TT 16: Poster: Transport

Time: Monday 15:00–18:00 Location: P2/OG4

TT 16.1 Mon 15:00 P2/OG4

Asymmetric and spatially resolved power dissipation in quantum transport — •Nico Leumer — Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Dissipation is a natural byproduct of quantum transport caused by various inelastic scattering events of electrons and their lost energy stimulates in turn the temperature profile of the underlying bulk material. Importantly though, electronic current may run only through a narrow part of the sample as, for instance, happens in the quantum Hall regime of graphene due to chiral edge channels (1); thus, dissipation has to be seen as a local quantity. The still rather recent invention of the Squid-on-tip technique in 2016 (2), paved the way to experimental access this challenge, where the temperature increases by merely a few hundred micro Kelvin on length scales of the order of nanometers.

Quantum point contacts (QPC's) are of particular interest in nanoscale transport, as electrons experience now a -perhaps energy dependent- transmission probability. On a hand waving level, QPC's increase the resistance electrons face from the sample locally, which is accompanied by areas of higher dissipation. In our recent project, we predict where and how much power is dissipated.

[1] A. Marguerite et al., Nature 575, 628 (2019)
[2] D. Halbertal et al., Nature 539, 407 (2016)

TT 16.2 Mon 15:00 P2/OG4

Resistive switching and peculiarities of conductivity of $TiTe_2$ point contacts — •Oksana Kvitnitskaya[1], Luminita Harnagea[2], Dmitri Efremov[3], Bernd Büchner[3,4], and Yurii Naidyuk[1] — [1]B.Verkin Institute for Low Temperature Physics and Engineering, NASU, Kharkiv, Ukraine — [2]Dep. of Physics, Indian Institute of Science Education and Research, Pune, Maharashtra, India — [3]Institute for Solid State Research, IFW Dresden, Dresden, Germany — [4]Institut für Festkörper- und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany

Ti-based dichalcogenides TiX_2 (X - S, Se, Te), display a variety of physical properties, depending on their lattice distortions, native defects, self-doping effects, intercalation, external pressure. They can exhibit semiconducting, semimetallic, CDW, and superconducting behavior, which together with their layered structure and unique properties upon exfoliation to monolayer limit, make them particularly interesting. Recently, we observed the resistive switching effect in $TiTe_2$ point-contacts (PCs). We attributed the effect to Se vacancy drift due to a high electric field in the PC core. Here we report the resistive switching in PCs with isoelectronic $TiTe_2$, where the ratio of the high resistance state to the low resistance state was so far up to several times, contrary to up to two orders of magnitude for $TiSe_2$. Additionally, we observed "camel-like" $dV/dI(V)$ spectra of $TiTe_2$ at helium temperature with two symmetric *vs* V=0 humps around +/-(200-300) mV, which vanished near 200 K.

TT 16.3 Mon 15:00 P2/OG4

Nonmonotonous Temperature Dependence of the Thermopower of Gold Atomic Contacts — Thomas Möller[1], •Marcel Strohmeier[1], Ruben Zerfass[1], Kim Nikolai Kirchberger[1], Danial Majidi[2], Juan Carlos Cuevas[3], Johannes Boneberg[1], Paul Leiderer[1], Wolfgang Belzig[1], and Elke Scheer[1] — [1]University of Konstanz, 78457 Konstanz, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38042 Grenoble, France — [3]Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We present measurements of the thermopower of atomic-size gold contacts realized by the mechanically controllable break junction (MCBJ) technique over a temperature range from 10 K to 295 K. While the conductance histograms confirm the quantum nature of the transport, we observe a non-monotonous temperature dependence of the ensemble-averaged thermopower (taking into account contacts between 1 and 20 $G_0 = 2e^2/h$) with a minimum of -2 μV/K at about 150 K. Our observations at low and high temperature are compatible with values reported in the literature [1-5], but the non-monotonous behavior in between disagrees with the expected linear increase of the thermopower for quantum coherent conductors described by the Landauer formula. We discuss several possible mechanisms, that may be at the origin of the deviation, such as phonon contributions or an energy-dependent transmission function. Both aspects can be addressed experimentally by analyzing current-voltage characteristics. We present here results obtained for Au and for Cu atomic contacts.

