TT 75: Poster Session: Transport 1

Time: Thursday 15:00–19:00 Location: P2-EG

TT 75.1 Thu 15:00 P2-EG

Keldysh-FRG Approach for Inhomogeneous One-Dimensional Fermi Systems with Finite-Ranged Interactions — •Lukas Weidinger, Dennis Schimmel, and Jan von Delft — LMU München, Theresienstraße 37, München

In a previous paper (arXiv:1609.07423), we have introduced an extended coupled-ladder approximation (eCLA) scheme for 2nd-order truncated functional renormalization group (fRG) calculations in the Matsubara formalism, capable of treating finite-ranged interactions. We applied it in a static approximation and at zero temperature to models of quantum point contacts (QPCs) and quantum dots (QDs).

In this poster, we present our current follow-up work on the implementation of a dynamical eCLA within the Keldysh formalism. We pursue this for two main reasons: First, to get additional insights by obtaining real-frequency data, allowing us, for example, to compute the interacting local density of states (LDOS). This enables us also to study the finite-temperature behavior of the conductance which turned out to be unfeasible in Matsubara fRG. Second, within the Keldysh formalism we are able to study non-equilibrium effects, e.g. by applying finite source-drain voltages or temperature gradients to our systems.

TT 75.2 Thu 15:00 P2-EG

Non-equilibrium transport through a disordered molecular nanowire — Patrick Thiessen[1], Francisco Dominguez-Adame[1,2], •Rudolf A Römer[2], and Elena Diaz[1] — [1]University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Universidad Complutense, E-28040 Madrid, Spain

We investigate the non-equilibrium transport properties of a disordered molecular nanowire. The nanowire is regarded as a quasi-one-dimensional organic crystal composed of self-assembled molecules. One orbital and a single random energy are assigned to each molecule while the inter- molecular coupling does not fluctuate. Consequently, electronic states are expected to be spatially localized. We consider the regime of strong localization, namely, the localization length is smaller than the length of the molecular wire. We also take into account the electron-vibron interaction that takes place in each single molecule. We investigate the interplay between disorder and electron-vibron interaction in response to either an applied electric bias or a temperature gradient. To this end, we calculate the electric and heat currents when the nanowire is connected to leads, using the Keldysh non-equilibrium Green's function formalism. At not very high temperature, scattering by disorder dominates both charge and energy transport. We find that the electron-vibron interaction enhances the effect of the disorder on the transport properties due to the exponential suppression of tunneling.

TT 75.3 Thu 15:00 P2-EG

Implementation of transmission functions for an optimized three-terminal quantum dot heat engine — •Christian H. Schiegg, Michael Dzierzawa, and Ulrich Eckern — Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

We consider two modifications of a recently proposed three-terminal quantum dot heat engine. First, we investigate the necessity of the thermalization assumption, namely that electrons are always thermalized by inelastic processes when traveling across the cavity where the heat is supplied. Second, we analyze various arrangements of tunneling-coupled quantum dots in order to implement a transmission function that is superior to the Lorentzian transmission function of a single quantum dot. We show that the maximum power of the heat engine can be improved by about a factor of two, even for a small number of dots, by choosing an optimal structure.

TT 75.4 Thu 15:00 P2-EG

Hierarchical equations of motion approach to transport through an Anderson impurity coupled to interacting Luttinger liquid leads — •Junichi Okamoto[1,2], Ludwig Mathey[1,2], and Rainer Härtle[3] — [1]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [3]Institut fuŕ Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

We generalize the hierarchical quantum master equations (HQME) method to investigate electron transport through an Anderson impurity coupled to one-dimensional interacting leads that can be described as Luttinger liquids [1]. In comparison to noninteracting leads, Luttinger liquids involve many-body correlations and the single-particle tunneling density of states shows a power-law singularity at the chemical potential. Using the generalized HQME method, we assess the importance of the singularity and the next-to-leading order many-body correlations. To this end, we compare numerically converged results with second and first-order results of the hybridization expansion inherent to our method. Cotunneling effects turn out to be most pronounced for attractive interactions in the leads. We also find that an interaction-induced negative differential conductance near the Coulomb blockade thresholds is suppressed compared to a first-order result. Finally, we discuss that the $n(\geq 2)$-particle correlations enter as a n-order effect and are, thus, not very pronounced at the high temperatures. [1] J. Okamoto, L. Mathey, R. Härtle, arXiv:1608.05399

