TT 38: Poster Session Transport

Time: Wednesday 14:00–18:00 Location: P3

TT 38.1 Wed 14:00 P3

Charge transfer statistics of double quantum dots in the Kondo regime — •David Breyel and Andreas Komnik — Institut für Theoretische Physik, Universität Heidelberg

We calculate the full counting statistics (FCS) for a system consisting of two quantum dots in the Kondo regime which are subject to different magnetic fields and are coupled to two metallic leads biased by a finite voltage. With certain restrictions on the coupling constants a transformation consisting of bosonization, rotation and refermionisation maps the Hamiltonian of the system to one of a noninteracting system as in [1,2]. We use the Schwinger-Keldysh-formalism for the Green's functions in order to derive the FCS along the lines of [3]. We concentrate on the Fano factor which can be calculated from the FCS as well as the effective transmission coefficients. We explain different features of the Fano factor depending on different system parameters. Furthermore, we succeed in linking the features of the effective transmission coefficients to individual transport processes. For instance we conclude that every transport process through the system is accompanied by a spin flip the the positions of the peaks in the transmission coefficient match the strength of the applied magnetic field. Finally, we discuss the experimental implications of the identified FCS features.
[1] V. J. Emery and S. Kivelson, Phys. Rev. B 46 (1992), 10812
[2] A. Schiller and S. Hershfield, Phys. Rev. B 58 (1998), 14978
[3] A. O. Gogolin and A. Komnik, Phys. Rev. Lett. 97 (2006), 016602

TT 38.2 Wed 14:00 P3

Magnetostrictive effects in ferromagnetic Dy break-junctions — •Marc Müller[1], Christoph Sürgers[1], Richard Montbrun[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

A characteristic property of the rare-earth metals are their large magnetostrictive strains which are related to the magnetocrystalline anisotropy through the elastic energy. We have investigated the electrical conductance G of mechanical break-junctions of a dysprosium wire at 4.2 K where Dy is in the ferromagnetic state. In zero magnetic field we find the usual variation of the conductance G vs. electrode distance x while breaking the wire mechanically, with a sequence of steps and more or less prominent plateaus. The behavior $G(x)$ is modified in magnetic fields $\mu_0 H$ up to 1 T due to the large magnetostriction of Dy. In addition, the conductance can be changed reproducibly by variation of H. For a number of contacts we observe discrete changes in $G(H)$ in the range of several $G_0 = 2e^2/h$. The behavior of $G(H)$ and its angular dependence can be quantitatively understood by taking into account the magnetostrictive properties of Dy. This first realization of a magnetostrictive atomic switch demonstrates the possibility of reproducibly tuning the conductance of magnetic nanocontacts by a magnetic field.

Work supported by the DFG Center for Functional Nanostructures (CFN).

TT 38.3 Wed 14:00 P3

Time-domain interferometry with single quantum dots — •Alexander Croy and Ulf Saalmann — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Coherent control of nanoscale devices is one of the main topics of current research on electron transport in systems on the nanometer scale. A very successful method for the coherent manipulation of charge and spin qubits in double quantum dots consists in using nearly rectangular voltage pulses. Moreover, recent experiments demonstrate that the creation of high-frequency pulse trains is feasible, which paves the way for observing new coherent transport phenomena.
Here we present numerical and analytical results demonstrating the influence of such pulse trains on the time-averaged occupation of a single quantum dot and the currents through the system. For very high and low frequencies coherent destruction of tunneling and adiabatic transport can be observed, respectively. Additionally, we consider random voltage pulse-trains given by a random telegraph process. In this case the coherent features cannot be observed.

TT 38.4 Wed 14:00 P3

Effects of Coulomb interaction on the dynamics of an open quantum dot system — •Benjamin Baxevanis and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg

We study the effect of Coulomb interaction on the time-dependent dynamics of a quantum dot system weakly coupled to an electronic reservoir. The two systems are assumed to be initially separated and we calculate the evolution from a non-equilibrium state to equilibrium as the interaction between the systems is instantly switched on. We determine the current flow from the reservoir to the single quantum dot in the sequential tunnelling regime using a master equation. The exact eigenstates of a finite number of correlated electrons in the quantum dot are taken into account provided by the exact-diagonalization method. We discuss the significance of the few-particle states which are involved in the charging of the quantum dot. We encounter signatures of Coulomb blockade in the transient regime of the current-voltage characteristics which emerged in recent experiments [1].
[1] B. Marquardt, M. Geller, B. Baxevanis, D. Pfannkuche, A. D. Wieck, D. Reuter, A. Lorke, preprint arXiv:1007.0392

TT 38.5 Wed 14:00 P3

Different time scales in the dynamics of an interacting quantum dot — •L.Debora Contreras-Pulido[1], Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[3] — [1]RWTH-Aachen University, Aachen, Germany — [2]Victoria University of Wellington, Wellington, New Zealand — [3]Universität Duisburg-Essen and CeNIDE, Duisburg, Germany