TT 16.4 Mon 15:00 P2/OG4

Analyzing vibrational instabilities arising from non-conservative current-induced forces in nanosystems with a semi-classical approach — •Robin L. Grether, Samuel Rudge, and Michael Thoss — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Deutschland

Understanding the electric properties of nanosystems such as molecular junctions is a crucial task for modern physics. For molecular junctions, these properties are often governed by an electronic-vibrational coupling, which can lead to an instability of the junction in some cases.

We provide an in-depth analysis of the vibrational instabilities caused by non-conservative current-induced forces in a molecular junction using a semi-classical approach that exploits the time-scale separation between the fast electronic dynamics and the much slower vibrational dynamics. In particular, we use a Born-Markov master equation for the electronic degrees of freedom in combination with a semi-classical Langevin equation for the vibrational dynamics [1]. Within this framework, we study the dynamics of a junction composed of two electronic levels and two harmonic vibrational modes [2] for various parameters.

[1] W. Dou *et al.*, J. Chem. Phys. **145**, 054102 (2016)
[2] J.-T. Lü *et al.*, Phys. Rev. B **85**, 245444 (2012)

TT 16.5 Mon 15:00 P2/OG4

Full counting statistics of electron transport through periodically driven quantum dots analysed with factorial cumulants — •Johann Zöllner, Eric Kleinherbers, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

The electron transport through quantum dots is a stochastic process. Factorial cumulants of full counting statistics can be used to analyse current and current fluctuations of electrons [1]. We present methods to calculate factorial cumulants for periodically driven systems. This makes it possible to investigate effects in which a periodic drive and noise both take part. An example for such an effect is stochastic resonance, which has already been observed in quantum dots [2]. We will explain the meaning of factorial cumulants for stochastic resonance.

[1] P. Stegmann, B. Sothmann, A. Hucht, J. König, Phys. Rev. B 92, 155413 (2015)
[2] T. Wagner, P. Talkner, J. C. Bayer, E. P. Rugeramigabo, P. Hänggi, R. J. Haug, Nat. Phys. 15, 330(2019)

TT 16.6 Mon 15:00 P2/OG4

Rational design of halide perovskite-based quantum dots using ab-inotio many body techniques — •Manaswita Kar, Benjamin Lenz, and Michele Casula — IMPMC, Sorbonne Université-CNRS, Jussieu, 75005 Paris, France

Quantum dots (QDs) have attracted increasing attention as next generation functional materials, because of their unique size dependent colour tunability, due to quantum-confinement effect. However, the cost of production of these QDs is very high, thereby limiting their large scale industrial applications. Halide perovskite-based QDs provide single photon emission at room temperature and can be manufactured comparatively easily. These perovskites have a complex structural form and bears a large compositional space. As a result of this, only a limited number of these perovskite QDs have been tested so far. Here, we aim to identify the most promising perovskite based QDs for coherent photon emission applications by characterising their optical properties from theoretical simulations. Towards this aim, we employ the many body Green's function (GW) and Bethe-Salpeter equation (BSE) techniques to study the excited state properties of the QDs, which are known to be not well captured by standard ground state methods, such as Density Functional Theory (DFT). From this study, we finally envision find the best halide perovskite based quantum dot, that is both structurally and thermodynamically stable and can be manufactured for large scale commercial applications.

TT 16.7 Mon 15:00 P2/OG4

Device and contact engineering of MoS_2 nanotubes and nanoribbons — •Konstantin D. Schneider[1], Robin T. K. Schock[1], Jonathan Neuwald[1], Matthias Kronseder[1], Luka Pirker[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Institute Jožef Stefan, 1000 Ljubljana, Slovenia

Even though low-temperature transport measurements of a MoS_2 nanotube have already demonstrated Coulomb blockade at 300 mK,[1] Fermi level pinning near the conduction band at the metal-MoS_2 interface requires reactive low-work function metals, which then damage the MoS_2. Recently, bismuth[2] was shown to drastically reduce contact resistances in planar MoS_2.

Here, we present millikelvin transport measurements on MoS_2 nanotubes and nanoribbons with bismuth contacts.[3] Our nanotubes are grown via a chemical transport reaction, yielding diameters down to 7 nm and lengths up to several millimeters. Nanotubes were either suspended or placed on hexagonal boron nitride (hBN) in order to reduce disorder from the SiO_2 substrate. The resulting devices show Coulomb blockade, with a rich set of features. Contacts are transparent, and the temperature dependence hints at single level transport.