TT 75.5 Thu 15:00 P2-EG

Quantifying system-bath correlations in biased quantum dot systems using the hierarchical quantum master equation technique — •Jakob Bätge and Rainer Härtle — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We consider quantum dot systems, where system-bath correlations emerge from a continuous exchange of electrons of the dot with its environment, that is leads representing macroscopic electron reservoirs. We analyze these correlations by investigating the transient dynamics in response to time-dependent electric fields, for example a sudden change of the applied bias voltage. To this end, we use the unique properties of the hierarchical quantum master equation technique [1,2], which allow us to turn on and off system-bath correlations completely or only selected parts, at any instant of time. Thus, we are able to define measures for system-bath correlations that can be used for a systematic and quantitative analysis. Here, we present first results of such an analysis, demonstrating the use of the new measures and how they can be accessed experimentally.

[1] Jin et al., JCP 128, 234703 (2008)
[2] Härtle et al., PRB 88, 235426 (2013)

TT 75.6 Thu 15:00 P2-EG

Switching the electrical conductance of double quantum dot and quantum dot spin valve systems exploiting exchange interactions — •Sebastian Wenderoth and Rainer Härtle — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Recently, sharp peaks in the conductance of double quantum dot and quantum dot spin valve systems have been reported [1,2,3]. Their origin has been traced back to the effect of interaction-induced renormalization [1,3] and coupling effects [2]. In this contribution, we investigate the possible use of the underlying phenomena to realize switching processes in electronic device applications by simple gate voltage operations. This includes a discussion of switching times, switching efficiencies, the underlying physical mechanisms and parameter dependencies. To this end, we employ the hierarchical quantum master equation approach, which allows us to obtain numerically converged, exact results as well as approximate results in terms of a hybridization expansion [1,3]. In particular, its time-local formulation allows us to study the switching behavior to all relevant time scales. We find that many-body interactions enhance the switching efficiency but also the switching times by an order of magnitude.

[1] Härtle et al., PRB 88, 235426 (2013)
[2] Hell et al., PRB 91, 195404 (2015)
[3] Wenderoth et al., PRB 94, 121303R (2016)

TT 75.7 Thu 15:00 P2-EG

Lab::Measurement — Measurement control and automation with Perl — Simon Reinhardt, Christian Butschkow, Alexei Iankilevitch, Alois Dirnaichner, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

For quickly setting up varying and evolving complex measurement tasks involving diverse hardware, graphical logic programming quickly reaches practical limits. We present `Lab::Measurement`, a collection

of Perl modules designed to control instruments connected by as various means as GPIB, USB, serial cable, Oxford Instruments IsoBus, or Ethernet. Internally, backends as e.g. Linux-GPIB or National Instruments' NI-VISA library are used as well as direct operating system calls. Dedicated instrument driver classes relieve the user from taking care of internal details. A high-level layer enables fast and flexible creation of nested measurement loops, where e.g. several input variables are varied and one or several output parameters are read for each setting. Metadata and device parameters are automatically protocolled. `Lab::Measurement` has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

TT 75.8 Thu 15:00 P2-EG

Unconventional superconductivity in quantum dots mediated by spin orbit coupling — •Isabel Oppenberg, Stephan Weiss, and Jürgen König — Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We study an interacting quantum dot with two electronic levels in the presence of spin orbit (SO) interaction and a static magnetic field. The quantum dot is coupled to two normal and one superconducting lead. We integrate out the superconductor in the limit $\Delta \to \infty$. This yields an effective model for the dot with finite conventional pairing amplitude. Due to finite SO coupling together with a (noncollinear) static magnetic field, singlets and triplets are coupled and finite unconventional pairing mechanism emerge. They are described by Gorkov's Greens functions [1]. We take the coupling of the system to the normal leads into account by a realtime diagrammatic method [2]. For a symmetric and non-symmetric lead coupling case, the density matrix elements, reflecting unconventional superconducting pairing, are analyzed for different sets of parameters. Furthermore, the calculation of the nonequilibrium Andreev current and the spectrum of Andreev addition energies allows us to investigate the interplay between SO coupling and unconventional superconducting correlations on the quantum dot.

