DS 6: Graphene: Theory (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 9:30–12:30 Location: H17

DS 6.1 Mon 9:30 H17

Instantaneous Quantum Time Reversal Mirror in Graphene — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics and Information Sciences, Northumbria University, Newcastle Upon Tyne, UK — [3]Ecole Supérieure de Physique et Chimie Industrielle, CNRS, PSL Research University, Paris, France

The physicists' fascination for time inversion goes back a long time, as testified by the famous 19th-century argument between Loschmidt and Boltzmann concerning the arrow of time. Both metaphysical and practical considerations intrigued generations of scientists, who have ever since strived to devise and implement time-inversion protocols – in particular, different forms of "time mirrors" for classical waves such as sound- and electromagnetic-waves (see e.g. [1-2]), and recently an instantaneous time mirror for water waves [3].

Here we propose the realization of instantaneous Time Mirrors for quantum systems. These are controlled time discontinuities acting on wavefronts as mirrors in time and leading to distinct wavefunction echoes. More precisely, our Quantum Time Mirror exploits up to now unrelated concepts of wavefront time inversion and population reversal in two-level systems, the latter quintessential to spin echoes. It can be implemented in a relativistic Dirac-like system, e.g. graphene.

[1]M. Fink , IEEE Trans. Ultr. Ferroel. Freq. Control, 39, 555, (1992)

[2]G. Lerosey, et al., Phys. Rev. Lett. 92, 193904 (2004)

[3]V. Bacot, et al., preprint (2015)

DS 6.2 Mon 9:45 H17

Plasmon signature in Dirac-Weyl liquids — •Johannes Hofmann — TCM Group, Cavendish Laboratory, University of Cambridge, UK

I shall discuss theoretically as a function of temperature the plasmon mode arising in three-dimensional Dirac liquids, i.e., systems with linear chiral relativistic single-particle dispersion, within the random phase approximation. It is found that whereas no plasmon mode exists in the intrinsic (undoped) system at zero temperature, there is a well-defined finite-temperature plasmon with superlinear temperature dependence, rendering the plasmon dispersion widely tunable with temperature. The plasmon dispersion contains a logarithmic correction due to the ultraviolet-logarithmic renormalization of the electron charge, manifesting a fundamental many-body interaction effect as in quantum electrodynamics. The plasmon dispersion of the extrinsic (doped) system displays a minimum at finite temperature before it crosses over to the superlinear intrinsic behavior at higher temperature, implying that the high-temperature plasmon is a universal feature of Dirac liquids irrespective of doping. This striking characteristic temperature dependence of intrinsic Dirac plasmons along with the logarithmic renormalization is a unique manifestation of the three-dimensional relativistic Dirac nature of quasiparticle excitations and serves as an experimentally observable signature of three-dimensional Dirac materials.

DS 6.3 Mon 10:00 H17

Finite temperature and electric field effects in the RKKY interaction in graphene and bilayer graphene — •Nicolas Klier[1], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in Bernal stacked bilayer graphene [1,2] is shown to have a particularly rich dependence on temperature and a layer symmetry breaking electric field. Depending on whether we consider the chemical potential or particle number as the fixed variable we find that an electric field may tune the RKKY between ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling, or an oscillatory and AFM coupling.

[1] N. Klier, S. Shallcross, and O. Pankratov, *P*hys. Rev. B **90**, 245118, 2014.

[2] N. Klier, S. Shallcross, S. Sharma, and O. Pankratov, *P*hys. Rev. B **92**, 205414, 2015.

DS 6.4 Mon 10:15 H17

The Electronic Structure of Graphene from Dyson-Schwinger Equations with Partially Screened Coulomb Interactions — •Manon Bischoff[1], Katja Kleeberg[2], Dominik Smith[2], Lorenz von Smekal[2], and Björn Wellegehausen[2] — [1]Johannes Gutenberg Universität, Mainz, Deutschland — [2]Justus Liebig Universität, Gießen, Deutschland

We have studied the possibility of a semimetal-insulator transition via spin-density or charge-density wave formation with partially screened Coulomb interactions in graphene from the coupled Dyson-Schwinger equations (DSEs) for the electronic excitations and their Lindhard screening on the honeycomb lattice. In the limit of purely static Lindhard screening these DSEs close on themselves and no further truncation is necessary. With appropriate boundary conditions they can then be solved numerically by fixed-point iteration. This is particularly efficient on graphical processing units (GPUs). After validating the static approximation from Monte-Carlo simulations on smaller lattices with appropriate boundary conditions, it allows to study much larger sheets than in the ab-initio simulations, e.g., to search for Miransky scaling, and to include cases where the latter break down because of a fermion-sign problem as for charge-density wave formation, for example.