The recent theoretical and experimental analysis of the controlled emission of charge (as well as current correlations) from a quantum capacitor, shows its potential application in quantum information, in nanoelectronics operating in Gigahertz frequencies, and also in the study of a few-particle physics, including the dynamics of nanoscale systems [1]. We extend the study presented in [2] for the time-dependent decay after a step pulse has been applied to a single-level quantum dot with Coulomb interaction and coupled to an electronic reservoir. Our results show that besides the independent decay of charge and spin, an additional time scale appears which we calculate up to second order in a perturbation expansion in the tunneling coupling. We relate the decaying quantity to deviations of the electron-hole occupation and the symmetry of the Anderson Model. Importantly, the decay rate is independent of the level position.
[1] See e.g. A. Mahé *et al.*, Phys. Rev. B **82**, 201309(R) (2010); M. Moskalets, P. Samuelsson, M. Büttiker Phys. Rev. Lett. **100**, 086601 (2008), and references therein.
[2] J. Splettstoesser, M. Governale, J. König, M. Büttiker Phys. Rev. B **81**, 165318 (2010).

TT 38.6 Wed 14:00 P3

Josephson current through interacting quantum dots — •Stephanie Droste, Janine Splettstoesser, and Sabine Andergassen — Institut für Theorie der Statistischen Physik RWTH Aachen & JARA-Fit, Germany

Motivated by recent experiments on transport through carbon nanotube double dots with superconducting leads, we study the effects of Coulomb interactions on transport through such a device. Richer physics due to the proximity effect is expected, as a consequence of the more complex level structure and differing interaction strengths between different dot levels. We extend a recent analysis [1] of Coulomb interaction effects in a single-level quantum dot to a serial double dot coupled to superconducting leads. We derive a local effective Hamiltonian including the atomic or molecular levels as well as the induced proximity effect on the quantum dot and compute the Josephson current as well as a Δ-dependent phase diagram. The effective Hamiltonian is the starting point of a detailed analysis of dissipative effects.
[1] T. Meng et al., Phys. Rev. B **79**, 224521 (2009).

TT 38.7 Wed 14:00 P3

Real-time renormalization group for quantum dots with normal and superconducting leads — •Jacek Swiebodzinski[1], Dirk Schuricht[2], Jürgen König[1], and Herbert Schoeller[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]Institut für Theorie der Statistischen Physik,

RWTH Aachen, 52056 Aachen, Germany

The real-time renormalization group in frequency space (RTRG-FS) is a formally exact perturbative renormalization group scheme from which the kernel of the kinetic equation for the reduced density matrix can be calculated. The method is applicable for small quantum systems, such as quantum dots, in contact with several particle or heat reservoirs. Since the formalism is based on a perturbative expansion in the system-reservoir coupling quantum systems with arbitrary large interaction strength can be treated. In its original form [1] the RTRG-FS was formulated for systems coupled to normal leads only. Here we present a generalization of the method to the case where the leads may be both normal or superconducting. In the latter case transport can be provided either by quasiparticle or Andreev tunneling giving rise to a rich variety of interesting physical phenomena. When several superconducting leads at different chemical potentials are present it is important to consider the energy contribution from the Cooper pair condensate in the leads. We in particular account for this situation. Finally we discuss some applications of the method.

[1] H. Schoeller, Eur. Phys. J. Special Topics **168**, 179 (2009).

TT 38.8 Wed 14:00 P3

Superconductivity-enhanced transport through a carbon nanotube quantum dot with Nb contacts — •Thomas Geiger[1], Kicheon Kang[1,2], Dmitry Ryndyk[3], Andreas Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Department of Physics, Chonnam National University, Gwangju 500-757, Korea — [3]Institute for Theoretical Physics, University of Regensburg, Germany

We present the effect of superconductivity in high quality Nb contacts ($T_c = 8.5$K, $B_c = 4.5$T in parallel field) on transport through a SWCNT quantum dot explored by means of high resolution charging diagrams. We find clear transport spectroscopy signatures of the superconductivity in the leads: Over a wide gate range density of states (DOS)-enhanced elastic cotunneling features are observed at an energy of twice the reduced gap of 500 μeV. In some gate regions, Andreev reflection (AR) causes low energy features near the degeneracy points and the contacts' DOS peaks are reflected in inelastic cotunneling lines.

The magnetic field dependence of these features shows an expected decrease following the gradual suppression of the gap-parameter in the leads. Remarkably, the sub-gap features at certain degeneracy points emerge and show a nonmonotonic temperature dependence: With just precursors visible close to base temperature, a rich structure of the AR features develops much more prominently at a few hundred mK.

[1] Grove-Rasmussen, K., Jørgensen, H. I., Andersen, B. M., Paaske, J., Jespersen, T. S., Nygård, J., Flensberg, K. and Lindelof, P. E.; Phys. Rev. B **79**, 134518 (2009)

TT 38.9 Wed 14:00 P3

Kondo effect in quantum dots: slave-boson Keldysh field theory — •Sergey Smirnov and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We consider a single impurity Anderson model, a quantum dot with a single spin degenerate level coupled to two contacts possibly at different chemical potentials. Assuming strong electron-electron interactions in the dot we restrict the dot Hilbert space to a subspace of the empty and singly occupied states at the expense of transforming to new fermions and introducing a slave-boson. Using this new fermi-bose representation we construct an effective Keldysh field theory suitable for both equilibrium and non-equilibrium situations. The conservation of the total number of the fermions and bosons leads to a constraint in the integration over the fermionic and bosonic fields. This mathematical complication, a consequence of the interacting nature of the problem, is dealt with by introducing an additional integration removing the constraint. After integrating over the fermionic fields of the dot and contacts we obtain an effective Keldysh action with respect to the dot slave-bosonic field. We further develop a saddle point analysis of this action equivalent to the mean field approach known from the imaginary time equilibrium field theories developed previously for the Kondo effect.

