TT 101: Transport - Poster Session

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

TT 101.1 Thu 15:00 P2

Non-equilibrium transport through a QD using Keldysh-fRG — •Dennis Schimmel[1,2], Florian Bauer[1,2], Jan Heyder[1,2], and Jan von Delft[1,2] — [1]Arnold Sommerfeld Center München — [2]LMU München, Germany

The functional renormalization group (fRG) is a powerful resummation technique which recasts the computation of diagrams into a diffential equation. We apply the non-equilibrium (Keldysh) version of it to a single impurity Anderson model and analyze various choices of the flow parameter. We focus on the weakly interacting region to establish the quality of the fRG-scheme. From previous studies, it is known that the truncation involved in fRG schemes inevitably leads to a violation of the particle-conservation law. As a consequence of this, physical quantities need to be computed without resorting to derivations using the particle-conservation law, unless the quantitative violation is negligible. The scheme used here can readily be generalized to quantum chain models, e.g. to treat nonequilibrium transport through (weakly) interacting quantum wires.

TT 101.2 Thu 15:00 P2

Nonequilibrium BCS-Anderson model- ISPI approach — •Stephan Weiss and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Using the scheme of iterative summation of real-time path integrals (ISPI) [1-2], we compute the $I(V)$ characteristics of a single spin-degenerate quantum dot tunnel coupled to superconducting (BCS) leads. By means of a Hubbard-Stratonovich transformation, the path integral is mapped to a finite spin sum inheriting nonlocal-in-time correlations among the spins. Anomalous Green's functions components are truncated according to the established rules [1-2] on the same footing as the normal Keldysh components. The remaining spin-path summation is capable for the ISPI scheme. Since we treat tunneling exactly to all orders, we are able to resolve the subgap structure in terms of multiple Andreev reflections (MAR). We present results of the $I(V)$ for the non-perturbative regime ($U/\Gamma, T/\Gamma, eV/\Gamma \gg 1$), whereas in the noninteracting limit we compare our results to previous analytical results [3]. For $U/\Gamma \ll 1$ we compare to a perturbative calculation [4] as well as to a real-time diagrammatic approach for $\Gamma_S \ll 1$ [5].

[1] S. Weiss, et al., Phys. Rev B, **77**, 195316, (2008).
[2] S. Weiss, et al., Phys. Status Solidi B **250**, 2298 (2013).
[3] A. Levy-Yeyati, et al., Phys. Rev. B **55**, 6137(R) (1996).
[4] L. Dell Anna, et al., Phys. Rev. B **77**, 104525 (2008).
[5] M. Governale, et al., Phys. Rev. B **77**, 134513 (2008).

TT 101.3 Thu 15:00 P2

Exact solutions of collective heat transport — •Gabriel Topp, Tobias Brandes, and Gernot Schaller — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

In the last decades a lot of different tools to describe transport processes in open quantum systems have been developed. Prominent examples include e.g. master equations or Green's functions. The model of a single impurity coupled to two reservoirs is therefore a well-known problem [1].

We show that several collective transport setups can be mapped to the single impurity model. Using exact solutions of the Heisenberg equations of motion we calculate stationary transport properties, both in fermionic and bosonic systems. With our proper solutions we investigate the validity of simple markovian master equations.

[1] G. Schaller, P. Zedler, and T. Brandes, Phys. Rev. A 79, 032110 (2009)

TT 101.4 Thu 15:00 P2

Electronic current switching at finite temperature by magnetic focusing in a soft-wall quantum dot — •Christian Morfonios and Peter Schmelcher — Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

We demonstrate a mechanism enabling efficient switching of the finite-temperature magnetoconductance in an electronic quantum dot with designed soft-wall confinement. The mechanism relies on the effective increase of the available area of motion within the dot with increasing energy, so that the magnetically deflected electron density retains invariant spatial characteristics at an optimal low field strength. Heavily suppressed background transmission can then be achieved along the entire ground propagation channel of the incoming electrons, while resonant states couple very weakly to the attached leads, even for a large number of dot levels. The presence of soft walls in an elliptically shaped quantum dot simultaneously aids collimated electron transport and high transmission for zero field, leading to efficient finite-temperature magnetoconductance switching at linear response. The effect is investigated in terms of the influence of the width of the soft wall and its profile at given temperatures, as well as for arrays of connected dots.

TT 101.5 Thu 15:00 P2

Spin-thermoelectric effects in metals — •Sebastian Tölle[1], Cosimo Gorini[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif sur Yvette, France

Via spin-orbit coupling, and even in the absence of magnetic fields, a temperature gradient applied to a two-dimensional electron gas can generate both spin currents and spin polarizations. These phenomena are the thermal counterpart of well-known ones such as the spin Hall effect and the voltage-induced spin polarization, and belong to the fast growing field of spin caloritronics. We study them by means of a generalized Boltzmann equation which takes into account spin-orbit coupling of both intrinsic and extrinsic origin within an $SU(2)$ formulation. We show, in particular, that a thermal gradient induces an in-plane spin polarization and a spin current transverse to the field and polarized out-of-plane (spin Nernst effect). We find that the interplay between intrinsic and extrinsic mechanisms is critical, and that the relation between spin currents and spin polarizations – well understood in the presence of simple electric drivings – is nontrivially affected by the thermal driving.

