TT 8: TR: Graphene 2 (jointly with MA, HL, and DY)

Time: Monday 14:00–18:30 Location: HSZ 304

TT 8.1 Mon 14:00 HSZ 304

Radiation-induced quantum interference in graphene based n-p junctions — •Mikhail Fistul[1], Sergey Syzranov[1], Anatoly Kadigrobov[1,2], and Konstantin Efetov[1] — [1]Ruhr-Universität, Bochum, Germany — [2]University of Gothenburg, Göteborg, Sweden

We predict and analyze *radiation-induced quantum interference effect* in low-dimensional graphene based n-p junctions.

In the presence of radiation the ballistic transport of electrons is determined by two processes, namely, by the resonant absorption of photons near the "resonant points", and by the strong reflection from the junction interface, occurring at the "reflection points". There are two paths corresponding to the propagation of electrons through the junction, and the interference between these two paths manifests itself by *large oscillations of the ballistic photocurrent* as a function of the gate voltage or the frequency of the radiation. This coherent quantum phenomenon resembles Ramsey quantum beating and Stueckelberg oscillations well-known in atomic physics.

A suitable radiation frequency may be in the THz or in the infrared optical region. The effect can be observed best in one- and two-dimensional n-p junctions based on carbon nanotubes, monolayer or bilayer graphene nanoribbons.

TT 8.2 Mon 14:15 HSZ 304

Resonant Scattering by Realistic Impurities in Graphene — •Tim Wehling[1], Shengjun Yuan[2], Alexander Lichtenstein[1], Andre Geim[3], and Mikhail Katsnelson[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Radboud University of Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom

We develop a first-principles theory of resonant impurities in graphene and show that a broad range of typical realistic impurities leads to the characteristic sublinear dependence of the conductivity on the carrier concentration. By means of density functional calculations various organic groups as well as adatoms such as H absorbed to graphene are shown to create midgap states within $\pm 0.03\,\mathrm{eV}$ around the neutrality point. A low energy tight-binding description is mapped out. Boltzmann transport theory as well as a numerically exact Kubo formula approach yield the conductivity of graphene contaminated with these realistic impurities in accordance with recent experiments. Consequences for spin-flip scattering are discussed.

TT 8.3 Mon 14:30 HSZ 304

Effect of Coulomb interaction on the gap in monolayer and bilayer graphene — Andreas Sinner and •Klaus Ziegler — Institut für Physik, Universität Augsburg

We study effects of a repulsive Coulomb interaction on the spectral gap in monolayer and bilayer graphene in the vicinity of the charge neutrality point by employing the functional renormalization-group technique. In both cases Coulomb interaction supports the gap once it is open. For monolayer graphene we correctly reproduce results obtained previously by several authors, e.g., an apparent logarithmic divergence of the Fermi velocity and the gap as well as a fixed point corresponding to a quantum phase transition at infinitely large Coulomb interaction. On the other hand, we show that the gap introduces an additional length scale at which renormalization flow of diverging quantities saturates. An analogous analysis is also performed for bilayer graphene with similar results. We find an additional fixed point in the gapless regime with linear spectrum corresponding to the vanishing electronic band mass. This fixed point is unstable with respect to gap fluctuations and can not be reached as soon as the gap is opened. This preserves the quadratic scaling of the spectrum and finite electronic band mass. Ref.:Phys. Rev. B, 82, 165453 (2010).

TT 8.4 Mon 14:45 HSZ 304

Dirac electrons in a spin-orbit periodic potential — •Lucia Lenz[1,2] and Dario Bercioux[1,2] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universitat, D-79104 Freiburg, Germany

In this talk we present a study of the the band structure of Dirac electrons in graphene in the presence of one-dimensional, periodically modulated spin-orbit interactions. It has been shown that the transmissions of the spin up and spin down channels are strongly dependent on the length of the barrier compared to the spin-precession length [1]. Based on the knowledge of the transfer matrix, we obtain an analytic equation for the band condition using the transfer matrix method [2]. We investigate how the band structure changes compared to potentials with no spin-orbit interactions [3], and give further interpretations to the additional eigenmodes of the transfer matrix.

[1] D. Bercioux, and A. De Martino, Phy. Rev. B **81**, 165410 (2010).
[2] B.H.J. McKellar, G.J. Stepheson, Phy. Rev. C, **35**, 2262 (1987).
[3] M. Barbier, F.M. Peeters, P. Vasilopoulos, J.M. Pereira, Phy.Rev. B **77**, 115446 (2008).