TT 38.10 Wed 14:00 P3

Shot-noise of tunnel current coupled to a local plasmon — •Fei Xu, Federica Haupt, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D- 78457 Konstanz, Germany

Current noise in mesoscopic conductors is an important tool to investigate quantum many-body effects in electron transport. If the noise is measured at frequencies in the quantum range, $\hbar\omega \gg k_BT$, the measurement amounts to the detection of photons produced by current fluctuations. This is important in view of recent experiments on photon-emission from tunnel junctions formed by a scanning tunneling microscope on a metallic surface [1,2]. These works showed a considerable intensity of photons emitted with a frequency larger than the applied bias voltage $\hbar\omega > eV$ [1,2]. While photons with frequency $\hbar\omega < eV$ can be readily interpreted in terms of fluctuations in single-electron transfer processes, over-bias ($\hbar\omega > eV$) photon emission is a fingerprint of electronic correlations. We address the problem of over-bias photon emission formulating it in terms of current fluctuations in a conductor interacting with an electromagnetic environment. The latter can mediate cooperative processes in which two electrons team up crossing the junction, emitting a single phonon with energy up to $2eV$ [3]. To describe the set-up of Ref. [1], we employ a minimal model consisting of a local tunnel junction coupled to an electric RLC circuit, whose dynamics mimics the local plasmon mode in the metal junction.

[1] G. Schull, *et al.* PRL 102, 057401 (2009).
[2] N. L. Schneider, *et al.* PRL 105, 026601 (2010).
[3] J. Tobiska, *et al.*, PRL. 96, 096801 (2006).

TT 38.11 Wed 14:00 P3

Laser induced electronic transport through metallic atomic-sized contacts — •Matthias Bädicker, Daniel Benner, Reimar Waitz, Johann Berres, Paul Leiderer, Johannes Boneberg, and Elke Scheer — Fachbereich Physik, Universität Konstanz

We investigate the influence of chopped laser light onto the electronic transport through a metallic point contact. It has been shown that there are several contributions to the laser induced effect like thermal expansion, plasmons and others. Here we concentrate on the thermal effects by varying the metal and the substrate material using correlation measurements of mechanical stress and optical excitation.

We use lithographically fabricated Mechanically Controllable Break-Junctions (MCBJs) operated at ambient conditions for fabricating atomic-size contacts and atomically-sharp tips of gold or platinum. The substrates we used are massive reflective and semi-transparent materials.

Detailed analysis of light-induced conductance changes has shown photo-assisted transport due to the excitation of high-energetic quasiparticles and collective effects such as surface plasmon excitation. We optimize the light-induced effects for the development of optoelectronic devices by studying systematically the effects on different metals (gold and platinum), wavelengths, position of the laser spot, and geometries (e.g. polarization of the laser light).

TT 38.12 Wed 14:00 P3

Magneto-resistance Measurements on Atomic Platinum Chains — •Christopher Espy, Florian Strigl, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Recently there have been many theoretical predictions that platinum, nonmagnetic in bulk, is indeed magnetic in nanostructures [1][2]. How and when this magnetism manifests is still a point of discussion [3]. Preliminary experiments investigating magnetic effects in nanostructures of various metals have been performed, however conclusive evidence confirming previous theoretical predictions regarding magnetism in platinum nanostructures has yet to be found [4].

In this contribution we present the study of suspended monatomic platinum nanowires, fabricated using the mechanically controllable break junction technique. Various experiments are carried out at low temperatures, T $<$ 4.2 K, and under cryogenic vacuum conditions, including the generation of conductance histograms, magneto-resistance investigations, and study of the current-voltage characteristics of the nanostructures. We find strong chain length-dependent magneto-resistive effects of considerable magnitude, up to 25%.

[1] Smogunov et al. Nat. Nanotechnol. 3 (2008) 22
[2] García-Suárez et al. Phys. Rev. B 79 (2009) 060408
[3] Thiess et al. Phys. Rev. Lett. 103 (2009) 217201
[4] Untiedt et al. Phys. Rev. B 69 (2004) 081401(R)

TT 38.13 Wed 14:00 P3

Higher-order perturbation theory applied to time-dependent electron transport processes — •Bogdan Popescu and Ulrich Kleinekathöfer — Jacobs University Bremen, Germany

In the present work, the electron transport through a quantum system, modelled as a linear chain of tight-binding sites and coupled to external fermionic leads, is investigated using a reduced density matrix

formalism [1]. This model may be applied to characterize a molecular wire or consecutive quantum dots coupled in series. The dynamics of the electrons tunnelling through the system is described by a quantum master equation derived in the framework of perturbation theory. The influence of higher-order terms [2] in the coupling to the leads has been investigated, i.e., the limits of the second-order perturbation theory have been shown. The present method is suitable to accurately describe stronger system-lead coupling. Additionally, this approach is able to accurately account for time-dependent effects of an external electric or magnetic field.