TT 101.6 Thu 15:00 P2

Magnetotransport in ferromagnetic Mn_5Ge_3 and $Mn_5Ge_3C_{0.8}$ thin films — •Christoph Sürgers[1], Patrick Winkel[1], Gerda Fischer[1], Inga A. Fischer[2], and Li-Te Chang[3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76049 Karlsruhe — [2]Institut für Halbleitertechnik, Universität Stuttgart, 70569 Stuttgart — [3]Device Research Lab., Dept. of Electrical Engineering., University of California, Los Angeles, CA 90095, USA

Ferromagnetic Mn_5Ge_3 and $Mn_5Ge_3C_{0.8}$ compounds with Curie temperatures of $\approx$ 300 K and 450 K, respectively, are potential electrode-materials for spin injection into Si and Ge due to their high resistivity and compatibility with CMOS technology [1]. We investigate the temperature dependence of the anisotropic magnetoresistance (AMR) and the anomalous Hall effect of sputtered thin films. The AMR changes sign from negative to positive with increasing temperature with a concomitant increase and sign change of the ordinary Hall coefficient R_0 while the anomalous Hall coefficient is independent of temperature. The correlation between the temperature dependence of R_0 and of the AMR ratio is discussed by considering a change of the different contributions arising from the electron-like minority-spin band and the hole-like majority-spin band to the conductance with increasing temperature. Magnetoresistance measurements in the Hanle geometry on $Mn_5Ge_3C_{0.8}$ electrodes deposited on highly doped n-Ge reveal that spin injection and spin extraction occur, however, at temperatures below 15 K.

[1] I. A. Fischer et al., Semicond. Sci. Technol. **28**, 125002 (2013)

TT 101.7 Thu 15:00 P2

Conductance Quantization in Rare-Earth-Metal Nanocontacts — •Oliver Berg[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76049 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe

We present conductance measurements of Gd, Dy, and Ce obtained on mechanically controlled break-junctions (MBCJ) made from polycrystalline wires at l-He temperatures. The contact formation and switching between metallic and tunneling conductance G is investigated in dependence of the electrode distance Δx. From a number of measurements of $G(\Delta x)$, exhibiting conductance plateaus, we ob-

tain conductance histograms. We focus on the conductance G^* of the last plateau before with increasing Δx, G enters the tunneling regime. While for Gd and Dy the last "plateau" occurs at $G^* \approx 0.6\,G_0$ and $0.9\,G_0$ ($G_0 = 2e^2/h$), respectively, $G^* \simeq 1.7\,G_0$ is observed for Ce. For Gd and Dy the $4f$ state is far below the Fermi level and does not contribute to the electronic transport. A possible explanation for the large G^* value of Ce is the additional contribution from the $4f$ state being shifted toward the Fermi level, when cooling the sample through the $\gamma - \alpha$ phase transition.

TT 101.8 Thu 15:00 P2

Renormalization of subband anticrossings in interacting quantum wires with spin-orbit interactions — •Tobias Meng[1], Jelena Klinovaja[1,2], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We discuss how electron-electron interactions renormalize the anticrossings between different subbands in quantum wires with spin-orbit interactions. Depending on the wire's parameters, interactions may either increase or decrease the width of the anticrossings. When the anticrossings are closed using a special combination of Rashba and Dresselhaus spin-orbit interactions, their width tends to zero as an interaction dependent power law of the spin-orbit couplings, which is a consequence of Luttinger liquid physics. Monitoring the closing of the anticrossings would allow to directly measure the related renormalization group (RG) scaling dimensions in an experiment.

TT 101.9 Thu 15:00 P2

Quantum transport and response to electric fields in non-Abelian systems with spin-orbit coupling and 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 and electron-electron interactions as well as spin-dependent meanfields is discussed. The appropriate quantum kinetic equation for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the spin and density dynamical responses to electric fields (polarized light) are calculated and several effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling, extended quasiparticle picture and polarization effect from correlated density. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found.

[1] EPL 104 (2013) 2700

TT 101.10 Thu 15:00 P2

Orbital dependent absorbing boundary conditions for nanoscale spin transport — •Sebastian Frank and David Jacob — MPI of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany

Atomic and molecular junctions containing magnetic atoms are an intriguing field of research that may give rise to the development of nanoscale spintronic devices [1]. This type of system is particularly challenging: it is infinite, but non-periodic in the transport direction. In order to model the effect of the leads, we implement a novel methodology making use of absorbing boundary conditions (ABC) [2,3] within the ab initio quantum transport method for nanoscale devices based on DFT [4]. Our method allows us to determine orbital dependent ABC. This is crucial for the correct description of transition metal leads which have s-, p- and d-orbital channels. The orbital-dependence is included via a non-empirical criterion. The two free parameters are chosen by comparision with exact results for infinite chains and prove to be universal, i.e. have to be chosen only once and can then be applied to all types of systems. We apply our method to transition metal nanocontacts and find smooth density of states and transmission functions in agreement with experimental data.

[1] A. R. Rocha, Nature Mater. 4 (2005) 335
[2] A. Goldberg et al., J. Phys. B 11 (1978) 3339
[3] F. Evers et al., CFN Lectures on Functional Nanostructures 2 (2011) 27
[4] J. J. Palacios et al., PRB 66 (2002) 035322

TT 101.11 Thu 15:00 P2

Electronic Properties of Spirobifluorene Molecules — •Amin Karimi[1], Michal Valasek[2], Fabian Pauly[1], Maya Lukas[2], Marcel Mayor[2], and Elke Scheer[1] — [1]University of Konstanz — [2]Karlsruhe Institute of Technology

The knowledge about the fundamental correlations between a molecule's functional chemical groups, its contacts, and surroundings and the resulting electronic properties is imperative for the design of future molecular electronic building blocks [1,2]. The electronic properties of multipodal molecules have been studied in recent years mainly by inserting them into mechanically controlled break junctions (MCBJ) [3] or by scanning tunneling microscopy (STM) [4]. We present charge transport measurements through single spirobifluorene tripodal molecules, performed with the help of the low-temperature MCBJ technique. Inelastic electron tunneling spectra are measured to study the influence of vibronic coupling on the conductance of molecular junctions and to obtain in this way knowledge about the contact geometry and electrode-molecule coupling.