TT 8.5 Mon 15:00 HSZ 304

Transmission through electrostatic and magnetic barriers in the $\mathcal{T}_3$-lattice — •Daniel F. Urban[1], Dario Bercioux[1,2], and Wolfgang Häusler[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [3]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

Albeit the $\mathcal{T}_3$-lattice exhibits a reciprocal lattice similar to graphene with two inequivalent Dirac-points at six corners of the hexagonal first Brillouin zone, where relativistic electron-hole symmetric bands touch, $\mathcal{T}_3$ differs and considerably generalizes graphene. A peculiarity of $\mathcal{T}_3$ is the occurance of an additional dispersionless energy band at energy $E = 0$ and an enlarged pseudo-spin $S = 1$ [1] instead of $S = \frac{1}{2}$ as for graphene. As a result, we find enhanced Klein tunneling through rectangular electrostatic barriers, compared to the case of graphene. Moreover, at the particular energy of half the barrier height we find even complete transparency, $T = 1$, irrespective of barrier thickness and of incidence angle. We also investigate rectangular magnetic barriers and in this case identify regimes of zero barrier transparency, qualitatively similar to the case of graphene [2].

[1] D. Bercioux, D. F. Urban, H. Grabert, and W. Häusler, Phys. Rev. A **80**, 063603 (2009).
[2] A. De Martino, L. Dell'Anna, and R. Egger, Phys. Rev. Lett. **98**, 066802 (2007).

TT 8.6 Mon 15:15 HSZ 304

Weak Localization versus Weak Antilocalization in Graphene — •Frank Ortmann[1], Alessandro Cresti[2], Gilles Montambaux[3], and Stephan Roche[4] — [1]INAC/SPRAM, CEA Grenoble, France — [2]IMEP-LAHC, Minatec, Grenoble, France — [3]Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France — [4]Institut Català de Nanotecnologia and CIN2, Universitat Autònoma de Barcelona, Barcelona, Spain

The understanding of quantum transport phenomena in graphene-based materials is the current subject of great excitation. In the presence of disorder, one of the predicted signatures of pseudospin is the change in sign of the quantum correction to the semiclassical Drude conductivity. This phenomenon, referred to as weak antilocalization (WAL), results from complex quantum-interferences of charge carriers in a disordered potential landscape and has been recently observed experimentally with weak-field magnetotransport measurements.

In this talk we present a numerical weak-field magnetotransport study of huge graphene samples and the influence of a realistic (long-range) disorder potential describing charges trapped in the gate oxide. Our simulations give clearly different magnetoconductance responses in different regimes which are fingerprint of either weak localization or WAL. Depending on the strength of the perturbing potential, the magnetoconductance can be tuned from positive to negative. The gate potential provides a second handle to modify these characteristics. Our results therefore shed new light on experiments and unveil the possible origin of crossovers from positive to negative magnetoconductance.

15 min. break

TT 8.7 Mon 15:45 HSZ 304

Graphene-based electronic spin lenses — •Ali G. Moghaddam[1] and Malek Zareyan[2] — [1]Theoretische Physik, Universität Duisburg-

Essen, 47048 Duisburg, Germany — [2]Institute for Advanced Studies in Basic Sciences (IASBS), P.O. Box 45195-1159, Zanjan, Iran

We have proposed a solid state electronic spin lens based on a ferromagnetic graphene which has an exchange potential higher than its Fermi energy. The key property is that an interface between such a spin-chiral ferromagnetic (FM) and a nomal (N) graphene region exhibits a negative electronic refractive index which has different signs for electrons with different spin-directions. We have shown that in a corresponding N-FM-N structure, an unpolarized electronic beam can be collimated with a finite spin-polarization producing a point spin accumulation with associated Friedel-like oscillations of spin-dependent local density of states. In this respect, our study reveals that magnetic graphene has the potential to be the electronic counterpart of the recently discovered photonic chiral metamaterials which exhibit a negative refractive index for only one direction of the circular polarization of the electromagnetic wave.
[1] A. G. Moghaddam and M. Zareyan, Phys. Rev. Lett. **105**, 146803 (2010).

TT 8.8 Mon 16:00 HSZ 304

Thermal fluctuations of free standing graphene — •Nils Hasselmann[1,3] and Fabio Braghin[2,3] — [1]MPIFKF Stuttgart — [2]Univ. Fed. de Goias, Goiania, GO, Brazil — [3]IIP, UFRN, Natal, RN, Brazil

We use non-perturbative renormalization group techniques to calculate the momentum dependence of thermal fluctuations of graphene, based on a self-consistent calculation of the momentum dependent elastic constants of a tethered membrane. We find a sharp crossover from the perturbative to the anomalous regime, in excellent agreement with Monte Carlo results for the the out-of-plane fluctuations of graphene, and give an accurate value for the crossover scale. Our work strongly supports the notion that graphene is well described as a tethered membrane. Ripples emerge naturally from our analysis.