[1] S. Welack, M. Schreiber and U. Kleinekathöfer, J. Chem. Phys. **124**, 044712 (2006).
[2] J. Jin, X. Zheng and Y. Yan, J. Chem. Phys. **128**, 234703 (2008).

TT 38.14 Wed 14:00 P3

Extension of the nonequilibrium Green's funtion towards systems with broken translational invariance — •Steven Achilles[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

Electronic structure calculations are nowadays an important tool for investigating and predicting physical effects of new materials on the nanometerscale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for two different types of geometries, planar junctions [3] and embedded clusters. Both implementations include the self-consistent treatment of systems under external bias using the nonequilibrium density between the chemical potentials of the left and the right lead.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for the two different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] C. Heiliger et al., J. Appl. Phys. 103, 07A709 (2008).

TT 38.15 Wed 14:00 P3

Effects of spin-orbit interaction on Andreev reflection in carbon nanotubes — •Anselm Schultes and Patrik Recher — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

We model transport through a carbon nanotube (CNT) in contact with a s-wave superconductor using the Dirac-Bogoliubov-de Gennes equation including spin-orbit interaction (SOI) in the CNT. For a transparent normal-superconductor (NS) interface the subgap conductance, which is dominated by Andreev reflection, is modified in the presence of SOI. Depending on the chirality of the CNT, transport can be spin-dependent. In a NSN junction the nonlocal conductance carried by crossed Andreev reflection and elastic co-tunneling is strongly influenced by SOI and can be manipulated by a gate voltage.

TT 38.16 Wed 14:00 P3

0.7 anomaly in QPC – temperature dependence of conductance in matsubara formalism — •Florian Bauer, Jan Heyder, and Jan von Delft — Arnold Sommerfeld Center, LMU München

To study the physics of the 0.7 anomaly in Quantum Point Contacts (QPCs), we calculate the conductance as a function of magnetic field and analyse the relevance of geometry. We study an extended 1D-Hubbard chain and model the QPC by a single smooth potential barrier. We use the functional renormalization group in Matsubara formalism to calculate the selfenergy and interaction vertex functions at Matsubara frequencies.

A calculation of the finite-temperature conductance for this chain model requires, in contrast to the SIAM, an analytic continuation to the real axis. We show that it is possible to avoid analytic continuation of the vertex function provided that the chain model is invariant under a L↔R parity transformation. For this case, we derive a conductance formula similar to the Meir-Wingreen formula, which expresses the conductance (including vertex contributions) purely in terms of two point correlators.

TT 38.17 Wed 14:00 P3

Geometry Dependent Spin Conductance in Quantum Dots with Spin-Orbit Interaction — •Vitalij Lutsker[1], Inanc Adagideli[2], Matthias Scheid[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Istanbul, Turkey

In a recent publication[1] it was demonstrated that the average two-terminal spin conductance of a cavity with Rashba spin-orbit interaction(SOI) depends on the orientation of the vector connecting the two terminals. This effect originates from an effect of the SOI on the electron dynamics, leading to a geometrical correlation, which survives in chaotic and diffusive dots. Here we present a systematic numerical analysis of this effect, based on a recursive Green's function approach to transport. We study statistics of the spin conductance, its dependence on the number of leads, and the role of additional linear and cubic Dresselhaus terms.

[1] I. Adagideli et al., Phys. Rev. Lett., in print (2010); arXiv:1008.4656

TT 38.18 Wed 14:00 P3

Effects of finite range exchange interactions in the RKKY spin density oscillations — •Sergey Smirnov — Institut für Theoretische Physik, Universität Regensburg

We study the impact of a finite spin distribution of a localized spin, embedded in a Fermi sea of noninteracting conduction electrons, on the induced spin density oscillations underlying the RKKY indirect exchange effect. Specifically, a one-dimensional (1D) ring at finite temperatures is considered. We show that any small but finite interaction radius always produces an essential change in the spin density oscillations if the number of electrons is large enough [1]. To understand the physical role, played by the impurity spin localization radius in the RKKY spin-density oscillations, we consider a system where those oscillations exist only if this radius is finite. The system represents a half-infinite 1D quantum wire with a magnetic ion placed at its edge. It is analytically demonstrated that the effect of the finite spin localization radius is to reduce the effective mass of the conduction electrons [2].

[1] S. Smirnov, Phys. Rev. B 79, 134403 (2009)
[2] S. Smirnov, Phys. Rev. B 81, 214425 (2010)

TT 38.19 Wed 14:00 P3

Spin-polarizing Beam Splitter Nanodevice — •Dietrich G. Rothe and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astrophysik, Würzburg, Germany

We present numerical calculations of a beam splitter device which can generate a spin-polarized current using the principle of birefringence at an interface of regions with different Rashba spin-orbit couplings. For our calculations we employ the non-equilibrium Green's function formalism, and make use of two-band as well as four-band models of the lowest subbands of the HgCdTe quantum wells. We find that the physics is governed by the interplay between Rashba and Dirac spin-orbit terms (the linear in k terms), where the latter leads to a spin polarization due to the confinement. We find that in the 4-band model, spin polarization can be measured by a helicity operator. When the interface with different Rashba SO regions is tilted at an angle well above the angle of total reflection, good spin polarization is achieved.