[1] J. C. Cuevas and E. Scheer, Molecular Electronics: An Introduction to Theory and Experiment, World Scientific, Singapore (2010).
[2] S. Aradhya and L. Venkataraman, Nature Nanotech. 8, 399 (2013).
[3] Y. Ie, T. Hirose, H. Nakamura, M. Kiguchi, N.Takagi, M. Kawai, and Y. Aso, J. Am. Chem. Soc. 133, 3014 (2011).
[4] M. Lukas, K. Dössel, A. Schramm, O. Fuhr, C. Stroh, M. Mayor, K. Fink, and H. v. Löhneysen, ACS Nano 7, 6170 (2013).

TT 101.12 Thu 15:00 P2

Transport measurements of diarylethene molecules with long conjugated linkers in solution — •Katharina Luka-Guth[1], Daniel Schmid[1], Jannic Wolf[2], Thomas Huhn[2], and Elke Scheer[1] — [1]Universität Konstanz, FB Physik — [2]Universität Konstanz, FB Chemie

We measure the conductance of several different diarylethene molecules via the mechanically controllable break junction (MCBJ) technique at room temperature. Diarylethenes are photochromic molecules that undergo a ring-opening ring-closure reaction upon irradiation with light with suitable wavelength. This reaction changes the conjugation of the pi-system of the molecules that are therefore discussed as optically driven molecular switches. To measure their transport properties, a solution of molecules is directly applied to the gold electrodes in a glass pipette sealed by a PDMS gasket. While opening and closing the MCBJ, molecules get into contact with the electrodes and bridge the gap between two electrodes. Simultaneously the conductance of the molecules is measured, from which conductance histograms are calculated. We compare our results to previous findings. The information is completed by current-voltage characteristics that enable us to determine the position of the current-dominating molecular orbital. We compare our findings with those from previous studies on diarylethenes with shorter linkers [1,2]. Furthermore, we discuss the role of the solvent.

[1] B. Briechle et al., Beilstein J. Nanotechnol. 3, 798 (2012)
[2] Y. Kim et al., Nano Letters 12, 3736 (2012)

TT 101.13 Thu 15:00 P2

Switching the Conductance of a Molecular Junction using a Proton Transfer Reaction — •Chriszandro Hofmeister[1], Pedro B. Coto[1], Óscar Rubio-Pons[1], Andrzej L. Sobolewski[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

The possibility of using single molecules as components in electronic circuits has motivated intensive experimental and theoretical research on the conductance characteristics of these systems. In this contribution, we present theoretical results suggesting that a molecular junction can work as a nano switch [1] using a mechanism that based on a ground state proton transfer reaction [2]. Employing density functional theory and the Landauer transport theory we show that the keto and enol forms of our selected molecule have different conductance characteristics which can be explained in terms of the different conjugation patterns exhibited by both tautomers. We also provide a proof of principle showing that both forms can be reversibly interconverted using an external electrostatic field. The dynamics of the process is investigated using a quantum master equation approach.

[1] B. Feringa, W. Browne, *Molecular Switches*, Wiley-VCH Verlag
[2] C. Benesch *et al.*, J. Phys. Chem. C 113, 10315

TT 101.14 Thu 15:00 P2

Effects of electronic correlations and magnetic field on a molecular ring out of equilibrium — •Martin Nuss, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology

We study effects of electron-electron interactions on the steady-state characteristics of a hexagonal molecular ring in a magnetic field, as a model for a benzene molecular junction. The system is driven out of equilibrium by applying a bias voltage across two metallic leads. We employ a model Hamiltonian approach to evaluate the effects of on-site as well as nearest-neighbor density-density type interactions in a physically relevant parameter regime. Results for the steady-state current, charge density and magnetization in three different junction setups (para, meta and ortho) are presented. Our findings indicate that interactions beyond the mean-field level renormalize voltage thresholds as well as current plateaus. Electron-electron interactions lead to substantial charge redistribution as compared to the mean-field results. It is shown that electron-electron interactions do not qualitatively change the current-voltage characteristics in magnetic fields as compared to the noninteracting case in a charge-neutral setup. We identify a strong response of the circular current on the electronic structure of the metallic leads. Our results are obtained by steady-state Cluster Perturbation Theory, a systematically improvable approximation to study interacting molecular junctions out of equilibrium, even in magnetic fields. The method is flexible and fast and can straight-forwardly be applied to effective models as obtained from ab-initio calculations.

TT 101.15 Thu 15:00 P2

Intramolecular interference in an extended benzenelike molecule, due to a three-path analogy — Tim Ludwig and •Carsten Timm — TU Dresden, Dresden, Germany

In the last few years so-called intramolecular interference gained attention. It is the effect of interference in electronic transport through single molecules, leading to proposals for devices in molecular electronics and spintronics. Previous works have investigated spatially symmetric molecules or structures with two degenerate many-body states, analogous to a semiclassical two-path setup. We report on electronic-transport calculations within the quantum master-equation-formalism, investigating an extended Hubbard model of a six-sided ring with an additional central site, inspired by, e.g., benzene-vanadium. One can archieve a threefold-degenerate groundstate by tuning the parameters of the central site corresponding to a semiclassical three path setup.