[1] Björn Sothmann, Stephan Weiss, Michele Governale and Jürgen König, PRB **90**, 220501(R) (2014)
[2] M. Governale, M.G. Pala and Jürgen König, PRB **77**, 134513 (2008)

TT 75.9 Thu 15:00 P2-EG

Utilizing SETs in single electron counting experiments — •David Reifert, Niels Ubbelohde, Ralf Dolata, Thomas Weimann, and Alexander Zorin — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig. Germany

We fabricate dynamic quantum dots through a shallow etch process of a GaAs/AlGaAs heterostructure. These quantum dots can be operated as single electron source by periodically modulating one of the barriers of the dot. The resulting current $I = e\,f$ depends only on the pumping frequency f and the electronic charge e, which enables us to use these pumps as a new quantum current standard. We utilize superconducting aluminum single electron transistors (SETs) as ultra sensitive charge detectors to characterize the performance of such electron pumps. To increase the measurement bandwidth of our detectors we use the RF-SET technology, where we put the SET in a resonant tank circuit and measure the reflectance of this resonator. Besides increasing the bandwidth this technique enables us to multiplex several detectors. We will show the fabrication and operation of our hybrid devices consisting of semiconductor electron pumps and metallic SET detectors. Furthermore, we investigate the performance of semiconductor based SETs as charge detectors and compare them with the superconducting metallic SETs. We then utilize these devices to perform single electron counting measurement, where the electron pump act as an electron source and the SETs detects these electrons, which then will enables us to validate the precision of the pump.

TT 75.10 Thu 15:00 P2-EG

Quantum transport and response with spin-orbit coupling in magnetic fields — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Electronic transport in spin-polarized systems with impurity interactions and spin-dependent meanfields is discussed. The coupled quantum kinetic equations for the scalar and spin components for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the RPA spin and density dynamical responses to electric fields (polarized light) are presented for arbitrary magnetic fields, Several known effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling. New transport coefficients occur due to the selfconsistent precession direction. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found and terahertz out-of plane resonances are predicted.

Europhysics Letters, 104 (2013) 27005, Phys. Rev. **B 92** (2015) 245425, errata Phys. Rev. **B 93** (2016) 239904(E), Phys. Rev. **B 92** (2015) 245426, Phys. Rev. **B 94** (2016) 165415

TT 75.11 Thu 15:00 P2-EG

Large anomalous Hall effect in the non-collinear antiferromagnet Mn_5Si_3 — •Christoph Sürgers[1], Thomas Wolf[2], Peter Adelmann[2], Wolfram Kittler[1], Gerda Fischer[1], and Hilbert v. Löhneysen[2] — [1]KIT, Physikalisches Institut — [2]KIT, Institut für Festkörperphysik

The anomalous Hall effect (AHE), which in long-range ordered ferromagnets appears as a voltage transverse to the current and usually is proportional to the magnetization, often is believed to be of negligible size in antiferromagnets due to their low uniform magnetization. However, recent experiments and theory have demonstrated that certain antiferromagnets with a non-collinear arrangement of magnetic moments exhibit a sizeable spontaneous AHE at zero field due to a non-vanishing Berry curvature arising from the quantum mechanical phase of the electron's wave functions. We show that antiferromagnetic Mn_5Si_3 single crystals exibit a large AHE which is strongly anisotropic and shows multiple transitions with sign changes at different magnetic fields due to field-induced rearrangements of the magnetic structure despite only tiny variations of the total magnetization. The presence of multiple non-collinear magnetic phases offers the unique possiblity to explore the details of the AHE and the sensitivity of the Hall effect on the details of the magnetic texture.

TT 75.12 Thu 15:00 P2-EG

Magnetotransport in Topological Insulator $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ — •Priyamvada Bhaskar, André Dankert, Dmitrii Khokhriakov, and Saroj Dash — Chalmers University of Technology, Göteborg, Sweden

Topological insulators (TIs) provide an excellent platform to study topological quantum physics and exploring spintronic applications due to their unique gap-less spin polarized helical metallic surface states. We explore novel semiconducting TI material $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ (BSTS) and report weak-anti localization (WAL) and quantum oscillations originating from surface states. Further, spin signals originating from spin-momentum locking were observed up to room temperature. From the temperature dependence of phase coherence length and the angle dependence of universal conductance fluctuations (UCF) it was inferred that the observed transport mechanisms originate from 2D, although coupling to the bulk leading to the formation of a single 2D channel cannot be ruled out. Although the angle dependence of WAL indicates surface state contribution, Shubnikov-de Haas oscillations provide for a low surface carrier concentration. However, magnetotransport in BSTS shows high spin polarization, thus showing promise as a spintronic TI. These studies provide a platform to pursue exotic physics and novel device applications predicted for TIs and its heterostructures with other 2D materials.

