TT 66: Poster Session Transport

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

TT 66.1 Thu 15:00 P2/EG

Simulating the nonequilibrium transport through quantum dots coupled to Holstein phonons using matrix-product states methods — •David Jansen and Fabian Heidrich-Meisner — Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Molecular nano structures play an increasingly important role in everyday technology and the field has experienced enhanced experimental and theoretical interest [1]. To better understand the influence of electron-phonon interactions on such structures we investigate a system consisting of two metallic leads connected by a quantum dot with vibrational degrees of freedom. We use matrix-product states based techniques that are designed for an efficient treatment of phonons [2] to calculate transport properties of the system when a bias voltage is applied. We first show that our results agree with those of a functional RG calculation [3]. By diagonalizing the reduced density matrix of the quantum dot we are also able to identify the optimal modes of the system. We show that taking advantage of these modes has computational benefits for our system and we analyze how these optimal modes and their structure are changed by the voltage.

This research is supported by the Deutsche Forschungsgemeinschaft via SFB 1073 (project B09).

[1] M. Galperin et al., J. Phys.: Condens. Matter 19, 103201 (2007)
[2] C. Brockt et al., Phys. Rev. B 92, 241106(R) (2015)
[3] A. Khedri et al., Phys. Rev. B 98, 195138 (2018)

TT 66.2 Thu 15:00 P2/EG

Kondo impurities in two dimensional Dirac semimetals — •Michael Turaev and Johann Kroha — Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany

In this work we study the effects of Kondo as well as static spin impurities on the surface of a three dimensional topological Kondo insulator, which is a Dirac semimetal. Recently there have been scanning tunneling spectroscopy measurements (STM) [1] of the surface state of Gd-substituted SmB_6. Gd has a half filled 4f shell, constituting to a static spin, and a single electron in the 5d shell that can be described as a Kondo impurity. The static spin impurity opens up a local gap and suppresses the local density of states whereas the Kondo impurity can lead to a Kondo peak in the density of states. A realistic theoretical description of the STM experiments requires both of these effects to be taken into account. We use T-matrix and non crossing approximation techniques to analyze a position dependent local density of states that is measured in [1].

[1] L. Jiao et al., Sci. Adv. 4, eaau4886 (2018)

TT 66.3 Thu 15:00 P2/EG

Applications of a general duality relation in fermionic open systems — •Jens Schulenborg[1], Valentin Bruch[2], Maarten Wegewijs[2,3], and Janine Splettstoesser[4] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Denmark — [2]Institute for Theory of Statistical Physics, RWTH Aachen, Germany & JARA-FIT — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Department of Microtechnology and Nanoscience, Chalmers University of Technology, Göteborg, Sweden

Complex Hamiltonians of closed quantum systems are successfully simplified with symmetries, topology or mappings to more easily understandable systems. The ubiquity of *open systems* thus makes an analogous treatment of their effective Liouvillian highly desirable. However, dissipation and memory due to the coupled environment can substantially reduce the number of symmetry relations to draw from.

For a large class of fermionic systems with bilinear system-bath couplings, one such relation derives merely from Pauli exclusion and the principle of total fermion-parity conservation: the *fermionic duality*[1]. This duality yields insights into the dynamics of the system by mapping it to a dual model with inverted energies. Focussing on weakly coupled, Markovian environments, this poster gives an overview of recent and potential future applications of fermionic duality. We address in particular non-equilibrium, stationary and time-dependent charge- and energy transport through nanoscale devices characterized by multiple orbitals with strong many-body interactions.

[1] J. Schulenborg et al.: Phys. Rev. B **93**, 081411 (2016)

TT 66.4 Thu 15:00 P2/EG

Current induced switching in atomic copper junctions — •Patrick Haiber, Martin Prestel, David Weber, and Elke Scheer — Universität Konstanz, Konstanz, Deutschland

Electromigration is intensively studied in micron-size conductors as it is a major cause of failure in integrated circuits. Though, not much is known about the phenomenon when downscaling the sample size to the atomic size.

Here, we study current-induced switching of atomic-size contacts of Cu, a metal that is used as backend in integrated circuits. We present the fabrication of thin-film mechanically controlled break-junctions, using electron beam lithography on a phosphor bronze substrate and thin-flm (80 nm) evaporation. The transport experiments are performed at low temperature under cryogenic vacuum. The conductance histogram obtained from hundreds of conductance vs. distance traces shows a pronounced maximum at $G = 1\ G_0$ as expected for monovalent metals [1] revealing the high sample quality.