TT 101.16 Thu 15:00 P2

Electrical Characterization of a Switchable Molecular Wire via Mechanically Controllable Break Junctions — •Torsten Sendler[1], Matthias Wieser[1], Jannic Wolf[2], Thomas Huhn[2], Elke Scheer[2], Francesca Moresco[3], Jochen Grebing[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]University of Konstanz, Germany — [3]Max Bergmann Center of Biomaterials, Dresden, Germany

Molecular electronics has been a field of big interest for the last years. Using the technique of mechanically controllable break junctions we characterize the Switchable Molecular Wire Oligo(phenylene ethynylene)-embedded Difurylperfluorocyclopentenes (SMW) in liquid environment. Via light irradiation the SMW can be switched between two well-defined conductance states.

Conductance and hysteresis measurements allow us to identify the two states providing the basis for a comprehensive study of the in situ switching process. Based on the analysis with the transport model assuming transport through a single molecular level, we confirm that a reliable contact of the molecules to the gold contacts is formed and extract the energy of the molecular levels and the coupling constants between molecule and electrodes.

TT 101.17 Thu 15:00 P2

Electronic structure of photosensitive molecular switches: A first-principle investigation — •Lokamani L[1], Daijiro Nozaki[1], Arezoo Dianat[1], Tahereh Ghane[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Sciences and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, Germany

The investigation of networks of nano-particles interconnected with functional molecular components is an active research field. Some potential applications include the realization of elementary computing units, able to act as memory nano-devices. However, to achieve this goal a detailed understanding of the electronic, structural, and electrical transport properties of potentially relevant molecular building blocks is mandatory. Here, we study such properties at the level of single molecules, for merocyanine derivatives, a photosensitive organic complex. In particular, we analyse the interplay between molecular conformation and corresponding modifications in the electrical response. First steps towards the inclusion of structural fluctuations via molecular dynamics simulations and its impact on the charge transport are also discussed.

TT 101.18 Thu 15:00 P2

Dynamics of a nano-electromechanical rotor driven by single-electron tunneling — •Alan Celestino[1], Alexander Croy[2], Marcus Werner Beims[3], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Chalmers University of Technology S-412 96, Göteborg, Sweden — [3]Federal University of Paraná, Curitiba, Brazil

We discuss a nano-electromechanical rotor driven by single-electron tunneling. A possible realization could be a nanotube with quantum dots attached on its extremities, which can freely rotate about a double-walled nanotube axis. The system is driven using a bias voltage between source and drain contacts. Using a few relevant parameters one can set the rotor's dynamics to either intermittent oscillations/rotations or continuous rotational motion. The connection between the dynamical regimes and the current through the device is established. The effect of tuning initial conditions is also addressed, showing a bistable behaviour in the system's phase space. Among the possible applications of such device stand out the signal amplification, current rectification and viscosity measurements.

[1] A. Croy and A. Eisfeld, EPL 98, 68004

TT 101.19 Thu 15:00 P2

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Electron Transport in Single-Molecule Junctions — •Christian Schinabeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

In this contribution we investigate vibrationally coupled transport in single-molecule junctions using the hierarchical quantum master equation approach [1,2]. This method allows a systematic convergence of the reduced dynamics of open quantum systems beyond the traditional Markovian rate equations. We consider a model consisting of a molecular level coupled to fermionic leads as well as a vibrational mode. For this system the numerically accurate results of the hierarchical quantum master equation approach are compared with Markovian rate equation calculations in different parameter regimes. The performance of the method with respect to numerical efficiency and convergence is analyzed in detail.

[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. 75, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).

TT 101.20 Thu 15:00 P2

Model study of nonadiabatic electronic-vibrational interactions in single-molecule junctions — •André Erpenbeck and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen- Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

The interaction between electronic and vibrational degrees of freedom in single-molecule junctions results from a dependence of the electronic energies on the nuclear displacement, but also from the dependence of the electronic states of the molecular bridge on the nuclear coordinates. The latter mechanism leads to a direct coupling between different electronic states and is referred to as nonadiabatic electronic-vibrational coupling. Employing a perturbative non-equilibrium Green's function approach, we study the influence of nonadiabatic electronic-vibrational coupling on the transport properties of model molecular junctions. In particular, we investigate the validity of the adiabatic approximation and show that nonadiabatic electronic-vibrational interaction gives rise to new transport channels. Furthermore, we explore the properties of nonadiabatic vibrational effects and their manifestation in observables such as the current-voltage characteristics.

TT 101.21 Thu 15:00 P2

Ab-initio phonon transport through single-molecule junctions — •Jan Klöckner[1], Robert Gossman[1], Thomas Hellmuth[2], Marius Bürkle[3], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Germany — [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the phononic contribution to thermal transport in single-molecule junctions. For this purpose we determine contact geometries and force constants on the level of density functional theory. The phonon transport is computed in the harmonic approximation by use of Green's function techniques. We study the following two basic problems: (i) Length-dependent transport and (ii) quantum interference effects. For (i) we study Au-alkane-Au junctions of varying molecular length. In (ii) we consider para- and meta-coupled Au-benzene-Au contacts to search for the phononic analogon of destructive electronic interference.

TT 101.22 Thu 15:00 P2

Real-time Dynamics in the Anderson-Holstein Model with phonon dependent hybridization — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We study the real-time dynamics after a quench in the one-lead Anderson-Holstein model with a modified hybridization term using the time-dependent numerical renormalization group (TD-NRG). In molecular devices hysteresis effects and negative differential conductions have been reported. Experiments give hints, that these physics are due to the electron-phonon interactions inside the molecule. In our model we show that the short time dynamics of an electronic level in contact with a electronic bath is strongly dependent on the coupling with a phononic mode. The expectation value of the occupancy of the electronic level oscillates with the frequency of the phonon. For long times we show that we reach the equilibrium expectation values.