[1] S. Reinhardt *et al.*, Phys. Stat. Sol. RRL **13**, 1900251 (2019)
[2] P. C. Shen *et al.*, Nature 593, **211** (2021)
[3] R. T. K. Schock *et al.* arXiv:2209.15515

TT 16.8 Mon 15:00 P2/OG4

Weak localization in semiconductor heterostructures with strong spin orbit interaction — •Simon Feyrer, Jaydean Schmidt, Michael Prager, Dominique Bougeard, and Christoph Strunk — Institute of Experimental and Applied Physics, University of Regensburg, Germany

We present measurements of weak localization (WL) and weak antilocalization (WAL) performed on quasi-1D wires patterned into an InAs based quantum well. Due to the confinement of the electrons along the wires, the D'yakonov-Perel spin relaxation is expected to be suppressed resulting in WL instead of WAL. As consequence of the spin orbit interaction anisotropy, the amplitude of the WL is sensitive to the direction of an applied in-plane magnetic field and provides an estimate of the ratio between the Rashba and Dresselhaus spin orbit coefficient [1,2].

By fitting the measured WAL and WL-curves, the highest spin relaxation rate was extracted for the wires orientated along the $[01\bar{1}]$ crystal axis. A clear suppression of spin relaxation was observed along the [001] wire direction.

[1] T. Nishimura et al., Phys. Rev. B **103**, 094412 (2021)
[2] A. Sasaki et al., Nat. Nanotechnol. **9**, 703 (2014)

TT 16.9 Mon 15:00 P2/OG4

Revealing the role of Klein tunneling in Aharanov-Bohm graphene rings — •Ching-Hung Chiu and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan City, Taiwan

Graphene, the ideal testbed of relativistic quantum mechanics, have been widely used to explore not only the exotic transport properties of Dirac fermions but also to confirm classic quantum-mechanical phenomena such as the Aharanov-Bohm effect. Motivated by a recent experiment [1], here we perform quantum transport simulations in the ballistic limit at zero temperature, considering an Aharanov-Bohm ring made of graphene with the same sample and gate geometry as the experiment. Preliminary properties from our simulations such as the gate and magnetic field dependence of the two-terminal conductance are rather consistent with the experiment, confirming their claim of the observed Aharanov-Bohm effect. To probe the effect of Klein tunneling, however, we propose a modified design using a local gate that makes pn interfaces perpendicular to the arm of the ring, different from the experiment. Based on our new design, we show that Klein tunneling may sharpen the Aharanov-Bohm oscillation frequency due to the screening of the transverse modes.

[1] J. Dauber et al., arXiv:2008.02556v3

TT 16.10 Mon 15:00 P2/OG4

Transport properties of pn junctions in 2D materials: Graphene vs MoS_2 — •Yu-Ting Xiao and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Graphene and monolayer MoS_2 both belong to the family of 2D materials. The former is known as a Dirac semimetal where electrons behave like relativistic Dirac fermions due to the gapless energy band linear in momentum, while the latter shows typical semiconducting behaviors due to the gapped energy band quadratic in momentum, with which electrons behave as standard Schrödinger fermions. In terms of transport, Dirac and Schrödinger electrons exhibit distinct behaviors, among which the so-called Klein tunneling [1] is perhaps one of the best known. To further identify their difference in transport properties, here we perform quantum transport simulations for pn junctions in various 2D systems, including graphene, MoS_2, and other toy models for 2D semiconductors. Our results identify transport properties that are unique to Dirac fermions as well as those that do not significantly differ from the two.

[1] M. Katsnelson, K. Novoselov, and A. Geim, Nat. Phys. 2, 620 (2006)

TT 16.11 Mon 15:00 P2/OG4

Quantum transport simulation for graphene devices with sawtooth-shaped n-p-n junctions — •Zhe-Bin Hsu and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Graphene, a gapless two-dimensional semimetal made of carbon atoms arranged in a honeycomb lattice, is an ideal platform for studying electron optics both experimentally and theoretically. Because of its lack of energy gap, n- and p-type carriers in graphene can be easily tuned simply by electrical gating. Typical graphene n-p-n junctions are created by local gates of rectangular shapes that exhibit Fabry-Pérot interference of electron waves in the clean limit. A recent experiment [1] realized a Dirac fermion reflector of graphene using sawtooth-shaped npn junctions, reporting not only the suppressed Fabry-Pérot interference but also resistance enhancement. Motivated by this experiment, we perform quantum transport simulations for graphene considering similar gate and sample geometries. Good consistency between our simulation and the experiment [1] will be shown. Further tests on other shaped top gates are performed in order to find the optimal gate geometry for best enhanced resistance. Our work shows that sawtooth-shaped graphene n-p-n junctions cannot work as a field-effect transistor (FET), even though the transmission can be reduced by a certain amount.