TT 75.13 Thu 15:00 P2-EG

Shot noise of contacts to Fe atoms and FeH_n on Au(111) — •Michael Mohr, Andreas Burtzlaff, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The ballistic transport through contacts to single Fe atoms on Au(111) surfaces is investigated with a 4 K scanning tunneling microscope. The shot noise of the current is measured to obtain information about its spin polarization. The influences of other Fe atoms close to the contact and of hydrogen in the contact are addressed

TT 75.14 Thu 15:00 P2-EG

Transmission through half-metallic NiMnSb under consideration of defects and correlations — •Andreas Prinz-Zwick, Wilhelm Appelt, Liviu Chioncel, and Ulrich Eckern — Universität Augsburg

Half-metallic materials are of particular importance for achieving spin dependent transport properties for various spintronic applications. We

study a (001) oriented heterostructure of epitaxial grown NiMnSb on Au and evaluate the transmission within the combined Density Functional and Non-Equilibrium Greens Function (NEGF) theory, implemented in SMEAGOL. The calculations include lattice defects such as vacancies and exchange of atoms. In addition the calculation for the clean system is compared with DFT+DMFT to quantify the influence of electronic correlations. Electronic correlations induce minority spin states in the half-metallic gap and significantly reduce the spin polarization of bulk NiMnSb. Surprisingly no significant change is seen in the transmission coefficient. These results demonstrate the localized nature of the many-body induced states in the half-metallic gap.

TT 75.15 Thu 15:00 P2-EG

Resonance phenomena in ferrocene-based single-molecule junctions — •Diana Slawig[1], Karthiga Kanthasamy[1], Markus Ring[3], Holger Butenschön[2], Christoph Tegenkamp[1], Fabian Pauly[3], and Herbert Pfnür[1] — [1]Inst. f. Festkörperphysik, Leibniz Universität Hannover — [2]Inst. f. organ. Chemie, Leibniz Universität Hannover — [3]FB Physik, Universität Konstanz

Ferrocene dithiol (FDT) molecules as molecular junctions and switches are particularly attractive because of their high conductance and their rotational flexibility. In our study of electrical transport through single FDT molecules between Au contacts via the break junction technique it turns out that the conductance depends strongly on the chemical end groups. This dependence allows tuning of the energy level alignment of HOMO and LUMO relative to the Fermi energy of the electrodes, as demonstrated by the comparison between ferrocene-1,1′-diamine (FDA) and FDT, making FDT a much better conductor than FDA. Comparison of the experimental results with DFT calculations based on the single level model suggest changes of binding geometries of the molecule at the electrodes as a function of electrode separation for both molecules. Particularly interesting are resonances in the IV-curves of FDT at fixed contact distances in the conductance range (at zero bias) between $0.1\,G_0$ to $0.56\,G_0$. This phenomenon can be described by the Fano resonance model, as verified for selected molecular binding geometries in DFT simulations, which, however yields a too high temperature dependence. Therefore, further possible contributions from inelastic transport processes will also be discussed.

TT 75.16 Thu 15:00 P2-EG

Constructing nanoelectronic circuits by top-down and bottom-up strategies — •Filip Kilibarda, Torsten Sendler, Dipjyoti Deb, Muhammad Bilal Khan, Bezu Teschome, and Artur Erbe — Helmholtz - Zentrum Dresden - Rossendorf, Dresden, Germany

The construction of nanoelectronic circuits requires the development of bottom-up strategies, which can be combined with top-down structuring. We show how reconfigurable silicon nanowires are produced using electron-beam lithography and reactive ion etching. Such structures can be used as large-scale electrodes to networks of self-assembled electronics on the nanoscale. As a first step towards the development of nanoscale circuits by self-organization, we demonstrate the construction of nanoscale metallic wires based on metallized DNA origamis. Active building blocks with smallest dimensions on the molecular scale are developed in single molecule contacts. The properties of those junctions need to be characterized. We have demonstrated that the mechanically controllable break junction (MCBJ) technique can be successfully used to determine the properties of electronic transport through single organic molecules and that the participating molecular energy levels and the metal-molecule coupling can be characterized using this technique. Further developments are based on the use of more complex molecules, which can, for example, be used as single molecule switches. We present the first demonstration of a single molecule junction, in which the molecule is switched in situ from the non-conducting off-state to the conducting on-state.

TT 75.17 Thu 15:00 P2-EG

Design rules for molecular electronics: Theoretical and experimental approach — Lokamani Lokamani[1], •Filip Kilibarda[1], Jannic Wolf[2], Peter Zahn[1], Thomas Huhn[2], Sibylle Gemming[1,3], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Universität Konstanz, 78457 Konstanz, Germany — [3]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Diarylethenes, a class of photosensitive molecules which exhibit photochoromism, can be switched between open- and closed-ring isomers. In break-junction experiments diarylethene derivatives in open and closed-ring forms can be distinguished by a low and high conductance state respectively with a difference in current levels of about one order of magnitude.