The electromigration experiments are performed for contacts with conductance between 1 G_0 and 7 G_0 by applying an alternating bias current [2]. With this process, bistable as well as monostable conductance switching is observed. We discuss the statistical behavior of the switching phenomena as well as the dependence of the switching process on the ramping speed of the alternating current.

[1] Agraït et al., 2003, Phys. Rep. 377, 81-279
[2] Schirm et al., 2013, Nature Nanotech. 8, 645-648

TT 66.5 Thu 15:00 P2/EG

Noise and transport measurements in atomic contacts of rare-earth and transition metals — •Marcel Strohmeier, Martin Prestel, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

We study the formation of atomic-scale magnetic ordering in rare-earth and transition metals. For Gd, a well-known Heisenberg ferromagnet with localized 4f electrons, theoretical studies predict a spin-polarized (SP) transport behavior in reduced dimensions [1]. Otherwise there are paramagnetic materials like Pd or Ir, where an emerging magnetic ordering in small dimension is expected due to the Stoner instability [2, 3]. Nonmonotonic magnetotransport has been reported for atomic contacts of Pt [4], Pd [5], and Ir [6]. Here, we extend the investigations by measurements of the shot noise. Shot noise allows insights into the channel configuration [7] and is sensitive to SP [8]. We study atomic contacts of Gd, Ir, Pd, Pt, and Co using the mechanically controllable break junction (MCBJ) technique at low temperatures. While no evidence for SP is observed for Pt and Pd, we find clear deviation from the usual shot-noise behavior for Gd and Ir.

[1] Olivera et al., PRB 95, 075409 (2017)
[2] Delin et al., PRL 92, 057201 (2004)
[3] Delin et al., PRB 68, 144434 (2003)
[4] Strigl et al., Nat. Comm. 6, 6172 (2015)
[5] Strigl et al., PRB 94, 144431 (2016)
[6] Prestel et al., PRB, accepted
[7] Kumar et al., PRL 108, 146602 (2012)
[8] Burtzlaff et al., PRL 114, 016602 (2015)

TT 66.6 Thu 15:00 P2/EG

A theoretical study of the interplay of electron and phonon transport in nanosystems — •Jakob Bätge and Michael Thoss — Institute of Physics, University of Freiburg, Freiburg, Germany

In view of the tremendous recent progress in experimental techniques to study charge and heat transport in nanostructures based on single atoms or molecules [1,2], theoretical research on basic transport properties of nanosystems is of significant interest.

Here, we investigate the mutual influence of electronic and phononic transport driven by voltage and temperature gradients through basic model systems from a theoretical perspective. For this purpose, we use the hierarchical quantum master equation approach [3], which generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of the results.

[1] L. Cui *et al.*, Science **355**, 1192 (2017).
[2] M. Popp *et al.*, Appl. Phys. Lett. **115**, 083108 (2019).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407(R) (2016).

TT 66.7 Thu 15:00 P2/EG

Spin-orbit coupling drives entangled dynamics in a single molecule junction — •Moritz Frankerl and Andrea Donarini — Institut für Theoretische Physik, Universität Regensburg, 93035 Regensburg, Germany

Experiments based on THz-STM have shown how to obtain both space and time resolution of single molecule vibrations on their intrinsic length and time scales [1]. We report here the theoretical investigations on electronic dynamics of a copper-phthalocynanine in a THz-STM set-up. The quasi-degenerate anionic states of the molecule allow for a coupled spin and pseudo-spin description [2]. The spin-orbit interaction on the metallic centre is responsible, in combination with the ligand, for an intrinsic molecular spin-anisotropy .The latter is modulated, in the junction, by the coupling to the ferromagnetic tip which moreover, generates exchange fields on the molecule [3,4]. We study the resulting entangled spin and orbital dynamics directly in the time domain within a generalized master equation approach.

