TT 42: Other Transport Topics

Time: Wednesday 9:30–12:45 Location: HSZ/0105

TT 42.1 Wed 9:30 HSZ/0105

Enhancement of the thermopower of Anderson impurity by Van Hove singularities in graphene nanoribbons — •Damian Krychowski and Krzysztof Wójcik — Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland

We present results from the numerical renormalization group theory of spin-1/2 ad-atom coupled to contacts made of zigzag graphene nanoribbons (ZGNRs). We propose tuning ZGNRs with a transverse electric field [1] and back gates such that they exhibit one of their asymmetric power-law Van Hove singularities at the Fermi level. We demonstrate that, under these conditions, the local spectral density of the ad-atom spin exhibits a sharp and asymmetric pseudo-gap despite complete Kondo screening. This ensures weak charge conductance and a large Seebeck coefficient at low and moderate temperatures, leading to a high figure of merit over a wide temperature range and impurity energy level. A similar enhancement of the Seebeck coefficient is observed in magic-angle twisted bilayer graphene with a highly particle-hole asymmetric band, though it occurs at a different energy scale [2]. At a set temperature, the sign of thermopower of Kondo-correlated system can be further tuned by dragging the singularity through the Fermi level with gate voltage.

[1] Y.-W. Son, M. L. Cohen and S. G. Louie, Nature 347, 444 (2006).
[2] A. K. Paul et al., Nat. Phys. 18, 691 (2022).

TT 42.2 Wed 9:45 HSZ/0105

Dynamical current as a spin-state discriminator in open-shell GNR's — •Nico Leumer[1], Geza Giedke[2], and Thomas Frederiksen[2] — [1]Wrocław Tech — [2]Donostia International Physics Center

The recent advances of surface synthesis unlocked the potential of open-shell physics in graphene nanoribbons (GNRs) which ever since have gained significant attention. Normally chemically unstable, these structures feature unpaired, localized p_Z-electrons pinned at zero energy, giving rise to the unique phenomenon of π-magnetism. At half-filling certain GNRs host quasi degenerate spin singlets/triplets states with a vanishing energy gap for long ribbons and without significantly increasing the gap conventional current-based measurements hardly distinguish these spin textures.

In our setup charge current $I(t)$ discriminates between the responsible states –even for a vanishing gap– by means of a Spin-Pauli blockade (SPB). We discuss how our setup preserves the states, how their distinct spatial profile causes different charging energies and such that a variation of the reservoirs chemical potentials allow the isolation of singlet/triplet signals.

Rather than considering only ensembles of measurements or repetitions, our setup allows for single-shot experiments simulated by Monte-Carlo trajectories. From relative frequencies, we estimate overhaul time-scale $\Delta t = 6\hbar/\Gamma$ for a successful identification of the spin. For experiments on shorter time scales, we report on the fidelity and the necessary time for a confident identification of the state.

TT 42.3 Wed 10:00 HSZ/0105

Single Spin-Flip Dynamics in the Ising Model — •Luca Cervellera, Fred Hucht, and Björn Sothmann — University of Duisburg-Essen, Duisburg, Germany

We investigate the real-time spin-flip dynamics of the 1D Ising model by means of waiting time distributions between subsequent spin flips. At large temperatures the waiting time distribution shows an exponential decay due to thermal excitation and relaxation of spins. At low temperatures, the waiting time distribution is dominated by an algebraic decay caused by domain wall motion. The latter can be suppressed by an external magnetic field. Our results are relevant to understand the dynamics of dimer flipping on the Si(001) surface [1].

[1] C. Brand et al., Phys. Rev. Lett. **130**, 126203 (2023).

TT 42.4 Wed 10:15 HSZ/0105

Universal relations between thermoelectrics and noise in mesoscopic transport across a tunnel junction — •Andrei Pavlov[1] and Mikhail Kiselev[2] — [1]TKM, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151 Trieste, Italy

We develop a unified theory of weakly probed differential observables for currents and noise in transport experiments. Our findings uncover a set of universal transport relations between thermoelectric and noise properties of a system probed through a tunnel contact, with the Wiedemann-Franz law being just one example of such universality between charge and heat currents. We apply this theory to various quantum systems, including multichannel Kondo, quantum Hall and Sachdev-Ye-Kitaev quantum dots, resonant impurity and two-stage Kondo models, and demonstrate that each of the microscopic theories is characterized by a set of universal relations connecting conductance and thermoelectrics with noise. Violations of these relations indicate additional energy scales emerging in a system.

TT 42.5 Wed 10:30 HSZ/0105

Relaxation to persistent and oscillating currents in simply and doubly frustrated spin systems coupled to fermionic baths — •Nikodem Szpak[1], Gernot Schaller[2], Ralf Schützhold[2,3], and Jürgen König[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We study relaxation dynamics in a strongly-interacting three and four-site Fermi-Hubbard system (quantum dots) coupled to environment represented by fermionic baths. We analyze the simply frustrated (trimer) and doubly frustrated (tetrahedron) spin geometries to observe the relaxation to steady states containing persistent or oscillating spin currents. Due to high sensitivity of these results to the coherence of the final state, we can test several variants of the Lindblad master equations, derived under different assumptions and parameter regimes: local and global, secular and coherent.