TT 38.20 Wed 14:00 P3

Adiabatic pumping through an interacting quantum dot with spin-orbit coupling — •Stephan Rojek[1], Jürgen König[1], and Alexander Shnirman[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]Institut für Theorie der Kondensierten Materie and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany

We study adiabatic pumping through a two-level quantum dot coupled to two normal leads in the presence of spin-orbit coupling. The variation of the two energy levels of the dot periodically in time leads to finite charge and spin currents. We calculate the pumped charge and spin using a diagrammatic real-time approach. Going beyond the case of noninteracting electrons on the quantum dot [1], we study the situation of finite Coulomb-interaction. For comparison, we show results for the limits of noninteracting and strongly interacting electrons. In both limits spin-orbit coupling provides the possibility for pure spin current. Furthermore, we discuss differences between the charge and spin transport characteristics.

[1] V. Brosco *et al.*, Phys. Rev. B **82**, 041309(R) (2010).

TT 38.21 Wed 14:00 P3

Probing of coherence in molecular and CNT transport — •Birgit Kiessig[1,2], Ralph Krupke[3], Regina Hoffmann[2], Dominik Stöffler[2], Kai Grube[1], Roland Schäfer[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe — [3]Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021 Karlsruhe

The advancing miniaturisation of electronic circuits has increased the scientific interest in transport properties of single molecules as the smallest available building blocks. Other promising candidates for ultrasmall electronic devices are carbon nanotubes (CNTs), which at the same time are already today far easier to handle than molecules.

We aim to probe a very special characteristic of transport through nanoscale devices, namely coherence. Its occurence in a single electronic building block leads to divergence of the behaviour of a combination of several such devices from the classical expectation.

Molecular transport measurements require the fabrication of conductive electrodes spaced only a few nm apart. To achieve such we chose a feedback controlled electromigration procedure for the preparation of our samples, which we investigated in detail.

Furthermore we also prepared and measured appropriate samples for coherence probing of transport through CNTs.

TT 38.22 Wed 14:00 P3

Inelastic transport through octane molecules and a single level model with light — •Thomas Hellmuth[1], Fabian Pauly[1], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institut of Technology (KIT) — [2]Institut für Nanotechnologie, Karlsruhe Institut of Technology (KIT)

We study the transport and vibrational modes of single-molecule junctions containing octandeamine and octanedithiol. For this we use a scheme based on density functional theory. We compare our results to experiments and map the calculated vibrational modes to the measured IETS [1]. We show the substantially different behavior for the different terminal groups, namely the pulling of gold chains for dithiols, while they are absent for the dimanines. In addition to these studies, we explore the inelastic rectification current of a light irradiated single level contact.

[1] Y. Kim, T. Hellmuth, F. Pauly, and E. Scheer (in preparation)

TT 38.23 Wed 14:00 P3

Ab-initio description of transport through biphenyl-based molecular junctions — •Marius Bürkle[1], Fabian Pauly[1], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology

Biphenyl molecules serve as prototype systems for transport through single molecule junctions. In combination with experiments, we study the electric and thermoelectric transport properties by means of density functional theory. We explore the effects of molecular conformation and anchoring groups on the electric transport in biphenyl dithiols, dinitriles, and diamines [1,2,3]. In addition, we show that they have also a strong influence on the thermoelectric properties. Namely, increasing torsion angle generally decreases the thermopower and, through doping via the anchoring groups, HOMO transport for dithiol and diamine linked molecules changes to LUMO transport for dinitriles.

[1] A. Mishchenko, D. Vonlanthen, V. Meded, M. Bürkle, C. Li, I. V. Pobelov, A. Bagrets, J. K. Viljas, F. Pauly, F. Evers, M. Mayor, and T. Wandlowski Nano Lett. 10, 156 (2010)
[2] A. Mishchenko, L. A. Zotti, D. Vonlanthen, M. Bürkle, F. Pauly, J. C. Cuevas, M. Mayor, and T. Wandlowski J. Am. Chem. Soc. (2010), accepted
[3] L. Venkataraman, J. E. Klare, C. Nuckolls, M. S. Hybertsen and M. L. Steigerwald, Nature 442, 904-907 (2006).

TT 38.24 Wed 14:00 P3

Optical Control of Single-Molecule Conductance — •Yaroslav Zelinskyy[1,2] and Volkhard May[2] — [1]Bogolyubov Institute for theoretical physics, National Academy of Science of Ukraine, 14-b Metrologichna str. UA-03680, Kiev, Ukraine — [2]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489, Berlin, Germany

A kinetic model is established for current formation through a single molecule embedded in between two metallic electrodes and irradiated by an external laser pulse. Focusing on the particular case of a molecule which can be moved in its excited electronic state if it became singly charged, an analytical expression for the steady-state current is presented. A detailed analysis of the current-voltage as well as conductance-voltage characteristics at the different wavelength of the applied laser light is carried out. Based on such computations a photo-switching effect between molecular states of low and height conductivity can be proposed. In the case of weak molecule-lead coupling a voltage region showing negative differential resistance is found. Its suppression due to laser pulse excitation is indicated.

