by experiments of Kogan et al. [1] we study the AC conductance and equilibrium current fluctuations of a Coulomb blocked quantum dot in the Kondo regime. To this end we apply the nonperturbative numerical renormalization group method in combination with the Kubo formalism [2] suitable for the nonperturbative calculation of finite-frequency transport properties. For frequencies smaller than the charge excitation energy $\min\{\epsilon_d, |U + \epsilon_d|\}$ we derive a formula for the frequency dependent current by extending [3]. This formula enables us to relate the spectral function with the linear AC conductance and the frequency-dependent equilibrium current fluctuations, respectively. We demonstrate that AC transport provides a new route to measuring the equilibrium spectral density (a key signature of Kondo physics) which so far has defied direct experimental observation.

- [1] A. Kogan, S. Amasha, and M.A. Kastner, Science 304, 1293 (2004).
 [2] W. Izumida, O. Sakai, and Y. Shimizu, J. Phys. Soc. Jpn. 66, 717 (1997).
 [3] A.-P. Jauho, N.S. Wingreen and Y. Meir, Phys. Rev. B 50, 5528 (1994).

TT 34.2 Mi 10:00 TU H104

Non-equilibrium Transport and Approximate Conductance Quantization in Multi-level Quantum Dot Systems — ●S. KIRCHNER¹, J. KROHA², and P. WÖLFLE³ — ¹Rice University — ²Universität Bonn — ³Universität Karlsruhe

Nanoconstrictions or quantum dots with several local levels or channels contributing to the conductance are prototypical systems for numerous quantum point contact devices, markedly for transport through single atoms, molecules or carbon nanotubes, many of them showing the tendency to conductance quantization. We discuss that for several local levels the lead-dot coupling matrix Γ_{nm} is, by principle, not left-right symmetric. As a consequence, within a generalized Landauer-Büttiker approach the conductance is determined by both, the local density of states and the local distribution functions, even in the linear response regime, thus drawing the connection to the Kubo formula. We consider the case of strong Coulomb correlations $U \gg |\Gamma_{nm}|$ within the quantum point contact. While for a single transmission channel the Friedel sum rule strictly enforces quantization of the zero-temperature linear conductance, we show that for several levels there are systematical deviations due to the appearance of multiple Kondo-like resonances near the Fermi level. For the case of two transmission channels, relevant for carbon nanotubes, we give an analytical conductance formula and present results of numerical calculations for the general case both in and out of equilibrium.

TT 34.3 Mi 10:15 TU H104

Spectral Properties and Spin Correlations in the 1D Kondo Box: a DMRG Study — ●TH. HAND, J. KROHA, and H. MONIEN — Universität Bonn

For more than 20 years it has been a mystery why the spin-spin

coupling between magnetic impurities embedded in a metal is in general short-ranged, despite the exponentially large spin coherence length $\xi_K = v_F/T_K$ induced by the impurity in the electron sea, with T_K the Kondo temperature and $v_F = \hbar k_F/m$ the Fermi velocity. Only recently it has been found by general physical arguments [1] and by perturbative calculations [2] that the relevant length scale is $\ell = (\pi \xi_K / k_F^{d-1})^{1/d}$, i.e. $\ell \ll \xi_K$ in dimensions $d \geq 2$. This suggests that in $d = 1$ quantum wires long-range coupling between magnetic impurities can be achieved. In the present work we check this expectation by numerically exact density matrix renormalization group (DMRG) calculations, suitable for nanoscopic wires with discrete energy spectrum. Good quantitative agreement with the analytical predictions is found, including powerlaw behavior of the spin correlations for distance $r < \ell$. We correlate the spin structure with Kondo features in the impurity spectrum and analyze their dependence on the parity of the electron number in the system (even/odd effect). The results may be relevant for recent experiments on carbon nanotubes and double quantum dot systems in the Kondo regime coupled through a bath with discrete spectrum.

- [1] W. Thimm, J. Kroha, J. v. Delft, PRL 82, 2143 (1999).
 [2] I. Affleck, P. Simon, PRL 86, 2854 (2001); P. Simon, I. Affleck, PRB 68 115304 (2003).

TT 34.4 Mi 10:30 TU H104

Structure of Quantum Critical Points in Impurity Models — ●HYUN-JUNG LEE¹, RALF BULLA¹, and NING-HUA TONG² — ¹Theoretische Physik III, Universität Augsburg — ²Institut für Theorie der Kondensierten Materie, Universität Karlsruhe

The numerical renormalization group method is used to investigate zero temperature phase transitions in single-impurity models, where an impurity couples to a non-trivial fermionic bath (Pseudogap Anderson model) or to a (sub)ohmic bosonic bath (Spin-Boson Model). In both cases, zero temperature phase transitions occur between two different phases whose fixed points can be built up of non-interacting single-particle states. These trivial phases are separated by lines of quantum critical points. The structure of these quantum critical points can be understood close to certain values of the bath exponents which turn out to play the role of upper and lower critical dimensions. A complete description of the quantum critical many-particle spectra is achieved using suitable marginal operators.