Here, we explore the underlying design rules for modulating electronic transport in derivatives of diarylethene. In particular, we analyze the effect on molecular orbitals due to various electron accepting and donating groups and in turn the modulation of the conductance properties of single molecules attached to gold electrodes.

We have demonstrated that the mechanically controllable break junction (MCBJ) technique can be used to classify and determine the properties of electronic transport through single organic molecules. We present an outlook on experimental methods for exploring the underlying design rules for diarylethene molecules and derivatives. As a result, we show how the addition of different side groups modifies electronic behavior of the molecules.

TT 75.18 Thu 15:00 P2-EG

Ab-initio Simulation of Quantum Transport through Silane Molecular Wires — •María Camarasa-Gómez[1], Haixing Li[2], Daniel Hernangómez-Pérez[1], Latha Venkataraman[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, United States

The transport properties of molecular wires are sensitive to the relative alignment of the energies of the molecular orbitals and the Fermi-energy of the contact electrodes. A natural expectation is that the alignment shifts when one contact material, e.g., Au is replaced by another material, e.g., Ag; to lowest order, the shift should reflect the difference in the work functions [1]. We have performed an elaborate set of ab-initio transport calculations that puts this hypothesis to a test.

Motivated by recent experiments, we adopt a silane molecular wire as a paradigm system. We calculate the transmission function for Au and Ag substrates, for thiol- and amino- anchor groups [2] and a variety of different contact geometries. While our results qualitatively confirm the original hypothesis, we also observe other electrode related mechanisms that appear to be of similar magnitude compared to the work function shift. Our theoretical analysis will be compared to experimental data.

[1] T. Kim et al., NanoLett. 13, 3358 (2013)
[2] Y. Kim et al., ACS Nano 5, 4104 (2011)

TT 75.19 Thu 15:00 P2-EG

Vibrational excitations in current-driven single-molecule junctions — •Joachim Reichert[1], Hai Bi[1], Carlos-Andres Palma[1], Yuxiang Gong[1], Mark Elbing[2], Marcel Mayor[2,3], and Johannes V. Barth[1] — [1]Physik-Department, Technische Universität München, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Department of Chemistry, University of Basel, Switzerland

In order to advance the development of unimolecular electronic devices, it is mandatory to improve understanding of electron transport and its loss mechanisms in single molecules. One fundamental challenge in molecular electronics is the quantitative determination of charge-vibrational coupling for well-defined single-molecule junctions.

Here we determine the charge-vibrational coupling for a current-carrying, chemically defined metal-molecule-metal junction by synchronous vibrational and current-voltage spectroscopy. Measuring the steady-state vibrational distribution during charge transport in a bis-phenylethynyl-anthracene derivative by Raman scattering allows us to quantify the charge-vibrational coupling constant in this single-molecule system. Our work provides means to directly measure inelastic losses in (macro)molecular circuitry and introduces a general technique to perform optical spectroscopy on single-molecule junctions.

TT 75.20 Thu 15:00 P2-EG

Large magnetoresistance in single radical molecular junctions — •Sebastian Hambsch[1], Ryoma Hayakawa[1,2], Amin Karimi[1], Jannic Wolf[1], Thomas Huhn[1], Martin Sebastian Zöllner[3], Carmen Herrmann[3] und Elke Scheer[1] — [1]University of Konstanz, 78457 Konstanz — [2]NIMS, Tsukuba 305-0044, Japan — [3]University of Hamburg, 20146 Hamburg

We present the charge transport properties of single radical molecule junctions formed by a break junction technique at 4.2 K in magnetic field B. In this study, stable and neutral radical molecules based on an oligo(p-phenylene ethynylene) (OPE) backbone (TEMPO-OPE) were

placed on a freestanding gold (Au) bridge. We observe large positive magnetoresistance (MR) up to 287 % at 4T from TEMPO-OPE molecules when B was applied perpendicular to the sample plane [R. Hayakawa et al. Nano Lett. 16, 4960 (2016)]. The averaged MR was one order of magnitude larger than that of the analogous non-radical OPE molecule. The analysis of the MR, of IVs and of inelastic electron tunneling spectra reveal an effective reduction of the electronic coupling between the current-carrying molecular orbital and the electrodes with increasing B. Our findings thus provide a new physical approach for tuning the charge transport via radical molecules.