TT 38.25 Wed 14:00 P3

Electrical Characterization of Short DNA Fragments — •Matthias Wieser[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhuo Tang[2], Andreas Marx[2], Elke Scheer[2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — [2]Universität Konstanz, D-78457 Konstanz

The electrical transport properties of DNA molecules are important for future molecular electronics applications. We characterized the electrical conductance of single DNA fragments in ambient condition and in buffer solution using a Mechanically Controllable Break Junction (MCBJ) setup which allows us binding molecules between two gold electrodes. We analyzed the electrical conductance of double stranded DNA and G-quadruplex molecules. G-quadruplex molecules consist of four guanine bases arranged in the shape of a square and a cation in the center. The electrical characterization is done by investigating the I-V curves characteristics of the molecules in different conditions.

TT 38.26 Wed 14:00 P3

Electronic transport through switchable molecules — •Bernd Briechle[1], Nikola Treska[1], Dima Sysoiev[2], Jannic Wolf[2], Youngsang Kim[1], Johannes Boneberg[1], Thomas Huhn[2], Ulrich Groth[2], Ulrich Steiner[2], Artur Erbe[3], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, Germany — [3]Forschungszentrum Dresden-Rossendorf, Dresden, Germany

We investigate transport properties of molecules in liquid solvent at room temperature. For that purpose we use lithographically fabricated Mechanically Controllable Break Junctions (MCBJs) to generate atomic-size contacts and atomically sharp tips to contact the molecules. We study molecular switches for which reversible switching from an opened to a closed conjugated backbone via light irradiation is expected. The molecular switches feature thiol- or nitrogen-based endgroups for a strong bond to the metal. Analysis is based on statistics of conductance traces recorded during opening and closing the junction, and on current-voltage characteristics taken at constant electrode distance. It has been shown that the latter can be described by a simple transport model involving a single broadened molecular orbital. Fitting the experimental current-voltage characteristics to this model, we can extract the strength of the molecule-metal bond as well as the energy of the molecular orbital next to the Fermi level. This analysis enables us to determine promising combinations of metal and molecule endgroup for stable and reproducible contacting which is a crucial requirement for our transport studies.

TT 38.27 Wed 14:00 P3

Time-dependent transport through a molecular level coupled to a nanomagnet — •Milena Filipovic, Federica Haupt, and Wolfgang Belzig — University of Konstanz, Konstanz, Germany

We study the transport through a single level quantum dot coupled to two leads in the presence of a magnetic field. The magnetic field is coupled to the quantum dot and the leads are treated as noninteracting. We use the Keldysh nonequilibrium Green function technique to derive and analyze the properties of the spin-dependent tunneling current and its linear response to the applied time-dependent magnetic field. We further analyze the transport through the single level quantum dot coupled to a precessing molecular nanomagnet.

TT 38.28 Wed 14:00 P3

Quantum Interference and Dephasing Due to Vibronic Coupling in a Single-Molecule Junction — •Michael Butzin, Rainer Härtle, and Michael Thoss — Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

We study quantum interference and dephasing effects in a biphenylacetylene-dithiolate molecular junction. To this end, we analyze the molecular orbitals relevant for charge transport through this junction and show that destructive interference effects suppress coherent transport processes. The coupling of the electronic degrees of freedom to the large number of vibrational modes of the junction strongly influences the respective current-voltage characteristics and induces a dephasing mechanism that counteracts the suppression of the current due to destructive interference. To analyze these phenomena we discuss generic model systems using a nonequilibrium Green's function approach [1]. Moreover, for a molecular junction that exhibits quantum interference effects, we identify the constructive and destructive parts of the corresponding transmission function [2]. Interestingly, in the presence of electron-electron interactions, such destructive interference effects provide a testbed for the elastic co-tunneling approximation [1], which we study employing the exact method of Gurvitz et al. [3].
[1] R. Härtle *et al.*, Phys. Rev. Lett. 102, 146801 (2009).
[2] G. C. Solomon *et al.*, Nano Lett. 6, 2431 (2006).
[3] S. A. Gurvitz, Phys. Rev. B 57, 6602 (1998).

TT 38.29 Wed 14:00 P3

Time-dependent approach to mesoscopic transport — •Tobias Kramer — Institute for Theoretical Physics, Uni Regensburg

Transport and scattering phenomena in open quantum-systems with a continuous energy spectrum are conveniently solved using the time-dependent Schrodinger equation [1]. In the time-dependent picture, the evolution of an initially localized wave-packet reveals the eigenstates and eigenvalues of the system under consideration. We discuss applications of the wave-packet method to mesoscopic systems and point out specific advantages of the time-dependent approach. In connection with the familiar initial value formulation of classical mechanics, an intuitive interpretation of transport emerges. For interacting many-particle systems, we discuss the efficient calculation of the self-consistent classical transport in the presence of a magnetic field.
[1] T. Kramer, Time dependent approach to transport and scattering in atomic and mesoscopic systems, arXiv:1011.3194
[2] T. Kramer, V. Krueckl, E. Heller, and R. Parrott: Self-consistent calculation of electric potentials in Hall devices, Phys. Rev. B, 81, 205306 (2010)