TT 34.5 Mi 10:45 TU H104

Bosonic Kondo effect of a magnetic impurity in a deconfined magnet — ●LARS FRITZ¹, SERGE FLORENS¹, MATTHIAS VOJTA¹, and KEDAR DAMLE² — ¹Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe — ²Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai, India

Recent works have proposed the occurrence of deconfined $s = \frac{1}{2}$ gapless bosonic degrees of freedom at the quantum critical point separating the Neel state from the valence-bond phase in some two-dimensional quantum antiferromagnets. We propose to couple such systems to a single magnetic impurity. We find within a large-N approach a quenching of the extra moment, which provides a bosonic analog to the Kondo effect in metals. This behavior is in strong contrast to the known Curie susceptibility shown in usual confining critical points, and could serve as a probe for deconfinement in critical antiferromagnets.

TT 34.6 Mi 11:00 TU H104

Quantum two-particle problem in finite systems — ●B. SCHMIDT¹, K. MORAWETZ^{1,2}, M. SCHREIBER¹, A. FICKER¹, and P. LIPAVSKÝ³ — ¹Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ²Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — ³Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16200 Praha 6, Czech Republic

The correlated two-particle problem is solved analytically in the presence of a finite cavity. The method is demonstrated here in terms of

exactly solvable models for both the cavity as well as the two-particle correlation where the two-particle potential is chosen in separable form. The two-particle phase shift is calculated and compared to the single-particle one. We find a Fano resonance behavior due to the interference of single- and two-particle channels. The two-particle bound state behavior is discussed and the influence of the cavity on the binding properties is calculated.

[1] K. Morawetz, M. Schreiber, B. Schmidt, A. Ficker, P. Lipavský, Phys. Rev. B submitted, cond-mat/0409325

TT 35 Correlated Electrons - Quantum Critical Phenomena

Zeit: Mittwoch 11:15–13:00

Raum: TU H104

TT 35.1 Mi 11:15 TU H104

Evidence for a ferromagnetic quantum critical point in CePd_{1-x}Rh_x — ●CHRISTOPH GEIBEL¹, JULIAN SERENI², ROBERT KÜCHLER¹, and TEODORA RADU¹ — ¹MPI für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — ²Centro Atomica Bariloche-CNEA, 8400 S.C. de Bariloche, Argentina

The behavior at the disappearance of magnetic order in Ce-based systems is presently a subject of strong interest. While there exist many Ce-based compounds showing an antiferromagnetic critical point, appropriate candidates for the study of the disappearance of a ferromagnetic (F) state are very scarce. Theories presently favor a first order critical point in pure systems, while disorder is suspected to lead to a continuous second order quantum critical point. One attractive candidate is the alloy CePd_{1-x}Rh_x reported to evolve from an F - Ce³⁺ state at $x = 0$ to a non-magnetic, valence fluctuating state at $x = 1$. However, the disappearance of its F state has never been thoroughly investigated. We report here a detailed investigation of this system by means of ac-susceptibility (χ'_{ac}), specific heat (C_p) and thermal expansion (β) measurements. Our results indicate a continuous disappearance of the F-state, with $T_c \rightarrow 0$ K at around $x_{cr} \approx 0.85$ as traced following the sharp $\chi'_{ac}(T)$ maximum. In the vicinity of the quantum critical point at x_{cr} , power law behavior is observed in $C_p(T)$ and in $\beta(T)$. These results shall be discussed in the context of present theories

TT 35.2 Mi 11:30 TU H104

Ferromagnetic Quantum Phase Transition of Single Crystalline CeSi_{1.81} under High Pressure — ●SANDRA DROTZIGER¹, CHRISTIAN PFLEIDERER^{1,2}, MARC UHLARZ¹, HILBERT V. LÖHNESEN^{1,2}, DMITRI SOUPEL³, WOLFGANG LÖSER³, and GÜNTER BEHR³ — ¹Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — ³Leibniz-Institut für Festkörper- und Werkstofforschung Dresden, PF 27 01 16, D-01171 Dresden, Germany

The rare-earth system CeSi_x develops ferromagnetic order at low temperatures for $1.50 < x < 1.85$. With decreasing Si concentration a structural phase transition between a α -ThSi₂ and a α -GdSi₂ structure occurs. We report the pressure dependence of the magnetisation of single crystalline CeSi_{1.81} for magnetic fields parallel to the crystallographic a -axis, being an easy magnetic direction. Our samples belong to a new generation of CeSi_x single crystals, in which the structural phase transition is observed at $x = 1.85$. With increasing pressure the ordered magnetic moment μ_S and the Curie temperature T_C disappear continuously above a critical pressure $p_c \approx 13 \pm 0.2$ kbar. This behavior is consistent with the existence of a ferromagnetic quantum critical point at p_c . In contrast to the existence of a quantum critical point, magnetic isotherms $M(B)$ do not show clear evidence of a divergence of the uniform susceptibility at p_c . The possible origin of these inconsistencies will be discussed.