TT 75.21 Thu 15:00 P2-EG

Beyond the Born-Oppenheimer approximation: Non-adiabatic processes in manganites — •Michael ten Brink[1], Peter E. Blöchl[2], Stephanie Mildner[3], and Christian Jooss[3] — [1]Institute for Theoretical Physics, University of Goettingen — [2]Institute for Theoretical Physics, Clausthal University of Technology — [3]Institute for Materials Physics, University of Goettingen

Non-adiabatic processes in the combined atomic and electronic dynamics are explored using two simple model systems, the Holstein model and the Jahn-Teller model. Numerically exact simulations demonstrate processes for the optical excitation and the subsequent relaxation into the ground state. The Holstein model is the classical model for polarons and its dimer allows to demonstrate the role of electronic and structural transitions in an optical excitation. We demonstrate (1) predominantly electronic interband excitations, which are Frank-Condon like, (2) predominantly structural intra-band transitions related to tunnel processes, and (3) an electronic transition that critically depends on the presence of thermal phonons. The latter gives rise to a distinct absorption band with strong temperature dependence. The dominant relaxation mechanisms lead through conical intersections, for which the Jahn-Teller model is the classical model system. We present the transition of a quantum mechanical, nuclear-electronic wave packet through the conical intersection. We discuss the results of measured optical absorption spectra in manganites in view of our theoretical findings.

This work is supported by the Deutsche Forschungsgemeinschaft via SFB 1073 through projects B03 and C03.

TT 75.22 Thu 15:00 P2-EG

Comparison of dephasing models for molecular wires — •Patrick Karasch[1], Verena Gupta[1], Gabriele Penazzi[1], Alessandro Pecchia[2], Dmitry A. Ryndyk[1], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, Universität Bremen, Germany — [2]CNR-ISMN, Roma, Italy

In this work, we investigate the decoherence effects which play an important role in the charge transport characteristics of quantum wires at room temperature. For molecular junctions and onedimensional molecular wires we investigate the distinct dephasing models to calculate and compare the effective resistances and investigate the crossover from coherent Landauer transport to ohmic behavior in long wires. First, we consider the Momentum Relaxing Dephasing (MRD) and the Büttiker Probe (BP) models. These approaches rely on the empirical coupling strength of electronic states to the environment. Then we introduce the electron-phonon dephasing model and consider different approximations including the first Born approximation (BA) and the self-consistent Born approximation (SCBA). Besides, we consider the interplay of disorder and dissipation. Our theoretical method is based on the nonequilibrium Green function approach to quantum transport. To go towards the atomistic ab initio theory, we implemented the method in combination with the density functional based tight binding (DFTB) theory [1] within the DFTB+ code and DFTB-NEGF transport method.

[1] G. Penazzi et al., J. Phys. Chem. C **120**, 16383 (2016)

TT 75.23 Thu 15:00 P2-EG

Parallel fabrication of an entire array of carbon nanotubes devices: a new approach to stamping techniques — •Christian Bäuml, Korbinian Mühlberger, Julian Heger, Christoph Strunk, and Nicola Paradiso — University of Regensburg

We present a new approach to the fabrication of devices based on carbon nanotubes (CNTs) in the low disorder regime. Our fabrication method consists of growing CNTs on a transparent quartz chip and stamping them on an array of tens of devices. The quartz chip and the recipient chip are designed in such a way that during the stamping process the CNTs do not touch any substrate and stays suspended on the electrodes of the recipient devices. The parallel transfer of tens of CNTs highly increases the average number of usable devices per chip. The resulting CNT-based devices are characterized via transport measurements at different temperatures down to the mK-regime. The separation of growth chip from the measurement chip allows one to freely choose the material for the electrodes, opening the way for the implementation of CNT-based devices with superconducting or ferromagnetic leads.

TT 75.24 Thu 15:00 P2-EG

Shot noise measurements on an ultra clean CNT quantum dot — •Michael Schafberger, Daniel Steininger, Nicola Paradiso, and Christoph Strunk — University of Regensburg

Shot noise measurements are a fundamental tool for studying the correlation between charge carriers in mesoscopic devices. Here we present simultaneous measurements of shot noise and conductance on an ultra clean carbon nanotube (CNT) quantum dot. In order to favor defect free and unperturbed CNTs, chemical vapor deposition growth is performed as last nanofabrication step on to Pt-contacts. The sample shows a four-fold symmetry in the Coulomb oscillations. Boson-like excitation lines are observed in certain gate-voltage ranges. We investigate the shot noise on the electron-side, as well as the hole-side of the carbon nanotube and discuss the results.

