HL 8: Transport and theory of electronic structure

Time: Monday 15:00–17:30 Location: H33

HL 8.1 Mon 15:00 H33

Anomalous microwave-induced resistance oscillations in double quantum well hetero-structures — •Jana Meyer[1], Jan Scharnetzky[2], Maik Hauser[3], Werner Dietsche[3], Werner Wegschneider[2], Lars Tiemann[1], and Robert H. Blick[1] — [1]Center for Hybrid Nanostructures, Hamburg University, 22761 Hamburg, Germany — [2]ETH Zürich, 8092 Zürich, Switzerland — [3]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Gallium arsenide double quantum well systems with various barrier thicknesses were exposed to microwave radiation at low temperatures and large magnetic fields. The double quantum well Hall bar samples employ structured top and back gates to control the electron densities and to electrically separate the two quantum wells.[1] At specific microwave frequencies and carrier densities, pronounced anharmonic oscillations in the longitudinal resistance emerge, which exhibit nodes at certain Landau level filling factors. The amplitude of these oscillations is very sensitive to the microwave power and variations of the carrier density. We propose this phenomenon to originate from plasmonic excitations.

[1] J. P. Eisenstein et al., Appl. Phys. Lett. 57, 2324 (1990).

HL 8.2 Mon 15:15 H33

Is the multifractal spectrum at the spin quantum Hall transition exactly parabolic? — •Daniel Hernangómez-Pérez[1], Soumya Bera[2], Ilya Gruzberg[3], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, India — [3]Department of Physics, Ohio State University, USA

The integer quantum Hall effect (IQHE) has recently been proposed to have an exactly parabolic multifractality spectrum [1, 2]. Due to strong corrections to scaling, however the corresponding exponents are very difficult to access numerically. A close relative of the IQHE (class A) is the spin quantum Hall effect (SQHE, class C). In contrast to IQHE, for SQHE analytical results for certain anomalous exponents are available [3]. Correspondingly, corrections to scaling are under better control. Thus motivated, we here present a numerical study of multifractality at the SQHE using the corresponding network model. Our results: The multifractal spectrum of SQHE obeys the expected symmetry relation [4]; the analytically known exponents for the LDoS moments, $x_2 = 1/4, x_3 = 0$, are reproduced with good precision: 0.2504 ± 0.008 and 0.000 ± 0.002. The spectrum exhibits significant deviations from parabolicity, i.e. $x_q/q(3-q)$ shows linear term $a_1 = 0.0021 \pm 0.0002$. We see our results as providing constraints for future analytical theories of the SQHE. [1] R. Bondesan, et al., Nucl. Phys. B **918**, 52 (2017). [2] M. Zirnbauer, arXiv:1805.12555 (2018). [3] F. Evers et al., Phys. Rev. B **67**, 041303(R) (2003). [4] A. Gruzberg, et al., Phys. Rev. Lett. **107**, 086403 (2011).

HL 8.3 Mon 15:30 H33

Magnetotunneling Spectroscopy of Imbalanced Double Quantum Wells — •Gunnar Lasse Schneider[1], Werner Dietsche[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Uni Hannover, Deutschland — [2]MPI for Solid State Research, Stuttgart, Germany

Since several years bilayer phenomena such as 2D-2D Tunneling [1], Coulomb drag [2] and excitonic Bose-Einstein condensates (BEC) [3] are observable within double quantum wells in the Quantum Hall regime. Most studies were focused on balanced systems (i.e. the BEC was first found to arise at balanced layer densities with the filling factor combination of 1/2 and 1/2). In our work we are investigating imbalanced layers, allowing a mapping of the magnetotunneling characteristics at various filling factor combinations and the evolution of the excitonic condensate in the charge carrier density space.

All measurements were performed on a MBE grown GaAs double quantum well separated by a 10 nm AlAs/GaAs barrier. Each layer is individually contacted using field gates for a local depletion [4]. Additional gates allow tuning the charge carrier densities between 1E10 and 4E10 per square centimeter. Our measurements show Quantum Hall selection rules in the magnetotunneling characteristics (Quantum Hall spin diode) and the transition towards excitonic condensation.