[1] E. Kleinherbers, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 101, 125131 (2020)
[2] G. Schaller, F. Queisser, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 105, 115139 (2022)
[3] N. Szpak, G. Schaller, R. Schützhold and J. König, Phys. Rev. B 110, 115131 (2024)

TT 42.6 Wed 10:45 HSZ/0105

Fluctuation Spectroscopy and Filament Simulations on HfO_2 RRAM devices — •Demian Ranftl[1], Yingxin Li[2], Tristan Stadler[1], Eszter Piros[2], Philipp Schreyer[2], Taewook Kim[2], Lambert Alff[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University, Frankfurt am Main, Germany — [2]Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Low-frequency noise spectroscopy plays a crucial role in understanding resistive switching mechanisms and filament dynamics in RRAM devices [1]. In this work, we compare the noise characteristics of undoped [2] and La-doped [3] HfO_2-based devices across multiple resistance states and during DC cycling. Measurements are complemented by phenomenological simulations that assume various states of a stable filament with differing amounts of surrounding defects. The results provide new insights into the roles of filament geometry and defect densities on resistance and noise behaviour. We identify multi-stage resistance-noise scaling relationships, highlighting the competition between trap numbers and system size. These findings offer deeper insight into switching dynamics and the role of doping in modulating noise sources, contributing to the optimisation of RRAM configurations for neuromorphic applications.

[1] J. Müller, Contemporary Physics **29** (2025)
[2] P. Schreyer, N. Kaiser *et al.*, ACS Appl. Mater. Interfaces (2025)
[3] T. Kim, M. Major *et al.*, Adv. Electron. Mater. (2025)

15 min. break

TT 42.7 Wed 11:15 HSZ/0105

Symmetry breaking in the non-degenerate parametric oscillator — •Jonathan Schluck, Steven Kim, and Fabian Hassler — Institute for Quantum Information, RWTH Aachen University, 52074 Aachen, Germany

Two harmonic oscillators that are parametrically driven at the sum of their natural frequencies exhibit an instability once the driving

strength exceeds the damping. Close to and beyond this instability threshold, nonlinearities must be taken into account. As a consequence of the instability, the system develops a separation of time scales, which can be used to derive an effective Liouvillian describing the long-time dynamics. The effective model possesses a U(1)-symmetry akin to that of a laser. Above the transition, a symmetry-broken state with a fixed phase exhibits an extended lifetime, indicating the symmetry breaking. The phase coherence of this state increases with increasing photon number, following the conventional Schawlow-Townes limit. We propose a measure of symmetry breaking that compares the photon lifetime to the dephasing time in the lasing regime.

TT 42.8 Wed 11:30 HSZ/0105

Reconfigurable Optoelectronics at the Single-Molecule Level — •Atif Ghafoor — Department of Physics, Nanoscience Center, University of Jyväskylä, Jyväskylä, Finland.

Controlling exciton and its coupling at the single-molecule scale is a fundamental challenge for nanoscale optoelectronics and quantum technologies. The ability to precisely reposition individual atom within a single-molecule to alter transition dipole moment, thereby enabling on-demand switching of light emission, remains an unrealized yet transformative goal in single-molecule optoelectronics. Here, by displacing the central metal atom of a planar phthalocyanine molecule adsorbed on decoupling layer, we demonstrate active control over its transition dipole moment, leading to suppression or enhancement of light emission via scanning tunneling microscopy-induced luminescence. Through this atomic-scale control, we designed a tunable homogenous dimer in three distinct optical states: a non-emissive state, a single-molecule-like emissive state, and a coupled state (subradiant and superradiant modes) directly revealing intermolecular dipole-dipole coupling. Furthermore, we realized a heterodimer, in which resonant energy transfer can be switched on or off simply by controlling the dipole of the acceptor molecule. Our strategy for manipulating transition dipole moment and optical emission, not only enables deeper exploration of plasmon-exciton coupling, tunable dipole-dipole interaction, and tunable energy transfer dynamics at the single-molecule level but also stimulates the development of single-molecule quantum engineering and atomically reconfigurable optoelectronic devices.