TT 8.9 Mon 16:15 HSZ 304

Transport through a quantum-spin-Hall-insulator/normal junction in graphene ribbons — •Georgo Metalidis[1] and Elsa Prada[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid, Spain

We have investigated a junction between a quantum-spin-Hall insulator and a metallic contact obtained by selectively doping a single graphene ribbon. In the absence of disorder, the transmission of the topological edge states through the junction is perfect due to the orthogonality of left- and right-movers. This is proven analytically by deriving exact wavefunctions for the topological edge states in armchair and zigzag ribbons. The wavefunction character depends fundamentally on the ribbon termination: the edge state width is only dependent on the spin-orbit coupling strength for armchair ribbons, whereas it is only weakly dependent of this parameter for zigzag edge states where the width becomes energy dependent instead. These observations are confirmed in numerical plots of the current density in the sample. When disorder is present, the orthogonality between left- and right-movers is destroyed and backscattering sets in. Nevertheless, the perfect transmission can be restored by increasing the ribbon width.

TT 8.10 Mon 16:30 HSZ 304

Edge magnetism in nanoribbons of graphene — •Hélène Feldner[1,2], Zi Yang Meng[3], Thomas C. Lang[4], Fakher Assaad[4], Stefan Wessel[3], Andreas Honecker[2], and Daniel Cabra[1] — [1]IPCMS, Strasbourg, France — [2]Institut für Theoretische Physik, Göttingen, Germany — [3]Institut für Theoretische Physik III, Stuttgart, Germany — [4]Institut für Theoretische Physik und Astrophysik, Würzburg Am Hubland, Germany

A simple tight-binding model is sufficient to describe most of graphene's properties, but a Hubbard model is needed to account for its magnetic properties. To be able to compute quantities in direct space and for big systems of realistic size with chosen geometry, we use a mean field approximation solved in a self-consistent way in the direct space. In agreement with known results, we find a Mott-Hubbard transition, and a magnetization of the zig-zag edge of finite samples. We have studied the accuracy of the approximation by a comparison of our results with those obtained by exact diagonalization and quantum Monte-Carlo simulations [1]. The main point of our current work consists of a study of the graphene zig-zag ribbons by mean field and quantum Monte-Carlo simulations. First we have looked at the static magnetism of the zig-zag edges and in a second part the local spectral function. These quantities allow us to study the influence of static magnetism on dynamical properties and the local density of states which is a quantity accessible experimentally by STM and shows different behavior on the edge with and without magnetic properties.
[1] Phys. Rev. B 81, 115416 (2010).

TT 8.11 Mon 16:45 HSZ 304

Screening of external electrical fields for different graphene nanoribbons — •Tobias Burnus[1], Gustav Bihlmayer[1], Daniel Wortmann[1], Yuriy Mokrousov[1], Stefan Blügel[1], and Klaus Michael Indlekofer[2] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Hochschule RheinMain, Unter den Eichen 5, 65195 Wiesbaden, Germany

Graphene nanoribbons (GNR) hold great future promise for field-effect transistor and quantum dot (QD) devices. The gate electrodes and the electric field distribution play a crucial role. In this talk the effect of the screening of an in-plane oriented external electric field due to the electrons in graphene nanoribbons is studied in the framework of density functional theory calculations based on the full potential linearized augmented planewave method. These calculations offer a direct link to the static dielectric constant in the ribbon. We compare armchair ribbons of different width to see the effect of the bandgap on the electric response, as well an orientation with zig-zag edges, which show a metallic edge state. The formation of QDs in structures with both types of edges in an external field is considered. The presence of metallic states, e.g. from a substrate, significantly modifies the behavior of QD states in the external field. The work is supported by the DFG Research Unit 912 "Coherence and Relaxation Properties of Electron Spins".

TT 8.12 Mon 17:00 HSZ 304

Color-dependent conductance of graphene with adatoms — •Jörg Schelter[1], Pavel Ostrovsky[2,3], Igor Gornyi[2,4], Björn Trauzettel[1], and Mikhail Titov[2,5] — [1]Institut für Theoretische Physik und Astrophysik, University of Würzburg, 97074 Würzburg, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [4]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [5]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK

We study ballistic transport properties of graphene with a low concentration of vacancies or adatoms. The conductance of graphene doped to the Dirac point is found to depend on the relative distribution of impurities among different sites of the honeycomb lattice labeled in general by six colors. The conductivity is shown to be sensitive to the crystal orientation if adatom sites have a preferred color. Our theory is confirmed by numerical simulations using recursive Green's functions with no adjustable parameters.