[1]N. Turner et al., Phys. Rev. B 54, 10614 (1996)
[2]C. Jörger et al., Physica E 6, 586 (2000)
[3]J.P. Eisenstein and A.H. MacDonald, Nature 432, 691 (2004)
[4]J.P. Eisenstein et al., Appl. Phys. Lett. 57, 2324 (1990)

HL 8.4 Mon 15:45 H33

Suppression of magnetic-field-induced electronic transitions in graphite microflakes — •Jose Luis Barzola Quiquia[1], Christian Precker[1], Markus Stiller[1], Mahsa Zoragui[1], Pablo Esquinazi[1], Tobias Foerster[2], and Thomas Herrmannsdoerfer[2] — [1]Felix-Bloch Institute for Solid State Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In this contribution we report a detailed study of the magnetoresistance of bulk and microflakes of different thickness prepared from a highly oriented pyrolytic graphite sample. Measurements have been done at different temperatures with pulsed magnetic fields up to 62 T applied parallel to the c-axis. The bulk and thicker samples show the well-known sudden jumps in the magnetoresistance in a restricted field region that were interpreted in the past as field-induced electronic phase transitions in graphite associated with, e.g., charge density waves. In the case of the thin graphite flakes the jumps in the magnetoresistance nearly vanish. In general, this suppression agrees very well with other thickness dependent results, such as the temperature dependence of the resistance, the absolute resistivity, the relative change in the magnetoresistance and the Shubnikov-de-Haas oscillations amplitude. Our results indicate that the electronic transport properties of bulk graphite are dominated by the two-dimensional electron gas formed at the interfaces between crystalline regions with the same or different stacking orders present in graphite.

HL 8.5 Mon 16:00 H33

Surface acoustic wave induced electrical current in graphene — •Pai Zhao, Lars Tiemann, and Robert H. Blick — Center for Hybrid Nanostructures, Hamburg University, 22761 Hamburg, Germany

Surface acoustic waves (SAWs) generated on a piezoelectric substrate are able to induce an acoustoelectric current that sweeps electrons along with the propagating waves.[1,2] Here, we show how to apply this acoustoelectric current as an alternative to a conventional current to study magnetotransport in monolayer graphene. We fabricated a pair of interdigitated transducers (IDTs) on a semi-insulating GaAs substrate, separated by 1,800 μm. A large CVD graphene sheet was transferred from a copper substrate onto the GaAs sample. In a photolithographic process we patterned a Hall bar structure centered between the two IDTs. Regular magnetotransport characterization of the graphene sample shows an intrinsic carrier concentration of $5.5\times10^{11}\mathrm{cm}^{-2}$ and a mobility of $600\mathrm{cm}^2/\mathrm{Vs}$. When the IDTs on the GaAs are excited at one of their harmonic resonance frequencies, we detect an acoustoelectric current passing through the graphene Hall bar, which follows the longitudinal resistance oscillations with magnetic fields up to 8 Tesla at 4.2 Kelvin.

[1] A. Wixforth et al., Phys. Rev. Lett 56, 2104 (1986).
[2] D. Kreft et al., Phys. Rev. B 94, 235305 (2016).

HL 8.6 Mon 16:15 H33

Explaining Charge Mobility Regimes in Amorphous Materials — •Markus Krammer[1], Chris Groves[2], and Karin Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Department of Engineering, Durham University, United Kingdom

Charge mobility in amorphous materials like disordered organic semiconductors is commonly evaluated assuming hopping transport, where charges are viewed to migrate via hopping between localised states. The charge motion is governed by a complex interplay of energetic disorder, electric field, interactions, temperature, and other parameters. While state-of-the-art simulation techniques like kinetic Monte Carlo or Master equation (ME) account well for this complex interplay, it is desirable to distinguish between field- and charge density related mobility regimes and transitions between them from a more fundamental point of view. We developed a new simulation technique providing this fundamental view. The technique is reminiscent of ME with the benefit that it can directly incorporate correlations and interactions.

The separation of field- and charge density related effects included in our new technique allows to interpret the corresponding evolution of the mobility. We will explore the mobility regimes from the perspective of steady state charge densities and occupation statistics. With simulations containing one charge carrier, we will explain the ideas behind our technique and discuss the reasons for the field dependence of the mobility. By increasing the number of charge carriers, the charge density dependence of the mobility will be elucidated.

HL 8.7 Mon 16:30 H33

Tunable disorder and localization in the rare-earth nickelates — •Changan Wang[1], Ching-Hao Chang[2], Angus Huang[3], Lin Yang[5], Roman Böttger[1], Manfred Helm[1], Ying-Hao Chu[4], Ramachandran Ganesh[6], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Dresden, Germany — [2]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [3]National Tsing Hua University, Taiwan — [4]National Chiao Tung University, Taiwan — [5]South China Normal University, Guangzhou, China — [6]The Institute of Mathematical Sciences, Chennai, India

The rare-earth nickelates are a rich playground for transport properties, known to host non-Fermi liquid character, resistance saturation and metal-insulator transitions. We report a disorder engineering in LaNiO3 by ion-irradiation generated scattering centres in a tunable fashion to induce localization. While pristine LaNiO3 samples are metallic, highly irradiated samples show insulating behaviour at all temperatures. Using irradiation fluence as a tuning handle, we uncover an intermediate region hosting a metal-insulator transition. In the high temperature metallic regime, we find a transition from non-Fermi liquid to a Fermi-liquid-like character. On the insulating side of the metal-insulator transition, we find behaviour that is consistent with weak localization. In the highly irradiated insulating samples, we find good agreement with variable range hopping, consistent with Anderson localization. Our results demonstrate that ion irradiation can be used to tailor transport and study the physics of localization.