TT 101.23 Thu 15:00 P2

Magnetostriction in Nanomechanical Beams — •Rasmus Hollaender[1], M. Pernpeintner[1], M. J. Seitner[2,3], J. P. Kotthaus[2], E. M. Weig[2,3], S. T. B. Goennenwein[1], R. Gross[1], and H. Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Center for NanoScience (CeNS) and Fakultät für Physik, LMU, München, Germany — [3]Fachbereich Physik, Universität Konstanz, Germany

Nanomechanical sensors have demonstrated excellent force sensitivity [1], allowing for the detection of individual spins on surfaces [2]. Here, we apply this sensor concept to the detection of magnetostriction in nanometer thick ferromagnetic cobalt films. To this end we experimentally investigate the eigenfrequency of a 25 μm long and 300 nm wide highly stressed silicon nitride beam covered by a 10 nm thin film of cobalt at room temperature as function of the direction and magnitude of the applied magnetic field in the plane of the film using optical interferometry. For magnetic fields applied in the direction perpendicular to the beam, we find a decrease in the resonance frequency by 7.6 kHz compared to fields applied along the beam direction. We explain this 10^{-4} change in the resonance frequency quantitatively by modeling the impact of the magnetization orientation dependent magnetostriction. This opens the path for further magneto-mechanical experiments in nanostructures. Financial support via the Nanosystems Initiative Munich is gratefully acknowledged.

[1] J. Moser *et al.*, Nature Nanotechnology **8**, 493 (2013)
[2] D. Rugar *et al.*, Nature **430**, 329 (2004)

TT 101.24 Thu 15:00 P2

Exploring mechanical material parameters from spectroscopy of nano-electromechanical systems — •Anh Tu Bohn[1], F. Hocke[1], M. Pernpeintner[1], X. Zhou[3,5], A. Schliesser[4], T. J. Kippenberg[3,5], R. Gross[1,2], and H. Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Department, TU München, Germany — [3]École Polytechnique Fédérale de Lausanne, Switzerland — [4]Niels Bohr Institute, University of Copenhagen, Denmark — [5]Max-Planck-Institut für Quantenoptik, Germany

The field of nano-electromechanics combines nanomechanical resonators with electrical circuits. In our nano-electromechanics experiments, we investigate a double layer nanomechanical beam consisting of Si_3N_4 and Niobium coupled to a superconducting microwave resonator. Using microwave noise spectroscopy, we determine the electromechanical coupling. Furthermore, the investigation of the nonlinear Duffing regime gives access to the Young's modulus of the nano-beam. We compare our results with finite element modelling corroborating our experimental data. Additionally, we show that our experimental results can be well modelled by standard beam theory. Our technique provides a new way to explore the mechanical parameters of nanomechanical beams and could be extended to other hybrid structures. Financial support via the Nanosystems Initiative Munich is gratefully acknowledged.

TT 101.25 Thu 15:00 P2

Spin relaxation of phosporus donors in silicon at millikelvin temperatures — •Christoph W. Zollitsch[1,2], Felix Hoehne[3], Martin S. Brandt[3], Rudolf Gross[1,2], and Hans Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching — [2]Physik-Department, Technische Universität München, Garching — [3]Walter Schottky Institut, Technische Universität München, Garching

In the field of quantum information processing spin ensembles are promising candidates for quantum memories. To allow for the transfer of quantum information to the memory, the spin ensembles used are typically coupled to a microwave resonator, acting as a quantum bus. Regarding practical realizations, phosphorus dopants in silicon are very attractive due to their long spin coherence times [1,2]. Here, we investigate the coupling between an ensemble of phosphorus donors in silicon and a superconducting coplanar waveguide microwave resonator (CPWR) at temperatures below 1.4 K and study the electron spin resonance (ESR) saturation behavior to extract the relaxation time of the spin system. We find the expected linear dependence of the relaxation time on temperature between 1.4 K and 200 mK [3]. Additionally, we present initial pulsed ESR experiments allowing to access the full dynamics of the system.

Financial support by the DFG via SFB 631 and the Excellence Initiative via NIM is gratefully acknowledged.

[1] A. M. Tyryshkin, Nat. Mater. **11**, 143 (2012)
[2] M. Steger, Science **336**, 1280 (2012)
[3] G. Feher, Phys. Rev. **114**, 1245 (1959)

TT 101.26 Thu 15:00 P2

Entangled photon pairs from three coupled optomechanical cells — •Zhi Jiao Deng[1,2], Steven Habraken[1], and Florian Marquardt[1] — [1]Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen,Germany — [2]Department of Physics, College of Science, National University of Defense Technology,Changsha,China

Optomechanics, which couples light to the mechanical motion of an object, is a very important research field both for fundamental studies of quantum physics and for potential applications. To show features different or superior to the classical counterparts, one major goal in the field of optomechanics is to generate nonclassical states such as squeezed states, entangled states, or states with negative Wigner functions for either or both the optical and mechanical degrees of freedom. In this work, we will discuss on how to generate entangled photon pairs from three coupled optomechanical cells, where each cell consists of a standard optomechanical system and different cells are coupled by photon tunneling. Due to the symmetry of the setup and with the help of mechanical motion, the photons in the driven optical normal mode will be scattered into the other two optical normal modes, where the entangled photon pairs correlated by frequency can be collected. We have investigated the squeezing and entanglement properties of the output light beams, and how these properties would be changed under the influence of the mechanical thermal noise and intrinsic optical losses. Moreover, we find that a suitable choice of parameters can lead to large steady-state entanglement in this proposed setup.

TT 101.27 Thu 15:00 P2

Quasiparticle induced qubit dephasing — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany

We investigate dephasing in superconducting qubits due to quasiparticle tunneling. Contrary to qubit relaxation dephasing cannot be treated with golden rule calculations. Nonetheless one can define a dephasing rate which has to be obtained self-consistently. However, we show that qubit dephasing doesn't obey a simple exponential decay

but has a more complex time dependence.