[1] S. Morikawa et al., Semicond. Sci. Technol. 32, 045010 (2017)

TT 16.12 Mon 15:00 P2/OG4

Electron correlation and confinement effects in quasi-one-dimensional quantum wires at high-density — Ankush Girdhar[1], Vinod Ashokan[1], Neil Drummond[2], •Klaus Morawetz[3,4], and Kare Narain Pathak[5] — [1]Department of Physics, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar (Punjab), 144 011, India — [2]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom — [3]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [4]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [5]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India

The correlation energy, pair-correlation function, static structure factor, and momentum density of ferromagnetic quasi-one-dimensional quantum wires are calculated using the quantum Monte Carlo (QMC) method for various wire widths b and density parameters r_s. The peak in the static structure factor at $k = 2k_F$ grows as the wire width decreases. The Tomonaga-Luttinger liquid parameter K_ρ is found to increase by about 10% between wire widths $b = 0.01$ and $b = 0.5$. The ground-state properties of finite thickness wires is compared to the first-order random phase approximation (RPA), which is exact in the high-density limit. Analytical expressions for the static structure factor and correlation energy are derived.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] Phys. Rev. B 101 (2020) 075130
[4] Phys. Rev. B 104 (2021) 035149
[5] Phys. Rev. B 105 (2022) 115140

TT 16.13 Mon 15:00 P2/OG4

Ground state properties of electron-electron biwire systems — Rajesh O. Sharma[1], Neil Drummond[2], Vinod Ashokan[1], Kare Narain Pathak[3], and •Klaus Morawetz[4,5] — [1]Department of Physics, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar (Punjab), 144 011, India — [2]Department of Physics, Lan-

caster University, Lancaster LA1 4YB, United Kingdom — [3]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [4]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [5]International Institute of Physics-UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Variational Monte Carlo (VMC) method is used to study the ground-state properties of a parallel infinitely-thin electron-electron quantum biwire system. The ground-state energy, the correlation energy, the interaction energy, the pair-correlation function (PCF), the static structure factor (SSF), and the momentum distribution (MD) function is calculated. As two parallel wires approach each other, inter-wire correlations increase while intra-wire correlations decrease. The SSF shows a peak at $2k_F$ at higher densities. A second peak starts to appear at $4k_F$ when $r_s = 2$ and $d = 0.2$ a.u. For lower densities, the first peak completely disappears and the height of the second peak keeps increasing with r_s and d. The behaviour of the PCF and SSF show that the electron-electron biwire system under goes into a quasi-Wigner crystalline state at densities higher compared to the case of a single wire.
[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] Phys. Rev. B 101 (2020) 075130
[4]Phys. Rev. B 104 (2021) 035149]

TT 16.14 Mon 15:00 P2/OG4

Integrating coplanar resonators and carbon nanotubes for microwave optomechanics — Akong Loh, Fabian Stadler, •Furkan Özyigit, Nicole Kellner, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

The optomechanical coupling of a carbon nanotube and a superconducting coplanar microwave resonator has been achieved [1,2] in our previous work. The carbon nanotube acts as a quantum dot, responding to gate voltages in a highly nonlinear way. This can be used to enhance the optomechanical coupling strength by several orders of magnitude. Recent work has focused on improving the electronic properties of the microwave resonators, to maximize quality factors in presence of the nanotube coupling electrodes. Currently, we redevelop insertion of carbon nanotubes as the mechanical counterpart. Here, we give an overview of recent improvements and ongoing measurements on this fascinating optomechanical system: at proper optimization, it can have figures of merit close to several interesting parameter regimes, as, e.g., strong optomechanical coupling (with hybridization of vibrons and photons) and the quantum coherent limit (where manipulation is faster than thermal decoherence).
[1] S. Blien *et al.*, Nat. Comm. **11**, 1636 (2020)
[2] N. Hüttner *et al.*, in preparation.