TT 75.25 Thu 15:00 P2-EG

Magnetic field control of the electron-vibron coupling in a carbon nanotube quantum dot — Peter L. Stiller, Daniel R. Schmid, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

Quantum dots defined in suspended single wall carbon nanotubes define a prototypical nano-electromechanical system: the quantized harmonic oscillator behaviour of the longitudinal vibration mode becomes clearly visible in low-temperature transport spectroscopy.

Here, we present measurements on a nanotube device tuned to the region of $0 \leq N \leq 2$ trapped electrons, i.e., close to the electronic band gap. A highly localized electronic system in strong Coulomb blockade is present. At finite bias, we demonstrate the emergence of Franck-Condon sidebands in single electron tunneling, corresponding to the longitudinal vibration, solely in a magnetic field along the carbon nanotube axis.

The magnetic field evolution of the Franck-Condon coupling factor g is analyzed. For the two-electron ground state it increases from $g = 0$ starting at $B \simeq 1.5\,\mathrm{T}$ and saturates around $B \simeq 3.3\,\mathrm{T}$, however, for different electronic quantum states differing vibronic side band behaviour is found.

We present tentative models, based on the influence of axial magnetic fields on the localization of the electronic wave function. The impact of spin/valley quantum numbers on the electron-vibron coupling is discussed.

TT 75.26 Thu 15:00 P2-EG

Determining the carbon nanotube chiral angle from electronic Fabry-Perot interference — Alois Dirnaichner[1,2], Miriam del Valle[2], Karl Götz[1], Felix Schupp[1], Nicola Paradiso[1], Milena Grifoni[2], Christoph Strunk[1], and •Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Institute for Theoretical Physics, Universität Regensburg, Regensburg, Germany

Connecting low-temperature transport spectroscopy features with a specific microscopic nanotube structure has been an elusive goal so far. While in Coulomb blockade many aspects of the discrete level spectrum are well-understood, a closer look leads to fascinating (and puzzling) hard questions. Here, we apply a complementary approach and analyze the Fabry-Perot interference pattern of a carbon nanotube strongly coupled to metallic leads. By tuning a gate voltage over a large range, the trigonal warping of the Dirac cones can be probed. This, in combination with the valley degree of freedom, leads to a superstructure in the interference pattern, i.e., a secondary interference.

Measurements on an ultraclean, long and suspended carbon nanotube device at millikelvin temperatures are complemented with tight binding calculations of the transmission for specific chiralities and analytic modelling. Taking symmetry classes of nanotubes, but also effects of symmetry breaking at the contacts into account, we show that the crucial parameter for the robust secondary interference pattern is the chiral angle. Consequently, the pattern provides valuable information for determining the structure of a carbon nanotube device.

TT 75.27 Thu 15:00 P2-EG

Towards GHz reflection on a suspended carbon nanotube — Pascal Brunner, •Stefan Blien, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

Applying GHz signals as bias of a single electron tunneling device, as, e.g., a carbon nanotube, poses an obvious challenge. The impedance mismatch of typical radiofrequency electronics at $Z_0 = 50\,\Omega$ and a quantum conductor at $Z_L \gg 6\,\mathrm{k}\Omega$ leads to predominant signal reflection. This effect can be avoided by using an impedance matching network. A specific circuit which has already been successfully used to that purpose in literature is the so-called stub tuner.

We present low-temperature reflection measurements on stub tuner geometries intended for the in-situ growth of "ultraclean" carbon nanotubes as loads. The utilized superconductor is a rhenium-molybdenum alloy highly resistant to the nanotube growth process. For a load resistance of $Z_L = 50\,\mathrm{k}\Omega$ impedance matching is demonstrated with a return loss $> 70\,\mathrm{dB}$. The stub tuner properties are consistent with previous material characterization. Finally we discuss fabrication challenges for devices integrating in-situ grown carbon nanotubes.

TT 75.28 Thu 15:00 P2-EG

Current flow paths in deformed graphene and carbon nanotubes — Erik Kleinherbers, •Nikodem Szpak, and Ralf Schützhold — Faculty of Physics, University of Duisburg-Essen, Germany

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of deformed graphene and bent carbon nanotubes. Since low-energy electronic excitations behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanoelectronic elements and nanosenors. Taking into account the curvature effects as well as an emerging inhomogeneous pseudo-magnetic field we calculate the current flow paths theoretically and compare them with numerical simulations of the full electronic transport.