[1] T. L. Cocker et al., Nature 539, 263-267 (2016)
[2] B. Siegert et al., Beilstein J. Nanotechnol. 6, 2452 (2015)
[3] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[4] A. Donarini et al. Nano Lett. 9, 2897 (2009)

TT 66.8 Thu 15:00 P2/EG

Electronic Transport through PEEB between Au(111) facets: A High-throughput Study — •Lokamani Lokamani[1,2], Florian Günther[3], Jeffrey Kelling[2], Torsten Sendler[1], Filip Kilibarda[1], Jannic Wolf[4], Thomas Huhn[4], Peter Zahn[1], Artur Erbe[1,5], and Sibylle Gemming[1,6] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Department of Information Services and Computing, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [4]Department of Chemistry, Universität Konstanz, Germany — [5]Department of Physics, Universität Konstanz, Germany — [6]Institute of Physics, Technische Universität Chemnitz, Germany

Electrical current transport through single molecules promises new possibilities for down-scaling electronic circuits. The family of p-phenylene-ethynylene derivatives provides excellent candidates for molecular electronics. Here, we present a study on the geometrical and electronic structure of 4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) between Au-electrodes, as it is realized in mechanical break-junction experiments. We identify energetically most favorable configurations of PEEB derivatives between pyramidal Au(111) facets and investigate the electronic transport properties with semi-infinite leads using the DFTB+ code. We discuss the electronic transport properties of single PEEB molecules with anchoring groups -SH, -NH_2 and -CN depending on the anchoring positions on the Au(111) facets.

TT 66.9 Thu 15:00 P2/EG

Characterization and classification of molecular IV data — •Filip Kilibarda[1], Alexander Strobel[1], Michael Mortensen[2], Kurt Gothelf[2], Thomas Huhn[3], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Centre for DNA Nanotechnology, Aarhus , Denmark — [3]University of Konstanz, Konstanz, Germany

Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ). Here we present two different kinds of measurements. One is performed in a liquid solution and under ambient conditions, and the other one in a cryogenic environment, under vacuum. As a testbed for these measurements, we use salen and C60 molecules respectively. We show how this data fits to the basic Single Level Model and what are the possible pitfalls of this approach. As an alternative, we offer modified versions of the SLM and compare them at predicting the transport properties of the molecules. Furthermore, due to the inherently stochastic processes of molecular binding to the nanoscopic junction, we propose an efficient approach based on the Machine Learning to further cluster the data into subsets. By using auto-encoders and decision trees with minimal amounts of supervised learning we can cluster large quantities of data. This allows us to evaluate different binding positions and events, with most appropriate models, and extract the underlying data.

TT 66.10 Thu 15:00 P2/EG

Hydrodynamic Bounds to the Entropy Production in 1D Systems — •Dennis Hardt, Philipp Weiss, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

A typical strategy of realizing an adiabatic change of state is to vary system parameters/quench very slowly in time τ. In the ideal case of adiabatic state preparation $\tau \to \infty$ the entropy production vanishes. This approach is hampered by hydrodynamic long-time tails, i.e. hydrodynamic fluctuations relax *algebraically slowly*. This behavior transfers to various observables. Therefore, a power-law decay of the entropy production $\sim \tau^{-\alpha}$ is expected for slow quenches.

We investigate the non-equilibrium dynamics of a classical diatomic gas with point like particles in 1D to study the entropy production as a function of τ. In order to model the long time behavior of such a system, we simulate a large number of scattering events ($\sim 10^9$) in a population of $\sim 10^5$ particles, over a relaxation timescale 10^5 times larger than the average scattering time.

The resulting curve of the entropy production shows a long-time tail $\sim \tau^{-1/2}$ matching to theoretical predictions from linear fluctuating hydrodynamics.

TT 66.11 Thu 15:00 P2/EG

Phase slip signatures in fully proximitized carbon nanotubes embedded in van der Waals stacks — •Christian Bäuml, Lorenz Bauriedl, Michaela Eichinger, Nicola Paradiso, and Christoph Strunk — University of Regensburg, Regensburg, Germany

Recently, Marganska et al. suggested that Majorana fermions (MFs) can occur in carbon nanotubes (CNTs) proximitized by superconductor (SC) in large fields perpendicular to the CNT axis [1].

In this work, we demonstrate the first building blocks of the proposed device. As a SC we chose a bilayer $NbSe_2$ crystal, an Ising SC capable to sustain large in-plane magnetic fields. A 7 μm-wide bilayer flake is stamped on top of a 9 μm-long CNT, laterally contacted via Au edge-contacts [2,3]. $NbSe_2$ and edge Au contacts turn out to be extremely transparent. Consequently, we observe a large supercurrent induced even in the 2 μm-long portion of CNT not directly proximitized by $NbSe_2$, with a 2-terminal conductance exceeding 120 e^2/h. Moreover, the conductance through the CNT shows sharp magnetic field-dependent dips, which we attribute to phase slippage events within the 1D superconducting system, a 1D analogue of what observed recently in 2D systems as $NbSe_2$ [4].