TT 35.3 Mi 11:45 TU H104

Quantum Critical Behavior in Yb_{1-x}La_xRh₂Si₂ Studied by Low Temperature Resistivity in Magnetic Fields and under High Pressure — ●MICHAEL NICKLAS, JULIA FERSTEL, CHRISTOPH GEIBEL, and FRANK STEGLICH — Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str.40, 01187 Dresden

The stoichiometric heavy fermion system YbRh₂Si₂ is situated close to a quantum critical point (QCP). At zero magnetic field very weak antiferromagnetic order occurs at $T_N = 70$ mK. Substitution of Si by larger Ge reduces T_N , however, difficulties in sample preparation prevent a complete suppression of T_N by Ge-doping. An alternative route to suppress

the antiferromagnetic order is the partial substitution of Yb by larger La in Yb_{1-x}La_xRh₂Si₂.

We present pressure studies of the electrical resistivity of the paramagnetic 5% and 10% La substituted Yb_{1-x}La_xRh₂Si₂. Applying pressure reduces the unit cell volume again and the system can be tuned through the critical volume. However, substitution of the magnetic ion by non-magnetic La at the Yb-site has more subtle effects and acts not just as chemical pressure on the system.

TT 35.4 Mi 12:00 TU H104

Magnetization dynamics of YbIr₂Si₂ — ●ARNO HIESS¹, OLIVER STOCKERT², MICHAEL M. KOZA¹, ZAKIR HOSSAIN³, and CHRISTOPH GEIBEL² — ¹ILL, Grenoble, France — ²MPI-CPFS, Dresden, Germany — ³IIT, Kanpur, India

Several intermetallic compounds containing cerium, ytterbium or uranium exhibit deviation from Landau-Fermi-liquid behaviour when tuned through a magnetic instability by means of a control parameter such as doping, hydrostatic pressure or magnetic fields. Within this class of compounds YbIr₂Si₂ occupies a special place as it exists in two crystallographic modifications: one (P-type) showing antiferromagnetic order below 0.7 K, the other (I-type) remains paramagnetic down to lowest temperatures. We here report on inelastic neutron scattering experiments investigating the magnetization dynamics in the paramagnetic state of both modifications. Magnetic scattering has been identified for energy transfers smaller 40 meV. Surprisingly, only the I-type modification shows two well-resolved crystal-field transitions whereas for the magnetically ordered P-type modification a broad (most-probable quasi-elastic) signal is observed. We discuss these observations in terms of the crystallographic local ytterbium site symmetry as well as in respect to their unusual thermodynamic (electronic) properties.

TT 35.5 Mi 12:15 TU H104

Field-tuned Quantum Critical Point in Antiferromagnetic Metals — ●INGA FISCHER and ACHIM ROSCH — Institut für theoretische Physik, Universität zu Köln

A magnetic field applied to an antiferromagnetic metal can destroy the long-range order and thereby induce a quantum critical point. Such field induced quantum critical behaviour is the focus of many recent experiments. We investigate theoretically the quantum critical behavior of clean antiferromagnetic metals subject to a static, spatially uniform, external magnetic field. The external field is not only a means for tuning the control parameter, it also influences the dynamics of the order parameter by inducing spin precession. This is described by an exactly marginal operator in the spin-fluctuation theory put forward by Hertz. We investigate how the interplay of precession and damping determines the correlation length, specific heat, magnetocaloric effect, and scattering rate. While critical exponents remain the same, the universal scaling functions are modified and even the sign of leading corrections e.g. to the specific heat can be changed.

TT 35.6 Mi 12:30 TU H104

NRG Study of the Quantum Critical Properties of the Sub-Ohmic Spin-Boson Model — ●NINGHUA TONG¹, MATTHIAS VOJTA¹, and RALF BULLA² — ¹Institute for Theory of Condensed Matter, University of Karlsruhe — ²Theoretical Physics III, Institute for Physics, University of Augsburg

Using the bosonic numerical renormalization group technique, we study the quantum critical properties of the sub-Ohmic spin-boson model. This model describes a two-level system imbedded in a bosonic bath

with power-law spectrum density $J(\omega) \sim \omega^s$. In the sub-Ohmic regime $0 < s < 1$, there exists a line of quantum critical points separating localized and delocalized phases. The critical exponents are calculated and the hyperscaling relations are found to be fulfilled in the range $0 < s < 1$. In small s limit, these results agree well with the perturbative RG calculation, but contradict the existing results for the corresponding long-range Ising model. We conclude that the naive quantum-classical mapping fails for the spin-boson model in the regime $0 < s < 1/2$.