TT 38.30 Wed 14:00 P3

Diagrammatic approach to noise in adiabatically time-dependent systems — •Roman-Pascal Riwar[1], Janine Splettstoesser[1], and Jürgen König[2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, D-52056 Aachen, Germany and JARA-Fundamentals of Future Information Technology — [2]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

Noise is an important feature in quantum electron transport. Current-current correlations carry information about the system which is not accessible via a current measurement only. Here, we are interested in the noise of interacting quantum dot systems, which are subject to time-dependent fields, as e.g. adiabatic quantum pumps. We investigate the zero-frequency noise of such systems, taking into account Coulomb interaction. For this purpose, a real-time diagrammatic approach for the treatment of adiabatic time dependence [1] is extended to the calculation of current noise (performed for the stationary case in Ref. [2]), within a perturbative expansion in the tunnel coupling.
[1] J. Splettstoesser *et al.*, Phys. Rev. B **74**, 085305 (2006)
[2] A. Thielmann *et al.*, Phys. Rev. Lett. **95**, 146806 (2005)

TT 38.31 Wed 14:00 P3

Effective two-spin models for measurement based quantum computing — •Daniel Klagges and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The cluster state is an universal resource for measurement based quantum computation. One might consider to prepare a cluster state by cooling a suitable chosen Hamiltonian into its ground state. Unfortunately there is no Hamiltonian only containing (realistic) two-spin interactions with the cluster state as its only ground state. But there exist microscopic models consisting solely of two-spin interactions for which the ground state is approximately the cluster state. Here we present high order series expansions of such Hamiltonians, in order to investigate their usability in the context of measurement based quantum computation.

TT 38.32 Wed 14:00 P3

Influence of adsorbate clustering on transport in graphene nanoribbons — •Sarah Stahl, Georgo Metalidis, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, D-76128 Karlsruhe

Until now no consensus has been reached on the dominant scattering mechanism in graphene. Several experiments have observed the adsorption of different atoms and molecules on a free-standing graphene surface and imaged the formation of clusters of such adsorbates. Clustering of adsorbates might have a major influence on the transport properties of graphene. In particular, single adsorbates form short-range scattering centers and will thus induce scattering between the two valleys in the graphene Brillouin zone breaking chirality. When they cluster together their scattering is of a longer-range and intervalley scattering will be absent (conserving chirality). We investigate the influence of clustering with a numerical Green's function technique to study the crossover between these two regimes. In particular, we determine the mean free path as a function of the cluster size, ribbon dimensions and disorder strength.

TT 38.33 Wed 14:00 P3

Spin and Vibrations in Carbon Nanotubes — •Christoph Ohm[1], Janine Splettstoesser[1], Christoph Stampfer[1,2], and Maarten R. Wegewijs[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, and JARA - Fundamentals of Future Information Technology, Germany — [2]Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, Germany

Carbon nanotubes are ideal systems to probe the interplay of quantized degrees of freedom. We theoretically study the influence of vibrations on the spin dynamics in carbon nanotube quantum dots. We consider various types of spin-phonon coupling mechanisms and their influence on transport.

TT 38.34 Wed 14:00 P3

Transport studies of microsoldered Graphene — •Nils Freitag[1], Marcus Liebmann[1], Viktor Geringer[1], Alexander Georgi[1], Bart Szafranek[2], Daniel Neumeier[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumethal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

We present transport measurements on microsoldered Graphene using a 300 mK/ 10 T He^3-bath cryostat. These are complementary to our previous scanning tunneling microscopy studies [1]. Amongst the determination of the mobility of the samples, a distinct half-integer Quantum-Hall effect appears at high fields, whereas the low-field regime is dominated by the weak localisation and antilocalisation features which are analysed in detail. Interestingly, the mobility of graphene exhibits a sudden change at the critical field of the superconducting In-contacts.
[1] V. Geringer, D. Subramaniam, A. K. Michel, B. Szafranek, D. Schall, A. Georgi, T. Mashoff, D. Neumaier, M. Liebmann, M. Morgenstern, Appl. Phys. Lett. **96**, 082114 (2010).

TT 38.35 Wed 14:00 P3

Four-wave mixing to detect wave-packet revivals on graphene — •Viktor Krueckl, Tobias Kramer, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

By applying a perpendicular magnetic field the quasi-relativistic electrons of graphene are quantized into non-equidistantly spaced Landau levels. Consequently the time-evolution of an excited wave-packet undergoes collapses and revivals similar to the dynamics of highly excited Rydberg states [1]. We investigate the detection of graphene revivals by means of four-wave mixing. A few cycle laser pulse is used to generate an excited state, which is probed by a second time-delayed pulse. We apply a non-pertubative wave-packet scheme which allows for the calculation of the complete angle resolved polarization. The resulting integrated signals show a clear correspondence between the time-delay of the probe pulse and the wave-packet revival time.
[1] Viktor Krueckl and Tobias Kramer, New J. Phys. **11** 093010 (2009)

TT 38.36 Wed 14:00 P3

Superlattice Effects on Graphene Nanoribbons — •Fedor Tkatschenko, Jan Bundesmann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg,

Germany

We study how an additional, spatially modulated electric field affects the electronic properties of graphene nanoribbons. Previous efforts [1, 2] investigated peculiar effects on the electronic structure of bulk graphene such as the emergence of new Dirac points in the energy spectrum and an anisotropic velocity renormalization. These new characteristics are also reflected in the density of states and the conductivity. Insted of the bulk we will here consider the influence of a periodic modulation, oriented along the direction of a graphene nanoribbon, on its bandstructure and transport properties. To this end we employ a numerical Green function method based on the tight binding graphene Hamiltonian.