TT 42.9 Wed 11:45 HSZ/0105

Negative electronic friction and non-Markovianity in charge transport through molecular nanojunctions — •Riley Preston[1], Samuel Rudge[1], Daniel Kosov[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg — [2]College of Science and Engineering, James Cook University

The electronic friction approach is a popular mixed quantum-classical method for modeling the dynamics of atoms and molecules at metal or semiconductor surfaces. If the electrons are far from equilibrium, such as in molecular nanojunctions at high bias voltages, the electronic friction coefficient can become negative, meaning it acts to amplify the nuclear vibrations in the molecular bridge rather than dampen them, triggering bond rupture and a loss of device functionality. The physicality of negative electronic frictions has long been debated, owing to the hierarchy of underlying assumptions upon which the electronic friction method is built. We investigate the emergence of negative electronic friction in a donor-acceptor model of a molecule in a molecular nanojunction. We observe that negative electronic frictions arise predictably at high bias voltage according to the geometry of the donor and acceptor on the molecular bridge, resulting in large vibrational excitations that are validated by comparison to numerically exact quantum data calculated with the hierarchical equations of motion approach. However, we also show that the same physical conditions that give rise to negative electronic friction are also suggestive of non-Markovian dynamics, challenging the underlying assumptions of the electronic friction approach.

TT 42.10 Wed 12:00 HSZ/0105

Vibrational Instabilities in Molecular Nanojunctions - The Role of Anharmonic Nuclear Potentials — •Martin Mäck, Samuel Rudge, Riley Preston, and Michael Thoss — Institute of Physics, University of Freiburg

Current-induced vibrational excitation is a key factor determining the stability of molecular nanojunctions. Beyond conventional Joule heating, a different mechanism caused by nonconservative current-induced forces has been reported for models with multiple vibrational modes, leading to vibrational instabilities already at low bias voltages [1].

So far, this mechanism has only been investigated for harmonic nuclear potentials [1,2]. A natural question, is whether this effect can also be observed in more realistic models with anharmonic potentials and if it has a measurable impact on observables such as the dissociation probability of the junction. In this contribution, we apply a mixed quantum-classical approach based on electronic friction and Langevin dynamics [2,3] to different anharmonic model systems, studying the influence of anharmonicity on the reported instability and the dissociation dynamics of the junction. The results show that, in our models, anharmonic nuclear potentials destroy the mechanism leading to vibrational instabilities.

[1] J.-T. Lü, M. Brandbyge, P. Hedegård, T.Todorov, D. Dundas, Phys. Rev. B **85**, 245444 (2012)
[2] M. Mäck, M. Thoss, S. Rudge, Phys. Rev. B **112**, 075430 (2025)
[3] R. J. Preston and D. S. Kosov, J. Chem. Phys. **158**, 224106 (2023)

TT 42.11 Wed 12:15 HSZ/0105

Thermodynamic and kinetic uncertainty relations in topological surface states — •Phillip Mercebach[1], Pablo Burset[1], and Sun-Yong Hwang[2] — [1]Department of Theoretical Condensed Matter Physics and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Theoretische Physik, Universitat Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Strong fluctuations in nanoscale devices can hinder output precision, while the unavoidable entropy production is detrimental to performance. Device operation can be optimized to achieve a strong output signal while minimizing noise, entropy, and frenesy. However, there are fundamental constraints between the output and these drawbacks: the thermodynamic uncertainty relation (TUR) quantifies the trade-off between signal-to-noise ratio (SNR) and entropy, while the kinetic uncertainty relation (KUR) describes the trade-off between SNR and frenesy. Both relations are especially interesting as quantum coherent processes can yield output precisions surpassing classical limits. Here, we study TUR and KUR in a ballistic junction comprised of a 3D topological insulator (3DTI) in proximity to a ferromagnet. The 3DTI surface states, in combination with the ferromagnet, enable near-Carnot efficiency, indicating low entropy production [1]. We demonstrate that the SNR in this device becomes very high at optimum temperatures and voltage bias, where the thermal and shot noises are rather suppressed.

[1] P. Mercebach et. al., arXiv:2508.20969

TT 42.12 Wed 12:30 HSZ/0105

Electromagnetic chiral anisotropy of the semiconducting $LaRhC_2$-enantiomorphs — •Volodymyr Levytskyi[1], Ulrich Burkhardt[2], Markus König[2], Eteri Svanidze[2], Yuri Grin[2], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

In past decades, the majority of research is focused on chiral crystalline solids due to their non-trivial spin and charge transport properties. However, the preparation of mono-chiral samples is a complicated task – perhaps explaining why the influence of chirality on electrical properties has remained almost unexplored. EBSD (electron backscatter diffraction) -based enantiomorph distribution maps allow the extraction and shaping of suitable microdevices from polycrystalline material by the FIB (focused ion beam) micropreparation method. Here, we present results on the electrical transport studied on the mono-chiral, crystallographically oriented, single-crystalline $LaRhC_2$ (space groups $P4_1$ or $P4_3$) microdevices. Significant anisotropy of the electrical resistivity is observed for each enantiomorph, both parallel to and normal to the fourfold screw axis. The different linear coefficients of the longitudinal magnetoresistivity probed along the fourfold screw axis for the nonmagnetic right-handed (4_1-axis) and left-handed (4_3-axis) $LaRhC_2$ crystals in the oriented magnetic field parallel and antiparallel to the current flow direction (*dc* regime), confirm the electromagnetic chiral anisotropy (eMChA) – a rarely studied effect.