DS 6.5 Mon 10:30 H17

Ab-initio lattice Monte-Carlo simulations of the Neck-disrupting Lifshitz transition in mono-layer graphene — •Michael Koerner, Dominik Smith, and Lorenz von Smekal — Institut fuer Theoretische Physik, Justus-Liebig-Universitaet Giessen

We study the effects of inter-electron interactions on the neck-disrupting Lifshitz transition, which is characterized by a change of topology of the Fermi surface. The Lifshitz transition is known to occur within a pure tight-binding description of mono-layer graphene when an external chemical potential drives the Fermi surface away from half-filling and across the saddles at the M-points. At these Van Hove singularities the density of states diverges logarithmically without interactions. We employ ab-intio Monte-Carlo simulations, which account for the full many-body physics of interacting electrons. We choose a partially screened Coulomb potential which combines the screening from localized electron states at short distances with the unscreened long-range Coulomb tails characteristic of graphene at half filling. Our goal is to determine whether interactions change the character of the topological transition, such that a real phase transition in the thermodynamic sense may occur, possibly in combination with chiral superconductivity.

DS 6.6 Mon 10:45 H17

Tight-binding description of spin-orbit coupling in graphene due to adatoms — •Susanne Irmer, Denis Kochan, Klaus Zollner, Martin Gmitra, Tobias Frank, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH3 [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsics, Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models.

This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013)

[2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015)

[3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

30 min. Coffee Break

DS 6.7 Mon 11:30 H17

Ab initio studies of excitations in monolayer black phosphorus — •Tobias Frank[1], Marcin Kurpas[1], Martin Gmitra[1], Rene Derian[2], Ivan Stich[2], and Jaroslav Fabian[1] — [1]Universität Regensburg, Regensburg, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia

Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

DS 6.8 Mon 11:45 H17

Phase structure of graphene from Hybrid Monte-Carlo simulations — •Pavel Buividovich[1], Lorenz von Smekal[2], Dominik Smith[2], and Maksim Ulybyshev[1] — [1]Regensburg University, Institute for Theoretical Physics, D-93053 Regensburg, Universitatstr. 31 — [2]Giessen University, Institute for Theoretical Physics, D-35392 Gießen, Heinrich-Buff-Ring 16

We study the phase structure of monolayer graphene in the parametric space of on-site and nearest-neighbour interactions using the Hybrid Monte-Carlo algorithm similar to those used in lattice QCD simulations. Our simulation code allows us to perform ab-initio simulations on lattices as big as 36x36 unit cells. We numerically determine the boundaries of the charge density wave, spin density wave and the Kekule distortion phases. We also confront the results with analytic studies based on Schwinger-Dyson equations, which allow to reach even larger lattice sizes, up to 5000x5000 unit cells.

DS 6.9 Mon 12:00 H17

Quantum Monte-Carlo study of graphene in external magnetic field — •Maksim Ulybyshev — Institute of Theoretical Physics, University of Regensburg, D-93053 Germany, Regensburg, Universitatsstrasse 31

Recent experimental results indicate that graphene turns into insulator in sufficiently strong magnetic field. However, the exact nature of this state is still elusive and there are some discrepancies between theoretical predictions and experimental results. To resolve this discrepancies extensive simulations of graphene in external magnetic field were performed using Hybrid Monte Carlo algorithm. Insulating state was observed in agreement with experiment. Mass gap and various order parameters were measured.

DS 6.10 Mon 12:15 H17

Interaction-induced conductance from zero modes in a clean magnetic graphene waveguide — •Laura Cohnitz[1], Wolfgang Häusler[2,3], Alex Zazunov[1], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

We consider a waveguide formed in a clean graphene monolayer by a spatially inhomogeneous magnetic field. The single-particle dispersion relation for this waveguide exhibits a zero-energy Landau-like at band, while finite-energy bands have dispersion and correspond, in particular, to snake orbits. For zero-mode states, all matrix elements of the current operator vanish, and a finite conductance can only be caused by virtual transitions to finite-energy bands. We show that Coulomb interactions generate such processes. In stark contrast to finite-energy bands, the conductance is not quantized and shows a characteristic dependence on the zero-mode filling. Transport experiments thereby offer a novel and highly sensitive probe of electron-electron interactions in clean graphene samples. We argue that this interaction-driven zero-mode conductor may also appear in other physical settings and is not captured by the conventional Tomonaga-Luttinger liquid description.