[1] M. Marganska et al., Phys. Rev. B 97, 075141 (2018)
[2] L. Wang et al., Science 614, 342 (2013)
[3] J.-W. Huang et al., Nano letters 15, 10 (2015)
[4] N. Paradiso et al., 2D Mater. 6, 025039 (2019)

TT 66.12 Thu 15:00 P2/EG

Electronic Tranport in Graphene Nanoribbons with Edge Disorder — •Tom Rodemund[1,2], Fabian Teichert[2], and Jörg Schuster[1,3] — [1]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Graphene possesses many interesting properties like high charge carrier mobilities and concentration. This makes it particularly suited for electronic applications. However, while using Graphene in form of nanoribbons (GNRs) edge disorder cannot be avoided. We study the influence of edge roughness on electron conductance using a density-functional-based tight-binding model to calculate the conductance of rough GNRs. We analyze large ensembles of GNRs with random edges and varying chirality in order to gain insight into the electronic structure.

A GNR represents a quasi-one-dimensional system with disorder and is thus expected to have strongly localized states. This leads to an exponential dependence of the conductance on the length of the ribbon with a characteristic localization length. We express the localization length as a function of roughness, width and chirality of the system.

TT 66.13 Thu 15:00 P2/EG

Adsorped or intercalated nickel atoms in graphene based materials: stability and electronic properties — •Daniel Dick[1,2,3], Florian Fuchs[2,3,4], and Jörg Schuster[2,3,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany — [3]Forschungsfabrik Mikroelektronik, Berlin, Germany — [4]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

Graphene based materials such as graphene fibers or thin films offer promising electrical properties, which can be further improved by adsorption or by intercalation of dopants. A variety of electron donating

species can be considered to fabricate intercalation compounds, many of which have not been studied yet.

We investigate structure, stability and electronic structure of nickel doped graphene, bilayer graphene and graphite using density functional theory. Different positions of the nickel atom are compared. We demonstrate that the energetically optimal position of the nickel atom depends on the nickel concentration. While the nickel atom is in the middle of a hexagon in graphene, it is located at an off-center position in graphite. Furthermore, the stability of the nickel intercalant decreases with increasing nickel concentration. The nickel atom introduces additional bands in the band structure. These bands are located near the Fermi level, leading to improved conductance.

TT 66.14 Thu 15:00 P2/EG

Angle-dependent magnetoresistance in ballistic semi-metals — •Felix Spathelf[1,2], Benoît Fauqué[2], and Kamran Behnia[1] — [1]Laboratoire de Physique et d'Étude des Matériaux (CNRS), ESPCI Paris, Université PSL, Paris, France — [2]JEIP, USR 3573 CNRS, Collège de France, Université PSL, Paris, France

We performed electric transport measurements on bismuth and tungsten single crystals of several shapes, orientations and qualities in mangetic fields up to 13.8 T and at temperatures down to 2 K. In order to study the angular dependence of the magnetoresistance, we applied a current parallel to a high symmetry axis and rotated the magnetic field in the plane perpendicular to it. Due to the Fermi surface topology, the Lorentz force depends on the angle between the crystal axes and the applied magnetic field. Therefore, the magnetoresistance is angle-dependent.

We observed that at low temperatures the magnetoresistance loses also the symmetry of the underlying crystal. This happens in both bismuth, which has a very small Fermi surface, and tungsten, whose Fermi surface is much larger. The observed behaviour is thought to be connected to the shape of the sample [1], but at least in the case of bismuth, the sample shape cannot explain completely this effect [2].

[1] O. A. Panchenko, P. P. Lutsishin, Sov. Phys. JETP 30, 841 (1970)
[2] Z. Zhu et al., Nature Phys. 8, 89-94 (2012)

TT 66.15 Thu 15:00 P2/EG

Detecting superconductivity out-of-equilibrium in extended Hubbard and t-J models — Sebastian Paeckel[1], Benedikt Fauseweh[2,3], •Alexander Osterkorn[1], Thomas Köhler[4,1], Dirk Manske[2], and Salvatore R. Manmana[1] — [1]Institut für Theoretische Physik, U. Göttingen, D-37077 Göttingen — [2]MPI für Festkörperforschung, D-70569 Stuttgart — [3]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [4]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

Recent pump-probe experiments, e.g., on underdoped cuprates suggest the existence of a transient superconducting state above T_c. This poses the question how to reliably identify the emergence of long-range order, in particular superconductivity, out-of-equilibrium. We investigate this by studying a quantum quench in an extended Hubbard model and a variant of the t-J model using matrix product state time-evolution schemes. We compute various observables, which are used to identify (quasi-)long-range order in equilibrium. Our findings imply that it does not suffice to study the time-evolution of the optical conductivity to unambiguously identify superconductivity. In turn, we suggest to utilize time-resolved pair-ARPES experiments to probe for the formation of a condensate in the two-particle channel.