TT 35.7 Mi 12:45 TU H104

Fermi surface symmetry breaking on a square lattice — ●HIROYUKI YAMASE¹, VADIM OGANESYAN², and WALTER METZNER¹ — ¹Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569, Stuttgart, Germany — ²Department of Physics, Princeton University, Princeton, NJ 08544, USA

TT 36 Superconductivity - Vortex Dynamics, Vortex Phases, Pinning

Zeit: Mittwoch 10:00–13:00

TT 36.1 Mi 10:00 TU H2053

Vortex Pinning and Magnetization Reversal Observed in Real Space by Magnetic Force Microscopy — ●ALEXANDER SCHWARZ¹, MARCUS LIEBMANN², UNG HWAN PI³, and ROLAND WIESENDANGER¹ — ¹IAP, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — ²Department of Mechanical Engineering, Yale University, 15 Prospect Street, New Haven, CT 06511, USA — ³ETRI, Gajeong dong Yuseong gu, Daejeon 305-350, South Korea

Vortex pinning mechanisms are important for an understanding of the magnetic properties of high temperature superconductors. Since magnetic force microscopy is able to image individual vortices and the surface topography in the same sample area, it is an ideal tool to study trapping characteristics of defects. In this study, we investigate a $\text{Bi}_2\text{SrCa}_2\text{Cu}_2\text{O}_{8+\delta}$ plate-like single crystal with artificial c -axis columnar defects and intrinsic line defects. The later can be identified as either stacking fault dislocations or surface steps. Columnar defects typically trap only one quantum flux. In regions where only columnar defects are present the vortex density follows the transversal Bean model. On the other hand, stacking fault dislocations can accommodate large numbers of vortices and exhibit an anisotropic pinning behavior, i.e., strong transversal, but weak longitudinal pinning [1]. As a result, they impede vortex propagation during magnetization reversal perpendicular to their orientation and strongly alter the flux distribution in their vicinity. Finally, surface steps apparently do not act as pinning centers at all.

[1] U. H. Pi *et al.*, Phys. Rev. B **69**, 094518 (2004).

TT 36.2 Mi 10:15 TU H2053

On the imaging of the flux-line lattice of a type-II superconductor by soft x-ray absorption microscopy — ●MANFRED FÄHNLE¹, JOACHIM ALBRECHT¹, THOMAS EIMÜLLER¹, PETER FISCHER^{1,2}, EBERHARD GÖRING¹, DANIEL STEIAUF¹, and GISELA SCHÜTZ¹ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — ²Center for X-ray Optics, E. O. Lawrence Berkeley National Laboratory, MS-400, 1 Cyclotron Road, Berkeley, CA 94720 U.S.A.

A new method is proposed for the imaging of the flux-line lattice of a type-II superconductor by soft x-ray absorption microscopy. The method is based on the fact that in the core of a flux-line with linear extension 2ξ (ξ = coherence length) the quasiparticle density of states is different from the one of the surrounding superconducting matrix. Like the scanning tunneling microscopy, the x-ray absorption microscopy therefore is sensitive to the spatial variation of the superconducting order parameter which is quite strong across the sample even for fields considerably larger than H_{c1} , whereas other imaging techniques are sensitive to the spatial variation of the magnetic field which becomes very small for large fields. The new technique has the potential to image in real space static and dynamical properties of the flux-line lattice at arbitrary magnetic fields and with single-flux-line resolution. Based on an estimate of the expected contrast it is shown that the new method is very demanding but probably realizable in the foreseeable future.

We analyze a mean-field model of electrons with pure forward scattering interactions on a square lattice, which exhibits spontaneous Fermi surface symmetry breaking with a d -wave order parameter. As a function of chemical potential, the phase transition is typically first order at low temperature (T) and second order at high T . It is, however, found that Fermi surface fluctuations near the first order transition can be strong. When a repulsive constant contribution to the forward scattering interaction is added, the first order transition is suppressed and tricritical points at the ends of the second order transition line are shifted to lower T . Although the shift is usually not strong enough to lead to a quantum critical point (QCP), we find a limited parameter region where a QCP can be realized. In the weak coupling limit, the transition of the Fermi surface symmetry breaking is characterized by universal functions of suitably rescaled parameters.

Raum: TU H2053

TT 36.3 Mi 10:30 TU H2053

Dendrite Propagation Velocity in Type-II Superconductors — ●BERND-UWE RUNGE¹, BJÖRN BIEHLER¹, ROMAN MINTS², and PAUL LEIDERER¹ — ¹University of Konstanz, Germany — ²Tel-Aviv University, Israel

We use the Faraday effect in combination with ultra-short fs-laser pulses to investigate the flux dynamics in type-II superconductors upon sudden heating. Under certain conditions a dendritic instability develops in those systems. The penetration velocity is measured using a pump-probe technique. A theory is proposed explaining the observed velocities. The theory is based on experimental observations and treats the dendrite as a moving flux jump instability. We can explain the observed “fast” and the well distinct “slow” regimes of flux penetration [1].

[1] U. Bolz *et al.*, Europhys. Lett. **64**(4) 517 (2003)

TT 36.4 Mi 10:45 TU H2053

Vortex Matching due to Periodic Pinning Center Arrays produced by Micellar Techniques — ●J. EISENMEGER, M. OETTINGER, C. PFAHLER, C. DIETRICH, F. WEIGL, B. KOSLOWSKI, A. PLETTL, H.-G. BOYEN, A. ETHIRAJAN, and P. ZIEMANN — Abteilung Festkörperphysik, Universität Ulm, 89069 Ulm