15 min. break

TT 8.13 Mon 17:30 HSZ 304

Edge effects on correlations in quasiparticle spectra of graphene billiards — •Jürgen Wurm[1], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

In this work, we study the energy spectrum of quasiparticles in chaotic billiards realized in nanostructured graphene. In particular, we focus on the different types of edges and show how they effect correlations in the spectrum. Previously we have investigated the effects of edges on the transport and spectral properties of graphene quantum dots, as well as on the conductance of graphene nanoribbons numerically [1,2]. Some edges can lead to effective time reversal symmetry breaking, others are effective intervalley scatterers. Here we describe the quasiparticle dynamics in graphene analytically using the effective 2D Dirac Hamiltonian and imposing appropriate boundary conditions that depend on the specific structure of the graphene edges. Starting from the multiple reflection expansion for the exact Green function, we develop a semiclassical theory for graphene and derive a trace formula for the oscillating part of the density of states. We then focus on correlations in the spectrum investigating the spectral form factor and its

dependence on the edge structure of the graphene billiard.
[1] J.Wurm, A.Rycerz, I.Adagideli, M.Wimmer, K.Richter and H.U.Baranger. Phys. Rev. Lett. 102, 056806 (2009)
[2] J.Wurm, M.Wimmer, I.Adagideli, K.Richter and H.U.Baranger. New J. Phys. 11, 095022 (2009)

TT 8.14 Mon 17:45 HSZ 304

Transport in Rough Quasi-One-Dimensional Systems — •Otto Dietz[1], Ulrich Kuhl[1,2], Hans-Jürgen Stöckmann[1], Felix M Izrailev[3], and Nykolay M Makarov[3] — [1]Universität Marburg, Germany — [2]Université de Nice, France — [3]Universidad de Puebla, Mexico

Scattering at rough disordered boundaries strongly influence the conductance of nanowires. For rough silicon nanowires a much higher ratio of electric conductivity to thermal conductivity has been reported than expected from the Wiedemann-Franz law [1]. These findings have not been explained yet.

In the case of bulk disorder it is well known that correlations can drastically change conductance properties [2]. Similar effects have been predicted for rough nanowires [3] but drew little attention before their applicability to conductivity in silicon nanowires became evident.

We present a first experimental test of this theory in microwave waveguides with rough walls. Because of the strict analogy between the 2d Schrödinger equation and the Helmholtz equation, the results can be directly applied to electron transport in nano structures. Microwave techniques can be helpful in this respect, since in contrast to real nanowires the surface roughness is both known and controllable. We could confirm that certain rough boundaries can block or enhance wave transport in given frequency windows. \newline [1] A. I. Hochbaum, et. al., Nature 451, 163 (2008). \newline [2] U. Kuhl, et.al., Appl. Phys. Lett. 77, 633 (2000). \newline [3] M. Rendón, et.al., Phys. Rev. B 75, 205404 (2007).

TT 8.15 Mon 18:00 HSZ 304

Strong suppression of thermal conductivity in defected graphene nanoribbons: Order-N methodology and thermoelectric properties — •Hâldun Sevinçli[1], Wu Li[1,2], Stephan Roche[1,3,4], and Gianaurelio Cuniberti[1] — [1]1Institute for Materials Science and Max Bergmann Center of Biomaterials, TU-Dresden, 01062 Dresden, Germany — [2]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [3]Institut Català de Nanotecnologia (ICN) and CIN2, Campus UAB, 08193 Bellaterra, Barcelona, Spain — [4]Institució Catalana de Recerca Avançats (ICREA), 08010, Barcelona, Spain

We investigate electron and phonon transport through defected graphene nanoribbons (GNRs). For phonon transport, we develop an efficient linear scaling method which is based on the Chebyshev polynomial expansion of the time evolution operator and the Lanczos tridiagonalization scheme, and also use molecular dynamics simulations. We show that edge-defects reduce phonon thermal transport dramatically in both armchair and zigzag GNRs, while in zigzag GNRs edge-defects are only weakly detrimental to electronic conduction. On the other hand, bulk defects suppress both charge and thermal transport for relatively high density of defects. The behavior of the electronic and phononic elastic mean free paths of zigzag GNRs with edge-defects points to the possibility of realizing an electron-crystal coexisting with a phonon-glass.

TT 8.16 Mon 18:15 HSZ 304

Orbital magnetism in ballistic graphene quantum dots — •Lisa Hesse[1], Jürgen Wurm[1], Inanç Adagideli[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

We study the magnetic response of quasiparticles in graphene quantum dots. To this end we derive the density of states (DOS) of graphene nanostructures including the effect of a small magnetic field, starting from an exact expansion for the Green function of a graphene flake with arbitrary types of edges. We then consider systems much larger than the Fermi wavelength, for which we can evaluate this expansion in the semiclassical limit and obtain the DOS. For graphene, the structure of the boundary has significant effects on both the average DOS and the DOS oscillations. We then calculate the orbital magnetic susceptibility that is closely related to the DOS and discuss the pecularities that arise due to the different types of edges and the pseudospin degrees of freedom of charge carriers in graphene.