HL 8.8 Mon 16:45 H33

Analytically tractable model for chirality-induced spin selectivity — •Areg Ghazaryan[1], Yossi Paltiel[2], and Mikhail Lemeshko[1] — [1]IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria — [2]Department of Applied Physics, Hebrew University, Jerusalem 91904, Israel

It is well established experimentally that electron transmission and tunneling through chiral molecules is spin selective. This phenomenon is termed as chirality-induced spin selectivity (CISS). Despite substantial advances on the experimental investigation of CISS, a theoretical understanding of the microscopic origin of the effect is still lacking. Previous theoretical efforts usually employed helical structure of the molecule for constructing the scattering or transport theories of CISS. The complicated geometry of the helix makes these theories intractable analytically. Here we develop a scattering theory for the CISS effect, by modelling the molecule as a combination of dipoles. These allows us to develop an analytically tractable model for analyzing the microscopic origin of the CISS effect. Different enantiomers are distinguished with different directions of the dipoles and the dipole moments can be directly measured using Stark effect measurements of the microwave spectrum of the molecules. Therefore, the parameters of our model can be directly obtained from the experimental results.

HL 8.9 Mon 17:00 H33

Ab-initio electronic structure calculations for random alloys: Accurate SiGe composition-dependent band gap at reduced computational cost — •Petr A. Khomyakov, Daniele Stradi, Ulrik G. Vej-Hansen, Maeng-Eun Lee, Jess Wellendorff, Søren Smidstrup, and Kurt Stokbro — Synopsys QuantumATK, Fruebjergvej 3, 2100 Copenhagen, Denmark

Semiconductor random alloys are commonly used in microelectronics, so first-principles calculations for the physical properties of random alloys are of great interest. This kind of calculations allow for obtaining the physical parameters for any alloy composition. However, configuration sampling of results for alloy supercells, which is the standard approach to capturing the effect of alloy disorder on the physical properties, can be computationally demanding.

In this study, we use the special quasi-random structures (SQS) approach for modeling SiGe random alloys over the entire range of alloy compositions. The SQS method alleviates the need for configuration sampling, reducing the computational cost considerably. At each alloy composition, we apply our recently-developed pseudopotential projector-shift (PPS) method for obtaining accurate band energies for silicon and germanium within the framework of the DFT-PBE functional approach. Using the SQS + PPS-PBE combination allowed us to obtain accurate SiGe band gaps across the entire range of alloy compositions, as compared to room-temperature measured gaps. Applying the HSE06 hybrid functional yields the composition-dependent SiGe band gaps in good agreement with low-temperature measured gaps.

HL 8.10 Mon 17:15 H33

Robust automatic Wannierisation — •Giovanni Pizzi[1], Valerio Vitale[2,3], Antimo Marrazzo[1], Nicola Marzari[1], Jonathan R. Yates[4], and Arash A. Mostofi[3] — [1]NCCR MARVEL and EPFL, CH — [2]Cavendish Laboratory, University of Cambridge, UK — [3]Department of Materials and Physics and Thomas Young Centre, Imperial College London, UK — [4]Department of Materials, University of Oxford, UK

In a recent work [1], the SCDM-k method has been successfully extended to obtain a set of localised Wannier functions in the case of entangled bands. The method relies on numerical parameters that need to be identified. Here, we first present the implementation of the method in Quantum ESPRESSO. Then, we provide a validation on ∼200 chemically different structures (including also lower-dimensional structures), discussing the robustness for the choice of the parameters with respect to the quality of the band interpolation and final spread of the localized orbitals. Thanks to this, we are able to provide a physical understanding of the parameters and present an automated protocol to select them, making use of the projectability of the states onto atomic-like orbitals. Finally, we present the implementation of this fully automated method into AiiDA workflows for Quantum ESPRESSO and Wannier90, that makes it possible to obtain automatically maximally-localised Wannier functions for any material without supervision.

[1] A. Damle, L. Lin, Disentanglement via entanglement: A unified method for Wannier localization, arXiv:1703.06958v1 (2017).