TT 101.28 Thu 15:00 P2

Fluctuations in the susceptibility of spin systems — •Pablo Schad[1], Boris Narozhny[1], Alexander Shnirman[1,2], and Gerd Schön[2,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Motivated by experiments in the context of 1/f flux noise in SQUIDs and Josephson qubits [1], which is widely attributed to magnetic impurities on the device surfaces [e.g. 2,3,4], we consider fluctuations in the susceptibility of spin systems. We use the Majorana fermion representation for spins [5] and take advantage of generalized relations between spin and Majorana correlators [6]. A path integral formulation allows us to study the role of slow modes and their influence on higher-order correlators, e.g. fluctuations of the spin susceptibility.

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TT 101.29 Thu 15:00 P2

Non-Markovian noninvasive measurements in coupled quantum systems — •Johannes Buelte and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457, Germany

The standard textbook introduction of quantum measurement uses the projection postulate implying a instantaneous collapse of the systems wave function in the measurement process. In many real systems a less invasive measurement is performed by coupling a detector to the measured system for a finite time and with a weak interaction. We investigate the generalized measurement scheme by positive operator-valued measures (POVM) in the weak coupling limit with a focus on a non-Markovian interaction [1]. Such a scheme with memory allows to directly measure nonsymmetrized correlations and is hence related to absorption and emission noise. We calculate the memory function which couples the detector to the system in general and for a harmonic oscillator as detector and discuss the resulting quasiprobabilities, in particular the possible violation of weak positivity [2] by second-order correlation functions.

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TT 101.30 Thu 15:00 P2

Resonance-assisted tunneling of Cooper pairs — •Pierre-Luc Dallaire-Demers and Frank Wilhelm-Mauch — Universität des Saarlandes, Saarbrücken, Deutschland

Superconducting tunnel junctions can be designed to have femtofarad capacitance with their charging energy larger than their Josephson energy E_J. When biased with a constant voltage V below the superconducting gap, the supercurrent starts to oscillate at a frequency $\omega = \frac{2eV}{\hbar}$. If the junction is capacitively coupled to an external electromagnetic environment, a net current appears through the junction as Cooper pairs tunnel and emit photons in the external modes, allowing for the spectroscopy of the environment. We investigate the situation where Cooper pair tunneling is coupled to a perfect LC mode, high order processes such as sequential coherent tunnel events involving many photons and pairs can contribute to the net current, departing significantly from the traditional picture of incoherent tunneling given by $P(E)$ theory. At low temperature, different regimes can be observed varying with the ratio of the mode frequency and the tunneling rate. We present the main diagrams contributing to each of those regimes and compute the asymptotic current in each case. Finally, the full perturbative series in E_J is cast in terms of a $P(E)$ framework in order to extend the method to more general environmental impedances.

TT 101.31 Thu 15:00 P2

Ab-initio calculation of local current-flow in functionalized graphene armchair nano-ribbons — •Jan Wilhelm, Michael Walz, and Ferdinand Evers — Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76133 Karlsruhe, Germany and Institut für Theorie der Kondensierten Materie, D-76128 Karlsruhe, Germany

We calculate the local current density in graphene armchair nanoribbons employing AITRANSS, our DFT-based transport simulation tool. [1,2] The simulations for pristine ribbons indicate that the current flows along streamlines. Neighboring streamlines are separated by stripes of almost vanishing flow. These streamlines form a strongly textured current pattern with gradients that exceed an order of magnitude on the scale of the lattice constant.

Due to the pronounced texture of current flows, the ribbon exhibits a very strong sensitivity to the placing of adsorbates. Backscattering off the adsorbates is strong, if they are located within a streamline and weak, otherwise. We observe that a single adsorbant, e.g., H or OH, when properly placed on the ribbon (width, e.g., 11 carbon atoms) can suppress the current by more than two orders of magnitude.

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TT 101.32 Thu 15:00 P2

Effects of disorder and contacts on transport through graphene nanoribbons — •Andreas Pieper[1], Gerald Schubert[2], Gerhard Wellein[3], and Holger Fehske[1] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17487 Greifswald, Germany — [2]Philips Healthcare, Äyritie 4, 01510 Vantaa, Finland — [3]Regionales Rechenzentrum Erlangen, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study the transport of charge carriers through finite graphene structures. The use of numerical exact kernel polynomial and Green function techniques allows us to treat actual sized samples beyond the Dirac-cone approximation. Particularly we investigate disordered nanoribbons, normal-conductor/graphene interfaces, and normal-conductor/graphene/normal-conductor junctions with a focus on the behavior of the local density of states, single-particle spectral function, optical conductivity, and conductance. We demonstrate that the contacts and bulk disorder will have a major impact on the electronic properties of graphene-based devices.

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TT 101.33 Thu 15:00 P2

Electron dynamics in graphene with gate-defined quantum dots — •Rafael Leslie Heinisch, Andreas Pieper, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald

We study transport through circular graphene quantum dots. We use numerically exact Chebyshev expansion and kernel polynomial methods in the framework of a tight-binding honeycomb lattice model [1]. Thereby, we confirm the scattering resonances and bound states for small dots found in the Dirac approximation. Our focus lies on the regime where individual modes of the electrostatically defined dot dominate the charge carrier dynamics. In particular, we discuss the scattering of an injected Dirac electron wave packet for a single quantum dot, electron confinement in the dot, the optical excitation of dot-bound modes, and the propagation of an electronic excitation along a linear array of dots.