[1] M. Barbier, P. Vasilopoulos, and F. M. Peeters, Phys. Rev. B **79** 115427 (2010)
[2] Li-Gang Wang, and Shi-Yao Zhu, Phys. Rev. B **81** 205444 (2010)

TT 38.37 Wed 14:00 P3

A route to strong p-doping of epitaxial graphene on SiC — •Udo Schwingenschlögl and Yingchun Cheng — PSE Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effects of Au intercalation on the electronic properties of epitaxial graphene grown on SiC0001 substrates are studied using first principles calculations. A graphene monolayer on SiC0001 restores the shape of the pristine graphene dispersion, where doping levels between strongly n-doped and weakly p-doped can be achieved by altering the Au coverage. We predict that Au intercalation between the two C layers of bilayer graphene grown on SiC0001 makes it possible to achieve a strongly p-doped graphene state, where the p-doping level can be controlled by means of the Au coverage [1].

[1] Appl. Phys. Lett. 97, 193304 (2010)

TT 38.38 Wed 14:00 P3

Surface quantum criticality in topological insulators — •Matthias Sitte, Lars Fritz, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The discovery of graphene has allowed to experimentally study a (2+1)-dimensional variant of quantum electrodynamics. It is known that a phase transition to a gapped phase with broken chiral symmetry can in principle be driven by varying the fine structure constant α. However, in graphene the tunability of α is quite limited. Recently, the surfaces of 3D topological insulators have shown to host states that are also described by massless relativistic Dirac fermions in 2+1 dimensions. In this work we study the tunability of α in materials such as HgTe and CdTe by driving the bulk towards its quantum critical point. We investigate under which conditions chiral symmetry breaking on the surface can be expected.

TT 38.39 Wed 14:00 P3

Charge-spin duality in non-equilibrium transport of helical liquids — •Jan Carl Budich, Chao-xing Liu, Patrik Recher, and Björn Trauzettel — Institute for theoretical physics and astrophysics, Wuerzburg, Germany

Non-equilibrium transport properties of charge and spin sector of two edges of a quantum spin Hall insulator are investigated theoretically in a four-terminal configuration. A simple duality relation between charge and spin sector is found for two helical Tomonaga Luttinger liquids (hTLLs) connected to non-interacting electron reservoirs. If the hTLLs on opposite edges are coupled locally or non-locally, the mixing between them yields interesting physics where spin information can be easily detected by a charge measurement and vice versa. Particularly, we show how a pure spin density in the absence of charge current can be generated in a setup that contains two hTLL and one spinful Tomonaga Luttinger liquid in between.

TT 38.40 Wed 14:00 P3

Edge transport and backscattering in a two-dimensional topological insulator in strong magnetic fields — •G. Tkachov and E. M. Hankiewicz — Würzburg University, Germany

Unlike ordinary band insulators, a recently identified class of materials - topological insulators - exhibit unusual conducting states on sample boundaries. Recently, a large body of experimental and theoretical work has been devoted to detection and characterization of such states in topological insulators (see, e.g. Refs. [1,2]). In this work we discuss how the edge states in a two-dimensional topological insulator can be probed by means of quasiballistic transport in strong magnetic fields. We find in particular that defects, which cause edge-state backscattering, can generate strong energy and magnetic- field dependences of the longitudinal conductance [3].

[1] M. König, H. Buhmann, L. W. Molenkamp, T. Hughes, C.-X. Liu, X.-L. Qi, and S.-C. Zhang, J. Phys. Soc. Jpn. **77**, 031007 (2008).
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[3] G. Tkachov and E. M. Hankiewicz, Phys. Rev. Lett. **104**, 166803 (2010).

TT 38.41 Wed 14:00 P3

Spin Transport in HgTe Quantum Wells — •Rolf W. Reinthaler, Dietrich G. Rothe, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We study the spin transport in the topological insulators HgTe quantum wells which are described within an effective four band model (conduction/heavy hole bands) including space inversion breaking terms [1]. In the ballistic regime, we find that the spin transport is governed by the Rashba term, i.e. the spin signal precesses with the electric field perpendicular to the plane of the quantum well. However, the precession length is modified due to the Dirac-like structure of the Hamiltonian. In particular, we find a large background signal near the topological insulator state as well as an enhanced spin rotation. We attribute these effects to the properties of the Hamiltonian and the confinement potential of the two-dimensional topological insulator.

We acknowledge the financial support of the German DFG grant HA 5893/1-1.

[1] D. G. Rothe, R. W. Reinthaler, C.-X. Liu, L. W. Molenkamp, S.-C. Zhang, and E. M. Hankiewicz, New Journal of Physics 12 065012 (2010).