It has been demonstrated that pinning centers can lead to an enhanced stability of a vortex lattice, if this lattice matches a regular array of pinning centers without disturbing its preferred triangular order. Less explored are these phenomena at $T \ll T_c$ where effective pinning centers should exhibit sizes in the nm-range, which are difficult to achieve with conventional lithography methods. To produce triangular arrays of pinning centers we use metal-salt loaded inverse micelles of diblock-copolymers. The metal islands are prepared by immersion of the sample into a solution of diblock-copolymer micelles in toluene which were loaded with a defined amount of metal precursor. Subsequent plasma-etching removes the polymer and reduces the precursor salt to metal islands with a size of about 10 nm. Such supported metal nano particles can be used in different ways to produce pinning centers in superconductors. One approach is overgrowing the metal islands directly with a superconducting (SC) layer, producing pinning centers by locally changed SC properties. In a second approach, nano particles serve as etching masks to pattern arrays of nano columns into the surface of the substrate. These columns are used to locally influence the SC properties of a thin film grown on top. A third possibility is pressing a sample with nano columns into a SC film leading to an array of antidots.

TT 36.5 Mi 11:00 TU H2053

AFM-Analyse von schmelztexturiertem $\text{YBa}_2\text{Cu}_3\text{O}_x$ mit nanoskaligen Einschlüssen — ●MICHAEL R. KOBLISCHKA¹, MARC WINTER¹, UWE HARTMANN¹, ANJELA KOBLISCHKA-VENEVA², N. HARI BABU³ und DAVID CARDWELL³ — ¹FR Experimentalphysik, Universität des Saarlandes, Postfach 151150, D-66041 Saarbrücken — ²Institut für Funktionswerkstoffe, Universität des Saarlandes, Postfach 151150, D-66041 Saarbrücken — ³IRC in Superconductivity, University of Cambridge, Madingley Road, Cambridge, U.K.

$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) ist immer noch der am besten geeignete Hochtemperatur-Supraleiter (HTSL) für Anwendungen, allerdings wäre eine grössere Stromdichte wünschenswert. Um dieses Ziel zu

erreichen, wurde bislang hauptsächlich versucht, die Grösse der beim Wachstumsprozess entstehenden Y_2BaCuO_5 -Partikel zu verringern. Diese sind jedoch bislang für effektive Pinningzentren zu gross und ausserdem nicht ideal verteilt. Mit Hilfe der Nanotechnologie besteht jedoch die Möglichkeit, gezielt nicht-reaktive Nanopartikel in die HTSL-Proben einzubringen. Kürzlich gelang es, YBCO-Proben mit $\text{Y}_2\text{Ba}_4\text{CuMO}_x$ -Partikeln ($M = \text{Zr}, \text{Nb}$) herzustellen, in denen die Nanopartikel Grössen zwischen 10 und 50 nm aufweisen. Mit Hilfe von AFM-Messungen untersuchen wir die Verteilung dieser Partikel und deren Grössenverteilung, und die Wechselwirkung zwischen diesen Partikeln und der umgebenden supraleitenden Matrix. Ausserdem wurden die lokalen Stromdichten mit Hilfe magneto-optischer Untersuchungen bestimmt.

Diese Arbeit wird unterstützt durch EFFORT und DAAD-PPP.

TT 36.6 Mi 11:15 TU H2053

Artificial modulation and anisotropy of flux pinning force in R123 composite films — ●CHUANBING CAI, JENS HAENISCH, THOMAS GEMMING, and BERNHARD HOLZAPFEL — IFW Dresden, D-01171 Dresden, Germany

Artificial flux pinning centers in R123 films has emerged much significant for both fundamental understanding and practical applications (especially for coated conductors). Using PLD technique, we prepared two types of composite films: i) superlattices consisting of three R123: $n \times (\text{Gd}_{123d}/\text{Nd}_{123d}/\text{Eu}_{123d})$, and ii) multilayer of R123/ Y_2O_3 : $n \times (\text{Y}_{123d1}/\text{YO}_{d2})$. They possess the potential of artificial flux pinning centers due to epitaxial strain fields and second phase additions, respectively. We show the tailorable flux pinning forces and their anisotropy by angular dependences of the transport critical current density. It is revealed that the strongest modulation of flux pinning takes place at field direction parallel to c while it is hardly variable at field direction perpendicular to c .

Pause

TT 36.7 Mi 11:45 TU H2053

Nanostrukturierte Flußhaftzentren in Hoch- T_c Supraleitern — ●M. WINTER¹, M. R. KOBLISCHKA¹, A. HU², M. MURALIDHAR², U. HARTMANN¹ und M. MURAKAMI³ — ¹FR Experimentalphysik, Universität des Saarlandes, Postfach 151150, D-66041 Saarbrücken — ²SRL/ISTEC, 1-10-13 Shinonome, Koto-ku, Tokyo 135-0062, Japan — ³Department of Materials Science and Engineering, Shibaura Institute of Technology, Shibaura 3-9-14, Minato-ku, Tokyo 108-8548, Japan