[1] A. Pieper, R. L. Heinisch, and H. Fehske arXiv:1311.6271

TT 101.34 Thu 15:00 P2

Dynamics of Dirac Electrons in a Photon Cavity — •Lisa Hesse, Viktor Krückl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We consider low energy excitations of monolayer graphene embedded in an optical cavity and exposed to a perpendicular constant magnetic field. The influence of an additional radiation field can yield resonant cyclotron transitions of the Dirac fermions of graphene which can be studied using techniques known from cavity quantum electrodynamics. The coupling of cavity photons with condensed matter has been realized in the context of electron gases[1] and very recently also proposed for graphene[2, 3] and therefore opens a new subfield of research in graphene. By considering the interaction of cavity photon modes with Landau quantized states in graphene numerically based on a realistic tight-binding model we aim at clarifying the recent contradicting issue[2, 3] concerning the existance of a superradiant ground state in such systems.

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TT 101.35 Thu 15:00 P2

Phonon-drag thermopower in monolayer and bilayer graphene - significance of flexural phonons — •Eugen Wolf and Dietmar Lehmann — Institut für Theoretische Physik, TU Dresden, 01062 Dresden, Germany

Recent realizations of suspended monolayer graphene (MLG) and bilayer graphene (BLG) samples have enabled a direct probe of their intrinsic properties. It turns out that MLG and its bilayer possess high magnitudes of electron mobility and thermopower, thus promising attractive applications. A detailed study of the (intrinsic) scattering mechanisms, like electron-phonon-interaction, is therefore of large interest. A quite sensitive tool for investigating the coupling of electrons to acoustic phonons is the phonon-drag thermopower S^{g}. In freestanding graphene, electrons couple noticeably not only to in-plane longitudinal and transversal phonons, but also to out-of-plane (flexural) phonons. In our study, we indicate the contribution of flexural acoustic phonons to S^{g} in graphene for the first time. We have calculated S^{g} in doped, suspended MLG and BLG as function of temperature for different carrier densities by using a generalized Cantrell-Butcher formalism up to 2-phonon processes. Electron-phonon coupling by a screened deformation potential (proportional to the local contraction or dilatation of the lattice) as well as by an effective gauge field (induced by changes in bond length and bond angle between the carbon atoms) are included. We find that for reasonable coupling constants the electron scattering by out-of-plane phonons below 10 K cannot be neglected, especially for MLG.

TT 101.36 Thu 15:00 P2

Magnetic impurities at the edge of a two-dimensional topological insulator — •Johanna Kleinen, Markus Garst, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Germany

We investigate the effect of a magnetic impurity in a helical Luttinger liquid representing the edge states of a two-dimensional topological insulator. Analyzing the renormalization group flow in the presence of Kondo- as well as Rashba-interactions, we find that the magnetic impurity always couples strongly to the spin-polarized electrons. Moreover, we identify, in principle, two strong-coupling fixed-points with completely different transport characteristics. The magnetic impurity might either be Kondo-screened and only forward-scattering the electrons or it could develop into a strong backscatterer effectively inhibiting transport along the edge.

TT 101.37 Thu 15:00 P2

Electronic correlations in bulk Bi-chalcogenide topological insulators and elemental bismuth — •Luis Craco[1] and Stefano Leoni[2] — [1]Instituto de Fisica, Universidade Federal de Mato Grosso, 78060-900, Cuiaba, MT, Brazil — [2]School of Chemistry, Cardiff University, Cardiff, CF10 3AT, UK

In recent years three-dimensional (3D) topological insulators (TIs) have attracted great fundamental interest as systems that can lead to new phases of quantum matter. Theoretical and experimental work have revealed that intrinsic spin-orbit (SO) coupling can drive qualitative new effects on the electronic structure of Bi-chalcogenide p-band systems in general. In this poster, we present our recent work on electronic structure and transport properties of bulk Bi_2Se_3 [1] and Bi_2Te_2Se [2] TIs. We will also revisit the long-standing issues of transport and magnetoresistance responses in elemental bismuth [3]. Basing ourselves on LDA+DMFT calculations we show that the interplay between SO and multi-orbital Coulomb interactions has quantitative new effects in their semimetal electronic structure. We show, for example, why the intricate interplay between local Coulomb and SO interaction promotes a spin-orbit Kondo state in elemental bismuth. Taken together our work represents a realization of complex dynamical correlation effects in p-band semimetals and in bulk Bi-chalcogenide TIs.
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TT 101.38 Thu 15:00 P2

Transition between n-type and p-type transport in MBE-grown topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films — Tobias Merzenich[1], •Melissa Schall[1], Christian Weyrich[1], Igor E. Batov[1,2], Gregor Mussler[1], Jörn Kampmeier[1], Yulieth Arango[1], Jürgen Schubert[1], Thomas Schäpers[1,3], and Detlev Grützmacher[1] — [1]Peter Grünberg Institute (PGI-9), Research Centre Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia — [3]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

We report on the transition between n-type and p-type conduction in the ternary compound $(Bi_{1-x}Sb_x)_2Te_3$ $(0 < x < 1)$ films grown by molecular beam epitaxy. They were grown on silicon on insulator (SOI) substrates with Si(111)-top layer harbouring. A top-gate was used to deplete the intrinsic n-doped bulk. By performing Hall measurements on several samples with varying x, we obtain a change of sign of the Hall resistivity at $x = 0.43$. This is attributed to compensation effects. For samples with $x < 0.43$ we obtain a n-type conduction, i.e. an electron transport, whereas samples with $x > 0.43$ show a p-type conduction, i.e. a hole transport. This transition is an evidence that the Fermi energy is initially located above the conduction band edge and is shifted into the valence band for higher Sb concentration.

