TT 13: Graphene (joint session TT/DY/HL)

Time: Monday 15:00–18:30 Location: HSZ 201

TT 13.1 Mon 15:00 HSZ 201

Edge state crossing behaviour in a multi-band tight-binding model of graphene — •Thorben Schmirander, Marta Prada, and Daniela Pfannkuche — I. Institut für theoretische Physik Universität Hamburg, Hamburg, Deutschland

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the d-orbitals results in a breaking of electron-hole symmetry which in turn changes the dispersion of the states around the Fermi energy. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene, because they may exhibit the Spin Hall effect [3]. The band gap crossing is discussed by comparing different expectation values computed from the edge states. These expectation values change under different influences, such as strain or an external electric field. Apart from qualitatively treating these influences on the crossing of the band gap, electron-electron interactions are included via a self-consistent mean-field approach.

[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81 125435 (2010)
[3] Kane, C. L . and Mele, E. J., Phys. Rev. Lett. 95, 226801 (2005)

TT 13.2 Mon 15:15 HSZ 201

Graphene grain boundaries for strain sensing: a computational study — •Delwin Perera and Jochen Rohrer — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene has been celebrated as a material with exceptional properties at various fronts of electronics. In this contribution we investigate the strain sensing capabilities of graphene containing grain boundaries by using the non-equilibrium Green function formalism. Our work is inspired by an enhanced piezoresistivity of nanocrystalline graphene found experimentally in 2015 [1]. We investigate how different structural realizations of the grain boundary impact the transport properties. In particular, we compute strain gauge factors solely from *ab initio* electronic structure calculations as a function of the grain boundary topology. Thereby, we can compare this popular figure of merit for strain gauges with experimental values.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)

TT 13.3 Mon 15:30 HSZ 201

Virtual experiments on negative refraction across graphene pn junctions — •Wun-Hao Kang and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Graphene is a promising 2D material exhibiting optics-like properties due to its relativistic electronic structure linear in momentum. When charge carriers pass through a bipolar junction, the group velocity component parallel to the interface changes sign, leading to a negative refraction angle and hence effectively a negative refraction index in Snell's law. Many groups have been working on negative refraction in graphene, both theoretically and experimentally. However, most studies focus on the design of Veselago lensing. Here, we revisit a recent experiment [1] and perform quantum transport simulations for the same device geometry, based on the scalable tight-binding model [2]. Under ideal conditions, our result shows clear conductance peaks due to electron focusing, which is a combined effect of Klein tunneling and negative refraction. To single out the effect of negative refraction, we have further proposed a simpler design for future experiments.

[1] G.-H. Lee et al., Nat. Phys. **11**, 925–929 (2015)
[2] M.-H. Liu et al., Phys. Rev. Lett. **114**, 036601 (2015)

TT 13.4 Mon 15:45 HSZ 201

Electronic properties in a Bernal bilayer graphene monitored by selective functionalization — •Ahmed Missaoui[1,3], Jouda khabthani[1], Didier Mayou[2], and Guy Trambly de Laissardière[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

The absence of a band gap in the monolayer graphene presents a great limitation of the fields of application. In a Bernal bilayer of graphene we can exceed its limits with induce a tunable band gap here by applying a gate voltage. In this context, we study the electronic properties of bilayer graphene in the presence of adsorbates such as hydrogene. We used a tight binding modelisation and DFT calculations for our study. We analyze [1] the effects of a selective distribution of adosrbats between the two sublattices A and B [2] on band structure and the microscopic conductivity with Kubo formalisim. The results show that in some cases depending on Fermi energy value and specific adsorbate distribution a gap appears, and in others cases, a linear dispersion with an increase in conductivity with the concentrations is reported.

[1] Jyoti. Katoch et al., Phys. Rev. Lett. 121, 136801 (2018)
[2] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018)

TT 13.5 Mon 16:00 HSZ 201

Zero-magnetic-field Hall effects in artificially corrugated bilayer graphene — •Sheng-Chin Ho[1], Ching-Hao Chang[1,2], Yu-Chiang Heish[1], Shun-Tsung Lo[1], Botsz Huang[1], Carmine Ortix[3,4], and Tse-Ming Chen[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, NL-3584 CC Utrecht, Netherlands — [4]Dipartimento di Fisica E. R. Caianiello, Universita di Salerno, IT-84084 Fisciano, Italy

We propose a new scheme that uses a lithographically-defined strain technology to modify the interlayer coupling and intralayer interaction of bilayer graphene (BLG). In this deformed BLG system, we demonstrate an unusual pseudo-magnetoresistance anisotropy and the so-called nonlinear Hall effect. These observations are the consequence of the Fermi surface anisotropy and tilted mini-Dirac cones, which originate from the non-zero first-order moments of the pseudo-magnetic field in both real- and momentum-spaces, i.e., the pseudo-magnetic field dipole and Berry curvature dipole. This new approach enables us to turn a simple bilayer graphene into an exotic phase of matter with nontrivial band dispersion generated by the strain engineering, on par with the creation of metamaterials or state-of-art twistronics engineering.

TT 13.6 Mon 16:15 HSZ 201

Spin-caloritronic transport in hexagonal graphene nanodots — Thi Thu Phùng[1], Robert Peters[2], •Andreas Honecker[1], Guy Trambly de Laissardière[1], and Javad Vahedi[1,3] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Department of Physics, Kyoto University, Japan — [3]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

First, we investigate magnetism in the Hubbard model for hexagonal graphene dots. Employing static respectively dynamic mean-field theory (DMFT) we show that magnetism can be generated at the zigzag edges beyond a critical interaction of the on-site Coulomb interaction U that decreases with increasing dot size. Building on these results, we apply the Landauer formalism in the framework of the non-equilibrium Green function method to calculate the spin and charge currents through these dots as a function of temperature. We show that in the "*meta*" configuration of a hexagonal dot subject to weak Coulomb interactions, a pure spin current can be driven just by a temperature gradient in a temperature range that is promising for device applications.