Die ideale Grösse für Haftzentren in Supraleitern liegt bei der doppelten Kohärenzlänge, z.B. 4,5 nm in der ab -Ebene von $\text{YBa}_2\text{Cu}_3\text{O}_x$ (YBCO). Nichtleitende Einschlüsse, wie (SE)211-Partikel (Y_2BaCuO_5) mit typischen Grössen von einigen hundert Nanometern bis hin zu Mikrometern wirken nur bei niedrigen Magnetfeldern als effektive Flußhaftzentren. Um hohe kritische Stromstärken auch bei hohen Feldern zu erreichen, müssen nanometergroße, nicht-supraleitende Strukturen innerhalb des gesamten Volumens des Supraleiters vorhanden sein. Wir haben schmelztexturierte ($\text{Nd}_{0,33}\text{Eu}_{0,28}\text{Gd}_{0,38}$) $\text{Ba}_2\text{Cu}_3\text{O}_x$, ($\text{Nd}_{0,33}\text{Eu}_{0,38}\text{Gd}_{0,28}$) $\text{Ba}_2\text{Cu}_3\text{O}_x$ - (NEG), ($\text{Sm}_{0,33}\text{Eu}_{0,33}\text{Gd}_{0,33}$) $\text{Ba}_2\text{Cu}_3\text{O}_x$ - (SEG) und $\text{SmBa}_2\text{Cu}_3\text{O}_x$ - (SmBCO) Proben mit Rasterkraft- und Rastertunnel-Mikroskopie an Luft untersucht. Im Vergleich zu YBCO-Kristallen zeigen die SEG und NEG-Kristalle regelmäßige Streifen- und Kreuzstrukturen, etwa eine Größenordnung größer als die Kohärenzlänge. Es handelt sich dabei um periodische Variationen der chemischen Zusammensetzung, die zu örtlich unterschiedlichen supraleitenden Eigenschaften führt, so daß gewisse Phasen bei hohen Strömen oder hohen Feldern normalleitend werden und als Flußhaftzentren wirken können.

TT 36.8 Mi 12:00 TU H2053

Charge density distributions induced by flux creep in superconducting YBCO films — ●VOLKER BORN and CHRISTIAN JOOSS — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

A moving vortex in a superconductor represents an electric dipole where the induced charge is distributed over its spatial magnetic extension. On mesoscopic length scales of $\approx 1\mu\text{m}$ (averaging over the spatial structure of individual vortices) all dipoles cancel, if ensembles of vortices move homogeneously. However, a mesoscopic charge density distribution arises if gradients of the vortex velocity perpendicular to their direction of motion exist. An excellent tool to study these charge densities is time and space resolved magneto-optics with spatial resolutions down to $\approx 1\mu\text{m}$. Here, we report on charge densities being induced into superconducting $\text{YBa}_2\text{Cu}_3\text{O}_7$ thin films by thermally activated flux creep in constant ex-

ternal magnetic fields. We discuss briefly our method how to obtain the total electric field, the polarisation distribution and the charge density distribution. The main focus is directed to the vortex motion at current domain boundaries, grain boundaries and circular defects which builds up complex patterns of charge density distributions.

TT 36.9 Mi 12:15 TU H2053

Investigation of the $j_c(T)$ -behavior to answer the question of pinning in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thin-films — ●SEBASTIAN BRÜCK¹ and JOACHIM ALBRECHT^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart, Germany — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Thin films of the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) grown on SrTiO_3 (STO) substrates which partly experience a moderate nanostructuring of the surface, show an imposing increase of the critical current density where the surface is treated. The magneto-optical imaging technique joint by a numerical inversion scheme is used to obtain the current density distribution in such films with high spatial resolution enabling one to directly compare j_c in different parts of the sample. It will be shown that a detailed investigation of the temperature behavior of j_c , taking into account the distinctions between untreated and structured part, can provide deeper insights into the actual pinning scenario. By comparing the experimental results with theoretical models, evidence is found for the important role of intergranular low-angle grain boundaries for the increase of j_c as well as for the pinning scenario in general.

TT 36.10 Mi 12:30 TU H2053

Origin of the Resistive Transitions Broadening in Superconducting MgB2 Films — ●A. S. SIDORENKO^{1,2,3}, V. I. ZDRAVKOV^{2,3}, E. NOLD⁴, TH. KOCH⁵, TH. SCHIMMEL^{1,5}, S. HORN², C. MÜLLER², A. WIXFORTH², and R. TIDECKS² — ¹Institute of Applied Physics, Universität Karlsruhe, D-76128 Karlsruhe — ²Institut für Physik, Universität Augsburg, D-86159 Augsburg — ³Institute of Applied Physics, MD-2028 Kishinev, Moldova — ⁴Institute of Materials Research I, Forschungszentrum Karlsruhe, D-76021 Karlsruhe — ⁵Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe

The discovery of superconductivity in MgB2, the material with hexagonal layered crystal structure, raised questions about its transport properties. The crystal structure of MgB2 and the band structure calculations suggest that the quasi-two-dimensional (2D) boron planes are mainly responsible for the charge transport. Therefore the superconducting properties of MgB2 are expected to reflect this 2D character. On the other hand, the layered structure should also influence the magnetic flux penetration and flux motion in the presence of an external magnetic field. In particular, thermally activated vortex creep processes (TAFF) play a crucial role in the resistive transitions broadening for MgB2 as well as for artificial multilayered systems. In the present work we report about experimental studies of the origin of resistive transitions broadening for MgB2 thin films.