TT 101.39 Thu 15:00 P2

Transport simulations of nanowires hosting Majorana Bound States — •Felix Weiner and Peter Schmitteckert — Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

Semiconductor nanowires with proximity-induced s-wave superconductivity and spin-orbit coupling have been shown theoretically to host Majorana Bound States (MBS) on the boundaries of topological segments. The unambiguous identification of these states in experiments is still an ongoing challenge. Several groups have reported the observation of a zero-bias peak in the differential conductance of tunneling experiments, which hints at the existence of a MBS at the end of the wire. We investigate numerically the transport properties of inhomogenous nanowires by means of wavepacket evolution. The aim is to address open questions regarding the I-V characteristic such as the signature of the excitation gap, which is expected to close when passing through the topological phase transition.

TT 101.40 Thu 15:00 P2

Real time dynamics of Majorana bound states — •Michael Sekania[1], Felix Weiner[2], Ronny Thomale[1], and Peter Schmitteckert[2] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

Majorana fermions have been attracting substantial interest during recent years. Considerable attention is devoted to the robust and unambiguous probing of Majorana bound states and the error-tolerant manipulations of them, particularly in the view of possible applications in topological quantum computing. Here we present the investigation of the real-time dynamics of the Majorana bound states in different lattice geometries and discuss application of the real-time simulations in a context of braiding of Majorana fermions.

TT 101.41 Thu 15:00 P2

Majorana Fermions: Anholonomy of Bound States — •Sourin Das[1] and Indu Satija[2] — [1]MPIPKS, Dresden, Germany & University of Delhi, India — [2]Department of Physics and Astronomy, George Mason University, USA

Majorana modes in p-wave superconducting quantum wires are shown to result in exotic quantum holonomy of both the eigenvalue and the eigenstates. Induced by a degeneracy hidden in complex Bloch vector space, Majorana bound states are characterized by Kohn branch point (also known as exceptional points) singularities leading to Mobius strip-like structure of the eigenspace. This may provide yet another elegant framework to characterize topological aspect of Majorana detection in p-wave superocndcutor. This topological characterization is shown to be valid also for the periodically driven superconducting wires that supports two species of Majorana.

TT 101.42 Thu 15:00 P2

Majorana fermions at the quantum spin Hall edge —

Shuo Mi[1], Dimitry Pikulin[1], •Michael Wimmer[1,2], and Carlo Beenakker[1] — [1]Universiteit Leiden, The Netherlands — [2]TU Delft, The Netherlands

One of the earliest proposals for Majorana fermions in condensed matter systems involves quantum spin Hall (QSH) insulators [1]. In fact, Majorana fermions appear naturally if QSH insulators are coupled to superconductors, and are in this setting also inherently more stable than for example the now very popular proposal of obtaining Majorana fermions in semiconducting nanowires.

Yet, the proposals for Majorana fermions in QSH always involved elements (magnetic insulators, or very strong magnetic fields) that pose experimental problems. Here, we present a much simpler setup involving only gates and a weak magnetic field that will allow for an unambiguous signature of Majorana fermions in this system. In addition, we explain how to prove the non-Abelian statistics in a QSH setup [2].

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TT 101.43 Thu 15:00 P2

Stability of Majorana metals — •Kevin O'Brien and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The topological nature of exotic quantum states with non-Abelian vortices, such as $p_x + ip_y$ superconductors, the Moore-Read quantum Hall state or certain heterostructures of topological insulators and s-wave superconductors, can be discussed in terms of Majorana fermion zero modes. If the non-Abelian vortices hosting these zero modes form a regular triangular lattice – a natural situation for an Abrikosov lattice in a superconductor or a Wigner crystal in the context of quantum Hall liquids – the corresponding model of Majorana fermions hopping on a triangular lattice becomes particularly tractable. In terms of symmetry classification, such a Majorana model is in class D and allows for three types of ground states – a trivial insulator, a Chern insulator and a thermal metal state. While the Chern insulator is found for uniform hopping [1], sufficiently strong sign-disorder in the hopping amplitudes will drive the system into the thermal metal state [2].

Here we investigate the stability of this thermal metal state when introducing an additional level of disorder – random bond or site depletion of the underlying triangular lattice. In particular, we are interested in addressing whether the thermal metal state is stable up to the respective percolation threshold of site/bond disorder.

First results will be discussed on this poster.

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TT 101.44 Thu 15:00 P2

Absorption and transport properties of quantum aggregates with heavy-tailed disorder — •Sebastiaan Vlaming[1], Sebastian Möbius[1], Victor Malyshev[2], Jasper Knoester[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Centre for Theoretical Physics and Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Molecular aggregates exhibit extraordinary absorption properties, depending on their geometrical conformation and inter-monomeric coupling. The narrowing of the absorption band for J-aggregates can be well described by diagonal Gaussian static disorder for individual site energies. Aggregates consisting of large molecules are usually embedded in complex environments, making it impossible to separate individual contribution to the energy fluctuations.

Recent developments in generating and trapping highly excited Rydberg atoms, allow for quantum simulations of molecular aggregates. We show that by controlling the environment, e.g. a polar background gas, non-Gaussian static disorder can be studied. We analyze how the environment generates disorder distributions with heavy tails, so called Lévy-stable distributions, and discuss novel effects in Lévy disordered systems such as broadening of the absorption bandwidth [1] as well as a subdiffusive exciton transfer.[2]

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TT 101.45 Thu 15:00 P2

Full counting statistics of energy dissipated by a driven two level system — •Philip Wollfarth[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Within the last decades fluctuation relations[1-4] have been established. Recent experiments have shown the validity of such fluctuation relations for entropy production in the microscopic regime[5]. However the extension of fluctuation relations of heat and work to the quantum regime is still under discussion, since non-ambiguous definitions for heat and work have not yet been established. In this context we consider the statistics of energy emitted by a driven two level system into a bosonic bath using the full counting statistics technique.

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