15 min. break.

TT 13.7 Mon 16:45 HSZ 201

Lévy flights and Hydrodynamic Superdiffusion on the Dirac Cone of Graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Insti-

tut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We show that the hydrodynamic collision processes of graphene electrons at the neutrality point can be described in terms of a Fokker-Planck equation with a fractional derivative, corresponding to a Lévy flight in momentum space. Thus, electron-electron collisions give rise to frequent small-angle scattering processes that are interrupted by rare large-angle events. The latter give rise to superdiffusive dynamics of collective excitations. We discuss the relevance of our results to experiments with injected electron beams, and show how the superdiffusive behavior makes it possible to obtain analytical results for transport coefficients relevant to the hydrodynamics of graphene electrons.

TT 13.8 Mon 17:00 HSZ 201

Gate-controllable graphene superlattices: Numerical aspects — •Szu-Chao Chen, Wun-Hao Kang, and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

We study transport properties of gate-controllable graphene superlattices by performing quantum transport simulations based on the scalable tight-binding model and calculations of miniband structures within the continuum method [1]. Good agreement between transport simulations and the corresponding miniband structures confirms the reliability of our calculations for electrostatic superlattices in graphene. Combined with realistic potential profiles obtained from finite-element-based electrostatic simulations, our transport simulations agree well with recent transport experiments for gate-controllable square superlattices. This work therefore paves the way toward exploring gate-controllable graphene superlattices of arbitrary lattices, such as honeycomb or Lieb.
[1] S.-C. Chen et al., arXiv:1907.03288 (2019).

TT 13.9 Mon 17:15 HSZ 201

Localization at the Van Hove singularity — •Peter Silvestrov[1] and Jakub Tworzydło[2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland

Van Hove singularities are found in the electron spectrum of many 2-dimensional materials of current interest, including graphene systems (twisted bilayer and monolayer on a substrate), transitional dichalcogenides, and 2-dimensional superconductors. They appear due to saddle points in the energy bands at certain momenta. Even though the effective kinetic energy corresponding to such saddle point is unbounded from both above and below, we show that exponentially localized electronic states generically appear here in the presence of a smooth potential $U(x, y)$ with sufficiently diverse landscape. We also consider high order Van Hove singularities, where we predict a discrete spectrum of non-exponentially localized states.

TT 13.10 Mon 17:30 HSZ 201

The optical conductivity of strongly interacting Dirac fermions: a bosonization approach to the Kadanoff-Baym self-consistent resummation — •Sebastián Mantilla and Inti Sodemann — Max Planck Institute for the Physics of Complex Systems

The optical conductivity of 2D Dirac fermions at low energies is controlled by fundamental constants of nature $\sigma_0 = e^2/16\hbar$. However, Coulomb interactions produce a non-trivial dependence of the conductivity with the frequency. We use a bosonization approach to implement exactly a self-consistent Kadanoff-Baym resummation of the electron-hole propagator by mapping the momentum space lattice onto a Heisenberg-type model of interacting spins and employ this approach to determine the frequency dependence of the optical conductivity for Coulomb repulsions. We recover the perturbative renormalization group results at small coupling and extend its predictions to strong coupling. We discuss the relevance of our results to Dirac materials such as graphene and 3D topological insulator surface states.

TT 13.11 Mon 17:45 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene I — •Marlon Nuske[1,3], Lukas Broers[1], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

We determine the origin of the light-induced Hall current in graphene recently reported by J. McIver, et al., Nature Physics (2019). The Hall current derives from the total Berry curvature of the occupied states of the light-induced Floquet bands, in addition to the kinetic contribution deriving from the band velocities. The occupation of these states of the light-driven material emerges as a steady state that is determined by dissipative processes balancing out the optical driving force. For low electric field strength we propose an intuitive explanation of the Hall current within a two-level Rabi picture.

TT 13.12 Mon 18:00 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene II — •Lukas Broers[1], Marlon Nuske[1,3], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

Inspired by the recent experiments by J. McIver, et al., Nature Physics (2019), we investigate the light-induced Hall current in graphene. We show that this Hall current derives from the Berry curvature and band velocity contributions of the occupied Floquet-states. To support this proposal we determine the energy and momentum resolved single particle correlation function. The resulting steady state momentum and energy distribution supports the interpretation as a Floquet induced mechanism. We find that for low driving intensity the main contribution to the Hall current emerges from the resonantly driven electron states of the Dirac cone. With increasing driving intensity, additional higher order resonances contribute, giving rise to the full Floquet-driven effect. We demonstrate this within a Master equation formalism, and obtain good quantitative agreement with the experimentally measured Hall current.

TT 13.13 Mon 18:15 HSZ 201

Lightwave valleytronics in graphene — •Hamed Koochaki Kelardeh[1], Alexandra Landsman[2], and Takashi Oka[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Ohio State University, Columbus, USA

We propose a valley-selective device based on graphene at a few-femtosecond timescale with charge separation at different sublattices, and correspondingly at nonequivalent valleys. We characterize the maximality condition of valley polarization and investigate the parameters and condition upon which we can coherently control the carriers and store data via valley degree of freedom. The valley polarization is controlled by the amplitude as well as the carrier-envelope phase of the pulse - one cycle optical field - and the curvature of the electron trajectory in the reciprocal space. We believe the results of our study will step forward the Valleytronics and shed light on ultrafast data storage and processing with uttermost reliability and robustness.