TT 36.11 Mi 12:45 TU H2053

Flux-lattice melting in two-dimensional disordered superconductors — ●THOMAS NATTERMANN¹ und LI MAI SUAN² — ¹Institut für Theoretische Physik der Universität zu Köln, Zùlpicher Str. 77, 50937 Köln — ²Institute of Physics, Polish Academy of Sciences,

The flux line lattice melting transition in two-dimensional pure and disordered superconductors is studied by a Monte Carlo simulation using the lowest Landau level approximation and quasi-periodic boundary condition on a plane. The position of the melting line was determined from the diffraction pattern of the superconducting order parameter. In the clean case we confirmed the results from earlier studies which show the existence of a quasi-long range ordered vortex lattice at low temperatures. Adding frozen disorder to the system the melting transition line is shifted to slightly lower fields. The correlations of the order parameter for translational long range order of the vortex positions seem to decay slightly faster than a power law (in agreement with the theory of Carpentier and Le Doussal) although a simple power law decay cannot be excluded. The corresponding positional glass correlation function decays as a power law establishing the existence of a quasi-long range ordered positional glass formed by the vortices. The correlation function characterizing a phase coherent vortex glass decays however exponentially ruling out the possible existence of a phase coherent vortex glass phase.

TT 37 Transport - Fluctuations and Noise

Zeit: Mittwoch 10:15–12:15

Raum: TU H3027

TT 37.1 Mi 10:15 TU H3027

High-frequency shot noise measurement of a quantum point contact — •UDO HARTMANN¹, FRANCK BALESTRO², EUGEN ONAC², LAURENS W. VAN BEVEREN², RONALD HANSON², YULI V. NAZAROV², and LEO P. KOUWENHOVEN² — ¹Physics Department and CeNS, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany — ²Kavli Institute of Nanoscience Delft and ERATO Mesoscopic Correlation Project, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands

We present an experimental realisation of a quantum dot (QD) high-frequency noise detector that measures the current shot noise produced by a nearby quantum point contact (QPC) by means of noise-assisted tunnelling. We investigate the dependence of the detector signal on the voltage across the QPC and on the QPC transmissions which is consistent with previous low-frequency measurements [1,2]. We observe and explain the saturation and quantum features in the detector signal.

[1] Y. P. Li, *et al.*, Appl. Phys. Lett. **57**, 774 (1990).

[2] A. Kumar *et al.*, Phys. Rev. Lett. **76**, 2778 (1996).

TT 37.2 Mi 10:30 TU H3027

Statistics of Current Fluctuations and Coulomb Interaction in Diffusive Conductors — •DMITRY BAGRETS — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe.

I evaluate the full current statistics (FCS) in the low dimensional (1D and 2D) diffusive conductors in the incoherent regime, $eV \gg 1/\tau_D$, τ_D being the diffusion time through the conductor[1]. It is shown that Coulomb interaction substantially enhances the probability of big current fluctuations for short conductors with $\tau_D \ll \tau_E$, τ_E being the voltage dependent energy relaxation time, leading to the exponential tails in the current distribution. These tails arise from the huge fluctuations of the current of electron-hole pairs which are excited by the low frequency classical fluctuations of the electromagnetic field in the system. The current fluctuations are most strong for temperatures below $1/\tau_D$, provided $\tau_D \sim \tau^*(V)$, where the time scale $\tau^*(V)$ is parametrically smaller than the energy relaxation time $\tau_E(V)$. Remarkably, the time $\tau^*(V)$ transforms to the decoherence time $\tau_\varphi(T)$, known from the theory of weak localization[2], if one substitutes voltage for the temperature.

[1] D. A. Bagrets, cond-mat/0406483, to appear in Phys. Rev. Lett.

[2] B.L. Altshuler, A.G. Aronov and D.E. Khmel'nitsky, J.Phys. C **15** 7367 (1982)

TT 37.3 Mi 10:45 TU H3027

Super-Poissonian Noise in Complex Quantum Dots — •WOLFGANG BELZIG — Department of Physics and Astronomy, University of Basel, Klingelbergstr. 82, 4056 Basel, Schweiz

We examine the full counting statistics of quantum dots, which display super-Poissonian zero-frequency shot noise. By an extension to a generic situation with many excited states we identify the underlying transport process. The statistics allows to clearly identify the bunching-processes which leads to the enhanced noise. The obtained results could be useful to determine transport characteristics in molecules and large quantum dots, since the noise (an higher cumulants) allow to identify the internal level structure, which does not show up in the average current.

TT 37.4 Mi 11:00 TU H3027

Tunneling through coupled quantum dots - Dephasing and Counting Statistics — •GEROLD KIESSLICH¹, PETER SAMUELSSON², ANDREAS WACKER², and ECHEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin — ²Dept. of Physics, University of Lund, Box 118, SE-22100 Lund, Sweden

The electronic transport through two coupled quantum dots (QDs) in series can be described either in a fully coherent approach (e.g. density matrix description) or in a simple sequential tunneling treatment (Pauli master equation with Fermi's Golden rule for coupling between the QDs). It turns out that both descriptions provide the same average current for noninteracting QDs [1]. In contrast, the zero-frequency spectral power density is different for intermediate coupling strengths between the QDs reflecting its sensitivity on coherence in the tunneling process. In a phenomenological escape model we study the influence of the transition between the sequential and coherent limit on the current fluctuations. In particular, the counting statistics is obtained by means

of a stochastic path-integral method [2]. The noise and the skewness are discussed in detail with respect to decoherence in the tunneling process.

