TT 14: Graphene

Time: Monday 15:00–19:00 Location: H22

TT 14.1 Mon 15:00 H22

The non-local hydrodynamic transport properties of graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Within a kinetic theory approach, we calculate the non-local transport properties of graphene in the hydrodynamic regime, in the limit of a small graphene fine structure constant. We find an exact solution to the kinetic equation and derive exact expressions for the non-local (i. e. finite momentum and frequency) conductivity and viscosity. Possible applications of our findings to the study of relaxation phenomena will be discussed.

TT 14.2 Mon 15:15 H22

Spin and Charge Transport in Doped Graphene — •Marie-Luise Braatz[1,2], Axel Binder[3], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany

Graphene in its pristine form is already a remarkable material, however it has certain shortcomings in its pure form, such as no sizeable bandgap. Materials modifications allow one to better tailor its properties to specific needs such as engineering the charge carrier density or the bandgap, which is often required for electronic applications. We use chemical doping to gradually modify the graphene lattice, which has been shown to have an effect on the electronic structure [1]. Heteroatom substitution with nitrogen leads to changes in the structure as well as the electronic and magnetotransport properties. The amount of dopants is systematically varied so different dopant concentrations can be compared. The samples are then analyzed by Raman and electron microscopy to elucidate the changes in structure. Measuring the magnetoresistance at various temperatures and fields allows us to correlate the structure to the charge transport properties [2].
[1] H. Wang et al., ACS Catal. 2, 781 (2012)
[2] M. Rein et al., ACS Nano 9, 1360 (2015)

TT 14.3 Mon 15:30 H22

Transport through time dependent magnetic barriers in graphene — •Nico Leumer[1] and Wolfgang Häusler[2] — [1]Fakultät für Physik, Universität Regensburg — [2]Fakultät für Physik, Universität Augsburg

Studies of tunneling through time dependent scalar potential barriers have a long history, starting with the seminal work by Büttiker and Landauer [1]. Since in graphene electrostatic barriers are inefficient to guide carriers, due to Klein tunneling, we study here, to our knowledge for the first time, *time dependent magnetic barriers*. We discuss the difficulty of induced electric fields. Contrary to the scalar case, the problem now becomes inherently 2-dimensional. While more involved, we employ a strategy in the spirit of [1] by using a suitable gauge. For periodic time dependence, we find analytically the transmission through side bands. Depending on parameters, however, side bands may entirely close.
[1] M. Büttiker and R. Landauer, Phys. Rev. Lett. 49, 1739 (1982)

TT 14.4 Mon 15:45 H22

Spin-orbit coupled graphene *pn*-junction in a magnetic field — •D. Bercioux[1,2] and A. De Martino[3] — [1]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]Department of Mathematics, City, University of London, London EC1V 0HB, United Kingdom

We present a theoretical investigation of the spectral and transport properties of a *pn* junction in single-layer graphene in the presence of a uniform perpendicular magnetic field. The spectrum consists of localized bulk Landau-like and unidirectional interface states [1,2]. Specifically, we consider the effects of spin-orbit interactions (SOIs) on the spectrum of the *pn* junction. We show that the Rashba SOI [3] lifts the two-fold degeneracy of the zero mode. This degeneracy lifting takes place only in the transition from *p*- to *n*-region, whereas the modes are still two-fold degenerate in the bulk. We evaluate different observables along the transition region; particularly, we find that the spin density is different for the two zero modes and exhibits an oscillatory behaviour with the period depending on the strength of Rashba SOI. Finally, we discuss also the effects of Coulomb interaction on these chiral edge states in terms of Luttinger liquid theory.
[1] D. A. Abanin & L. S. Levitov, Science **317**, 641 (2007)
[2] L. Cohnitz, A. De Martino, W. Häusler & R. Egger, Phys. Rev. B **94**, 165443 (2016)
[3] D. Bercioux & A. De Martino, Phys. Rev. B **81**, 165410 (2010).

TT 14.5 Mon 16:00 H22

Thermoelectric efficiency in three-terminal graphene nanojunctions — Zahra Sartipi[1], Amir Hayati[2], and •Javad Vahedi[1,3] — [1]Department of Physics, Sari Branch, Islamic Azad University, Sari, Iran — [2]Faculty of Mazandaran Technical and Vocational University, Technical and Vocational University, Iran — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France

The thermoelectric efficiency of a thermal machine consisting of a triangular graphene nano-junction connected to three electrodes in the linear response regime is studied. Using the Onsager formalism and a combination of semi-empirical tight-binding calculations as well as Greens function theory, the efficiency at maximum output power which can be written in terms of generalized figures of merit is investigated. The results for a set temperature and chemical potential parameters have shown that adding a third terminal improves the efficiency at maximum output power compared to the two-terminal setup.