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TT 66.16 Thu 15:00 P2/EG

Thermal and nonthermal responses of the low temperature charge order in $IrTe_2$ to femtosecond laser pulses — •Gregor Jecl[1], Venera Nesretdinova[2], Yaroslav Gerasimenko[1], Claude Monney[3], Fabian von Rohr[4], and Dragan Mihailovic[1,2] — [1]Department for Complex Matter, Jozef Stefan Institute, Slovenia — [2]Center of Excellence on Nanoscience and Nanotechnology, Slovenia — [3]Département de Physique and Fribourg Center for Nanomaterials, Université de Fribourg, Switzerland — [4]Department of Chemistry, University of Zürich, Switzerland

$IrTe_2$ is a layered material which exhibits a structural transition at $T_{C1} = 275$ K to a low temperature (LT1) phase which is accompanied by the appearance of stripe order. A second transition (LT2 phase) at $T_{C2} = 180$ K changes the dominant periodicity of the stripes. Superconductivity can be introduced below 3.1 K by doping or in undoped samples at surface patch domains of hexagonal symmetry. We have investigated the dynamics of all three phases on sub-picosecond timescales by means of ultrafast optical spectroscopy in a temperature range between 8 and 295 K. Additionally, by imaging the surface after photoexcitation in STM, we have investigated the degree to which the stripe order can be controlled by ultrafast optical pules on long timescales. At helium temperatures and under high fluence photoexcitation we observe a non-thermal photoinduced response of the transient reflectivity. Additionally, exposure to high fluence pulse trains results in the stabilisation of the LT1 phase at low temperatures and to changes in the orientation of the stripe phase.

TT 66.17 Thu 15:00 P2/EG

Microwave cavity-free hole burning spectroscopy of Er^{3+}:Y_2SiO_5 at sub-Kelvin temperatures — •Nadezhda Kukharchyk[1], Anton Mladenov[1], Natalya Pankratova[2], Dmitriy Sholokhov[1], Alexey A. Kalachev[3], Sebastian Probst[4], Vladimir Manucharyan[2], and Pavel A. Bushev[1,5] — [1]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany — [2]Department of Physics, Joint Quantum Institute and Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, USA — [3]RFC Kazan Scientific Center of RAS, 420029 Kazan, Russian Federation — [4]Quantronics group, SPEC, CEA, CNRS, Universite Paris-Saclay, CEA Saclay 91191 Gif-sur-Yvette Cedex, France — [5]JARA-Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52428 Jülich, Germany

Spectral hole burning technique is well-deployed in optical inhomogeneously broaden medium for realization of slow light and optical memory based on atomic frequency combs. First implementation of this technique into the microwave regime has been recently demonstrated with NV-centers coupled to a cavity [1]. Here, we develop this idea by applying spectral hole burning technique to Erbium spin ensemble in a cavity-free regime. We investigate Erbium-doped Y_2SiO_5 crystal coupled to a superconducting transmission line. Here, we show the influence of the magnetic field and temperature on the dynamics of the attained spectral hole and discuss processes governing it.

[1] Putz, S., Angerer, A., Krimer, D. et al. Nature Photon **11**, 36-39 (2017)

TT 66.18 Thu 15:00 P2/EG

Damping of the Anderson-Bogolyubov mode in Fermi mixtures by spin and mass imbalance — •Piotr Zdybel and Pawel Jakubczyk — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

We study the temporally nonlocal contributions to the gradient expansion of the pair fluctuation propagator for spin- and mass-imbalanced Fermi mixtures. These terms are related to damping processes of sound-like (Anderson-Bogolyubov) collective modes and are relevant for the structure of the complex pole of the pair fluctuation propagator. We derive conditions under which damping occurs even at zero temperature for large enough mismatch of the Fermi surfaces. We compare our analytical results with numerically computed damping rates of the Anderson-Bogolyubov mode.

[1] P. Zdybel and P. Jakubczyk, Phys. Rev. A 100, 053622 (2019)