TT 75.29 Thu 15:00 P2-EG

Coherent exciton transport in double-bilayer graphene — •Bogusz Bujnowski[1], Dario Bercioux[1,2], Jerôme Cayssol[3], and Sebastian Bergeret[1,4] — [1]Donostia International Physics Center (DIPC) - Manuel de Lardizabal 5, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [3]LOMA (UMR-5798), CNRS and Université Bordeaux - F-33045 Talence, France — [4]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU E-20018 Donostia-San Sebastián, Basque Country, Spain

We study exciton condensate formation and coherent transport in a system of two graphene bilayers that are separated by hexagonal boron-nitride. A variety of excitonic-phases has been identified by varying separately the carrier density in the graphene sheets of each bilayer as well as the distance between the bilayer sheets [1]. The richness of the phase diagram could be the key to understand the interesting transport properties observed in recent experiments [2,3]. We aim to explain some key experimental features in terms of peculiar transport properties associated to excitonic condensates [4].

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[2] J.I.A. Li *et al.*, Phys. Rev. Lett., **117** 046802 (2016).
[3] K. Lee *et al.*, Phys. Rev. Lett. **117**, 046803 (2016).
[4] M. Rontani & L. J. Sham, Phys. Rev. Lett. **94**, 186404 (2005).

TT 75.30 Thu 15:00 P2-EG

Spin and Charge Transport in Tailored Carbon Allotropes such as Doped Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Hai I. Wang[1], Axel Binder[3], Mischa Bonn[4], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Graphene exhibits extraordinary properties, however, pristine graphene does not show a band gap as needed for many applications. One of the routes to change that is chemical doping [1]. Here we investigate the effect of heteroatom-dopants on the structure and on the electronic and magnetic properties of graphene. The growth conditions are systematically varied to achieve different dopant concentrations. The resulting structural properties are characterized by Raman and electron microscopy while the charge transport is probed by THz spectroscopy. To correlate the structure and charge properties with magnetotransport we determine the magnetoresistance as a function of temperature and field [2].

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[2] M. Rein et al., ACS Nano 9, 1360 (2015)

TT 75.31 Thu 15:00 P2-EG

THz Magnetooptical Conductivity in epitaxially grown Graphene Samples — •Markus Göthlich[1], Cay-Christian Kalmbach[2], Mattias Kruskopf[2], Klaus Pierz[2], Franz-Josef Ahlers[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Graphene – first isolated in 2004 – has a remarkable Landau quantization given by $E_L = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar v_F^2 e|Bn|}$ with Landau-level index n and band gap 2Δ (if one is opened). This leads to a strong separation of Landau-levels of low indices even at low magnetic fields. This strong Landau-level separation can be used for the detection of radiation in the THz spectral range by cyclotron resonance as shown theoretically in Phys. Stat. Sol. C **8**, 1208 (2011). In this contribution we are investigating the conductivity of graphene in the case of cyclotron resonance absorption in the THz spectral range. The carrier concentration of the device can be tuned by photo chemical gating. The samples are first characterised by Shubnicov-da Haas-measurements. Then, our photoresponse measurements are done in a cryostat at 4 K, in a magnetic field tunable up to 10 T and with a pGe-Laser with a tunable emission wavelength in the range of 120–180 μm corresponding to $\hbar\omega_{\mathrm{photon}} \approx 10\,\mathrm{meV}$. Our aim is a photodetector device based on epitaxial graphene on Si-face SiC that is responsive and spectrally selective and that can be used at elevated temperatures and low magnetic fields.

TT 75.32 Thu 15:00 P2-EG

Simulation of Electron Transport through Graphene-Molecule Junctions — •Dominik Weckbecker[1], Susanne Leitherer[1], Konrad Ullmann[2], Pedro B. Coto[1], Heiko B. Weber[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg — [2]Chair of Applied Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg

While most experiments on single-molecule junctions have employed metal electrodes, recent works demonstrate that graphene has a number of advantages over metallic leads [1-2]. In this contribution, we investigate charge transport in graphene-molecule junctions employing a theoretical approach that combines first-principles electronic structure methods with nonequilibrium Green's function transport theory. Specifically, we consider zigzag and armchair graphene terminated leads and two molecule-lead coupling regimes: (i) strong coupling with covalent binding and (ii) weak coupling, in which the molecular bridge is anchored to the leads by weak bonding interactions. We analyze how the different termination of the graphene electrodes and the molecule-lead coupling affects the transport characteristics [3]. The effect of the structure of the molecular bridge on the conductance properties of the junctions is also discussed [1].

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[2] C. Jia et al., Science 352, 1443 (2016)
[3] I. Pshenichnyuk et al., J. Phys. Chem. Lett. 5, 809, (2013)