TT 14.6 Mon 16:15 H22

Interatomic forces in current-carrying graphene nanojunctions — •Susanne Leitherer, Nick R. Papior, and Mads Brandbyge — Department of Micro- and Nanotechnology, Technical University of Denmark

The interplay between the applied field, current and the atomic structure in ballistic nanoscale conductors carrying a substantial current, as seen in experiments [1,2], is still not well understood. In this contribution, we study the non-equilibrium charge transport through nanojunctions with graphene electrodes, employing first principles electronic structure and transport calculations based on density functional theory combined with non-equilibrium Greens functions (DFT-NEGF) [3]. We calculate the forces on the atoms which are induced by a finite bias voltage. The junctions are gated to increase their conductance and to allow switching between electron and hole-dominated transport [4]. We discuss the role of the potential drop in the junction, and show how the forces can be rationalized in terms of bond-currents, charge redistribution and overlap populations.
[1] C. Schirm, M. Mat, F. Pauly J.C. Cuevas, P. Nielaba and E. Scheer, Nat. Nanotechnol. 8, 645-648 (2013)
[2] H. Sadeghi, J. A. Mol, C. S. Lau, G. A. D. Briggs, J. Warner and C. J. Lambert, PNAS 112, 2658 (2015)
[3] N. Papior, N. Lorente, T. Frederiksen, A. Garcia and M. Brandbyge, Comput. Phys. Commun. 212, 8 (2017)
[4] N. Papior, T. Gunst, D. Stradi and M. Brandbyge, Phys. Chem. Chem. Phys. 18, 1025 (2016)

TT 14.7 Mon 16:30 H22

Current splitter and valley polarizer in elastically deformed graphene — •Nikodem Szpak[1] and Thomas Stegmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Instituto de Ciencias Fisicas, UNAM, Mexico

Elastic deformations of graphene can significantly change the flow paths and valley polarization of the electric currents. We investigate these phenomena in graphene nanoribbons with localized out-of-plane deformations by means of tight-binding transport calculations. Such deformations can split the current into two beams of almost completely valley polarized electrons and give rise to a valley voltage. These properties are observed for a fairly wide set of experimentally accessible parameters. We propose a valleytronic nanodevice in which a high polarization of the electrons comes along with a high transmission making the device very efficient. In order to gain a better understanding of these effects, we also treat the system in the continuum limit in which the electronic excitations can be described by the Dirac equation cou-

pled to curvature and a pseudo-magnetic field. Semiclassical trajectories offer then an additional insight into the balance of forces acting on the ballistic electrons and provide a convenient tool for predicting the behavior of the current flow paths. The proposed device can also be used for a sensitive measurement of graphene deformations.
[1] T. Stegmann and N. Szpak, New J. Phys. 18 (2016) 053016
[2] T. Stegmann and N. Szpak, 2D Materials (in press, DOI: 10.1088/2053-1583/aaea8d)

15 min. break.

Invited Talk TT 14.8 Mon 17:00 H22
Gate-defined quantum point contacts and quantum dots in bilayer graphene — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich GmbH

Graphene and bilayer graphene (BLG) are attractive platforms for spin qubits, thanks to their weak spin-orbit and hyperfine interaction, promising long spin-coherence times. This has motivated substantial efforts in studying quantum dot (QD) devices based on graphene and BLG. The problem of edge disorder in etched graphene can be completely circumvented in BLG, thanks to a tunable band-gap in the presence of a perpendicularly applied electric field, a feature that allows introducing electrostatic confinement in BLG. However, until very recently, essentially all devices were limited by leakage currents due to shortcomings in opening a clean and homogeneous band gap. A very recent breakthrough in this field has been the introduction of graphite back-gates. Together with the technology of encapsulating BLG in hexagonal boron nitride (hBN), giving rise to high quality hBN-BLG-hBN heterostructures, the use of a graphite back gate allows for a homogeneous and gate tunable band gap in BLG. We will show that this technological improvement allows for an unprecedented quality of quantized conductance measurements and most importantly, allows realizing complete electrostatic current pinch-off. The latter finally offers the possibility of electrostatically confining carriers in BLG and allows implementing quantum dots with a high level of control and low disorder.

TT 14.9 Mon 17:30 H22
Gap opening and quantum transport in a functionalized Bernal graphene bilayer — Ahmed Missaoui[1,3], Jouda J. Khabthani[1], Didier Mayou[2], and •Guy Trambly de Laissardiere[3] — [1]Laboratoire de la Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS - Univ. Grenoble Alpes, France — [3]Laboratoire de Physique théorique et Modélisation, CNRS - Univ. de Cergy-Pontoise, France

We describe numerically the electronic properties in Bernal bilayer graphene in presence of a random distribution of vacant atoms that simulate resonant adsorbates. The values of fundamental quantities such as conductivity, elastic mean free path, localization length are computed. In a Bernal graphene bilayer, carbon atoms belong to two inequivalent sub-lattices A and B of each layer. Therefore, selective functionalizations on only a sub-lattice can significantly change its electronic properties [1]. In particular, we find that for some selective functionalizations, a mobility gap of the order of 0.5 eV is formed near the Dirac energy at concentration of adatoms larger than 1
[1] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018).