TT 16.15 Mon 15:00 P2/OG4

Description of defective graphene by means of the Dirac equation coupled to curvature and torsion — •Enkeleta Berisha and Nikodem Szpak — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany

The continuum theory of lattice defects (dislocations and disclinations) offers a practical description of the electron transport at the mesoscale at which the microscopic (ab initio) models become too complex. It can be linked to the geometrical concepts of curvature and torsion whithin the Riemann-Cartan geometry. In General Relativity there is an ongoing discussion about the equivalence of these two objects. In solid state physics both objects have concrete interpretations in terms of disclinations and dislocations. The application to a two-dimensional system can shed new light on this problem. We focus on graphene whose electron dynamics is described by the Dirac equation which exhibits such defects. This leads to the coupling of the effective Dirac equation to curvature and torsion, thus opening the possibility of mapping these objects onto each other. We study particular lattice configurations and interpret them in terms of curvature or torsion. Moreover, we compare the quantum current flows with the semiclassical trajectories in the effective Riemann-Cartan geometry.

TT 16.16 Mon 15:00 P2/OG4

Strain-induced pseudo-Landau levels in semimetals from dimensional reduction — •Fabian Köhler and Matthias Vojta — Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

Non-uniform strain applied to graphene's honeycomb lattice can induce pseudo-Landau levels in the single-particle spectrum. We generalize this procedure to d-dimensional hyperdiamond-lattices and solve the corresponding continuum theory. The unstrained tight-binding Hamiltonian has semimetallic bandstructure with a (d-2)-dimensional nodal manifold, which transforms into a series of relativistic Landau levels under suitable strain. We show that a mechanism of dimensional reduction is at play here that goes beyond the conventional minimal coupling framework. This mechanism generates two-dimensional Landau-level problems with identical level spacing at each point of the nodal manifold.

TT 16.17 Mon 15:00 P2/OG4

Semi-classical vibrational dynamics in molecular junctions: Anharmonic potentials and non-linear couplings — •Martin Mäck, Samuel Rudge, and Michael Thoss — Physikalisches Institut, Universität Freiburg

Non-conservative current-induced forces can lead to vibrational instabilities in molecular junctions, even at low bias voltages [1]. A common approach is to treat the vibrational dynamics semi-classically as influenced by quantum mechanical electronic degrees of freedom. Within these treatments, the vibrational modes are often assumed to be harmonic and linearly coupled to the electronic degrees of freedom. However, at the onset of vibrational instabilities, such harmonic potentials might no longer realistically describe the dynamics.

In this contribution, we use a recently developed hierachical equations of motion (HEOM) approach [2] to semi-classical Langevin dynamics [3] to study systems for which the introduction of anharmonic potentials and non-linear electron-vibrational coupling might play an important role for the vibrational dynamics of the system.
[1] J.T. Lü, M. Brandbyge, and P. Hedegård, Nano Lett. 2010, 10, 5, 1657
[2] C. Schinabeck, A. Erpenbeck, R. Härtle, and M. Thoss, Phys. Rev. B 94, 201407
[3] S. L. Rudge, Y. Ke, and M. Thoss, arXiv: 2211.14215

TT 16.18 Mon 15:00 P2/OG4

Solving non-interacting open bosonic systems — •Steven Kim and Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University

Open quantum systems that interact with their Markovian environment are described by a Lindblad master equation. We study non-interacting bosonic systems that are subject to single photon loss. The corresponding Liouvillian superoperator is at most of quadratic order in ladder operators. An analysis of the eigenvalues can give insight into possible instabilites as well as phase transitions. Especially the latter has gained growing interest for PT-symmetric systems. The difficulty in solving such systems for its eigenmodes lies in preserving the canonical commutation relation, which is why the standard way of diagonalization is not possible. In this work, we propose a new method to obtain the diagonalized form of any non-interacting bosonic system using symplectic transformations. We are able to diagonalize a general complex matrix, while maintaining the symplectic form that encodes the commutation relations of the bosonic ladder operators. We show that non-Hermitian Hamiltonians naturally appear while solving the Lindblad master equation and that the eigenmodes can be obtained by solving a reduced system. Including counting fields into the Lindbladian makes the efficient calculation of the cumulant generating functions of arbitrary observables possible.