[1] H. Sprekeler, G. Kießlich, A. Wacker, and E. Schöll. Phys. Rev. **B**, 125328, (2004)

[2] S. Pilgram, A.N. Jordan, A.V. Sukhorukov, and M. Büttiker. Phys. Rev. Lett. **90**, 206801 (2003)

TT 37.5 Mi 11:15 TU H3027

Correlations in noisy Landau-Zener transitions — •STEFAN SCHEIDL¹ and VALERY L. POKROVSKY^{2,3} — ¹Institut für Theoretische Physik, Universität zu Köln — ²Department of Physics, Texas A&M University, College station — ³Landau Institute for Theoretical Physics, Chernogolovka

We analyze the influence of colored classical Gaussian noise on Landau-Zener transitions during a two-level crossing in a time-dependent regular external field [1]. Transition probabilities and coherence factors become random due to the noise. We calculate their two-time correlation functions, which describe the response of this two-level system to a weak external pulse signal. The spectrum and intensity of the magnetic response are derived. Although the noise enters the equation of motion for the Bloch vector in a multiplicative way, non-perturbative analytic results are obtained by a resummation of diagrams in the limit of a short noise correlation time. Our results also cover regimes where fluctuations are of the same order of magnitude as averages.

[1] V.L. Pokrovsky and S. Scheidl, Phys. Rev. B **70**, 014416 (2004)

TT 37.6 Mi 11:30 TU H3027

Shot noise in AC-driven nanoscale conductors — •SIGMUND KOHLER, MICHAEL STRASS, JÖRG LEHMANN, SÉBASTIEN CAMALET und PETER HÄNGGI — Institut für Physik, Universität Augsburg, 86135 Augsburg

An ac driving force can significantly modify the electron transport through nanoscale conductors. Some paradigmatic effects in such systems are the current enhancement by resonant driving, the induction of a ratchet or pump current, and the suppression of the DC current by the purely coherent influence of the driving field [1,2]—their experimental observability depends crucially on whether the current flows at a tolerant noise level. For the investigation of the current noise in the mentioned situations, we employ a Floquet theory for periodically time-dependent coherent conductors which provides both the current and its noise properties. If the driving frequency is either large or close to a resonance, the time-dependent transport setup can be approximated by a static effective system which consists of a renormalized conductor Hamiltonian and an effective distribution function for the lead electrons. The analytical results are tested against an exact numerical solution.

[1] S. Camalet, S. Kohler, P. Hänggi, Phys. Rev. B **70**, 155326 (2004)

[2] S. Kohler, J. Lehmann, and P. Hänggi, submitted to Phys. Rep.; cond-mat/0409251.

TT 37.7 Mi 11:45 TU H3027

Shot noise in tunneling transport through molecules and coupled quantum dots — •JASMIN AGHASSI^{1,2}, AXEL THIELMANN¹, MATTHIAS HETTLER¹, and GERD SCHÖN^{1,2} — ¹Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, 76021 Karlsruhe — ²Universität Karlsruhe, Institut für Theoretische Festkörperphysik

We consider charge transport through a nanoscopic object such as single molecules or coupled quantum dots, that is weakly coupled to metallic electrodes. We explicitly account for the electronic interactions and the resulting many-body states of the molecule/quantum dots, and allow for relaxation of the excited states. The current-voltage characteristics as well as the current noise are calculated within first-order perturbation expansion in the coupling strengths. For the case of a semi-quantitative model of benzene we predict negative-differential-conductance accompanied with super-poissonian noise. For a series coupled quantum dots, we analyze the shot noise in the various regimes of transport depending on the inter-dot coupling and participating many-body states.

TT 37.8 Mi 12:00 TU H3027

Schwingungseigenschaften und Wärmeleitfähigkeit ungeordneter Festkörper — •WALTER SCHIRMACHER — Physik-Department E13, TU München, 85747 Garching

Eine Theorie der anomalen thermischen und Schwingungseigenschaften ungeordneter Festkörper wird vorgestellt. Grundlage ist die Modellvorstellung räumlich fluktuierender elastischer Konstanten. Mit Hilfe feldtheoretischer Methoden werden Mean-Field-Näherungsausdrücke für die Zustandsdichte und den Energiediffusionskoeffizienten hergeleitet. Hieraus lässt sich die spezifische Wärme und die thermische Leitfähigkeit

berechnen. Die niederfrequente Erhöhung der Zustandsdichte ("Bosonpeak"), sowie das Plateau in der Temperaturabhängigkeit der thermischen Leitfähigkeit ergeben sich als Resultat der eingefrorenen Unordnung. Diese führt zu einer verstärkten Streuung im Frequenzbereich des Bosonpeaks und darüber.