TT 14.10 Mon 17:45 H22
Valley subband splitting in bilayer graphene quantum point contact — •Rainer Kraft[1], Igor V. Krainov[2], Vanessa Gall[1,3], Alexander P. Dmitriev[2], Ralph Krupke[1,4], Igor V. Gornyi[1,2,3], and Romain Danneau[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [3]Institute for Condensed Matter Theory, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [4]Department of Materials and Earth Sciences, Technical University Darmstadt, Darmstadt, Germany

Here we present a study of the 1D confinement in a bilayer graphene quantum point contact, i.e. a system with fourfold degeneracy (spin and valley). The constriction is designed electrostatically with dual-gated nanostructures in edge-connected bilayer graphene-hexagonal boron nitride van der Waals heterostructures, employing the possibility of local band gap engineering in bilayer graphene. While quantized conductance due to size-quantization is observed in steps of $4\,e^2/h$ down to the lowest subband, the valley-degeneracy of the 1D subbands is lifted under a perpendicular magnetic field and a peculiar pattern of splitting and merging from two non-adjacent subbands arises.

TT 14.11 Mon 18:00 H22
Anisotropic Andreev reflection in twisted bilayer graphene — •Christophe De Beule[1] and Patrik Recher[1,2] — [1]Institute for Mathematical Physics, TU Braunschweig — [2]Laboratory for Emerging Nanometrology, Braunschweig

We consider Andreev reflection at a normal-superconducting interface in twisted bilayer graphene where superconductivity is introduced via proximity effect, for twist angles in the range where both valley coupling and localization are weak. Due to the anisotropic band structure, the conductance depends strongly on the orientation of the tunneling junction with respect to the twisted bilayer graphene when the Fermi energy is near the Van Hove singularity. This can be understood from the opening of a scattering channel between parts of the Fermi surface that are localized in different layers. Moreover, Andreev (normal) reflection in this interlayer channel can be specular (retroreflective) even at Fermi energies much larger than the superconducting gap.

TT 14.12 Mon 18:15 H22
Charge density wave orders in twisted bilayer graphene — •Markus Klug and Jörg Schmalian — Karlsruher Institut für Technologie, Karlsruhe, Deutschland

The observation of unconventional superconductivity in twisted bilayer graphene (TBG) at small twisting angles attracted great interest in the recent year, though the underlying mechanism remains still unknown. Instead, understanding the nature of the insulating phases neighbouring the superconducting pocket on the electron- and hole-doped side might shed light on the origin of superconductivity in TBG. In this work, we use an effective electron model, which is valid in the small twist-angle / low-temperature regime, to discuss possible candidates of the insulating phase. We present various types of charge order formations with a tendency towards Wigner crystallisation. Our results are supported by numerical simulations based on the unrestricted Hatree-Fock Method.

TT 14.13 Mon 18:30 H22
Tuning anti-Klein to Klein tunneling in bilayer graphene — •Ming-Hao Liu[1], Renjun Du[2], Romain Danneau[2], and Klaus Richter[3] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [3]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

More than a decade ago, monolayer and bilayer graphene pnp junctions were shown to exhibit perfect transmission and perfect reflection upon normal incidence [1], known as Klein tunneling and anti-Klein tunneling, respectively. When the bilayer graphene is gapped by breaking the layer symmetry, however, the anti-Klein tunneling has been recently shown to be broken due to the departure of the Berry phase from 2π toward π [2]. A simple question naturally arose: Is it possible to tune the Berry phase from 2π of a gapless bilayer graphene to π of a largely gapped bilayer graphene, such that the anti-Klein tunneling becomes Klein tunneling? We have given an affirmative answer to this question in our latest work [3], involving both experiment and theory.
[1] M. I. Katsnelson, et al., Nat. Phys. **2**, 620 (2006)
[2] A. Varlet et al., Phys. Rev. Lett. **113**, 116601 (2014)
[3] R. Du et al., Phys. Rev. Lett. **121**, 127706 (2018)

TT 14.14 Mon 18:45 H22
Quantum transport in graphene/hBN Moiré superlattices: A numerical aspect — •Szu-Chao Chen[1], Klaus Richter[2], and Ming-Hao Liu[1] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Transport properties of graphene/hBN Moiré superlattices are studied by performing quantum transport simulations based on the scalable tight-binding model [1], combined with calculations of miniband structures and density of states within the continuum model. Both of the two-terminal conductance simulation and the calculated spectrum of the density of states reveal extra dips corresponding to satellite Dirac points due to the implemented model superlattice potential. Despite the simplicity of the adopted model which takes into account

only the scalar potential term, our preliminary results already capture main features of the Moiré superlattice, and therefore shed light on further simulating more complicated transport experiments involving graphene/hBN samples, such as Fabry-Pérot interference [2] and transverse magnetic focusing [3] in the presence of Moiré superlattice potential.

[1] M.-H. Liu et al., Phys. Rev. Lett. 114, 036601 (2015)
[2] C. Handschin et al., Nano Lett. 17(1), 328-333 (2017)
[3] M. Lee et al., Science 353(6307), 1526-1529 (2016)